Notes for Classical Mechanics PG course, CMI, Autumn 2013

Govind S. Krishnaswami, updated: 13 Sep, 2020

Some books on classical mechanics are mentioned on the course web site http://www.cmi.ac.in/∼govind/teaching/cm-pg-o13. These lecture notes are very sketchy and are no substitute for attendance, class participation and taking notes at lectures. Please let me know (via govind@cmi.ac.in) of any comments or corrections.

Contents

1 Two body central force problem

1.1 Inverse problem: Universal law of gravity from Kepler's laws

• Based on astronomical observations (especially of Tycho Brahe) Kepler formulated (1606-1619) three laws of planetary motion around the sun: (1) Planetary orbits are ellipses with the Sun at a focus (in particular each orbit lies on a plane, the ecliptic plane of the planet); (2) The radius vector connecting the sun to a planet sweeps out equal areas in equal times and (3) The square of the period of revolution is proportional to the cube of the semi-major axis, with a proportionality constant that is approximately the same for all planets $r^3 = KT^2$ where $K \approx 7.5 \times 10^{-6}$ $(\text{AU})^3/(\text{day})^2 = 3.4 \times 10^{18}$ m^3/s^2 is 'Kepler's constant'. An astronomical unit AU is roughly the mean sun-earth distance, approximately 150 million km. Let us see how these laws led to the universal law of gravitation and how they could be understood using Newtonian mechanics.

• We use spherical polar coordinates (r, θ, ϕ) for the planet's location $\mathbf{r}$ with sun at the origin. The plane of the planet's motion is taken as the $x - y$ plane, so that $\theta = \pi/2$. If the angular momentum $\mathbf{l} = \mathbf{r} \times \mathbf{p}$ were conserved (at least in direction), then the orbit would have to lie on a plane perpendicular to $\mathbf{l}$. Moreover, the angular momentum $\mathbf{l} = l_z \hat{z} = (xp_y - yp_x)\hat{z} = mr^2\dot{\phi}\,\hat{z}$. Now Kepler's second law is used to deduce that the magnitude of angular momentum is constant in time. Indeed, the infinitesimal area swept out by the line joining the sun to the planet in a small time dt while the planet's angular position changes $d\phi$ is $d\text{Ar} = \frac{1}{2} r \times r d\phi$[1]. So constancy

[1] We ignore here the small change in area that results from a change in r, for this area is 2nd order in

of $\dot{\text{A}}\text{r} = \frac{1}{2}r^2\dot{\phi}$ implies angular momentum is conserved. It is an independent mathematical fact of Newtonian dynamics that angular momentum is conserved in a central potential. This suggests that the gravitational force is central $\mathbf{F} = -f(r)\hat{r}$ ($-$ for attraction). The inverse-square nature of the force is guessed from Kepler's third law $T^2 \propto r^3$. The eccentricity of several planetary orbits is fairly small (.02 for the Earth) and they approximately describe uniform circular motion around the sun. Kepler's law certainly applies to these planets and let us see what it implies. Equating the centripetal acceleration to the gravitational force gives

$$m_e\frac{v^2}{r} = f(r) \quad \text{with} \quad v = \frac{2\pi r}{T} \quad \Rightarrow \qquad f(r) = \frac{4\pi^2 K m_e}{r^2} \tag{1}$$

Besides its inverse square nature, the above gravitational force on the Earth due to the sun is proportional to the Earth's mass m_e so that the Earth's acceleration is independent of its mass. Newton postulated that this must be true also of the force felt by the sun due to the Earth (his 3rd law) and concluded that $K \propto m_s$. Thus we guess the universal (both terrestrial and celestial) law of gravitation

$$\mathbf{F} = -\frac{Gm_s m_e}{r^2}\hat{r} \quad \text{where} \quad G = \frac{4\pi^2 K}{m_s} = 6.67 \times 10^{-11}\ \text{Nm}^2/\text{kg}^2. \tag{2}$$

We will often abbreviate $\alpha = Gm_e m_s$, $m_e = 6 \times 10^{24}$ kg and $m_s = 2 \times 10^{30}$ kg. Kepler's first law on elliptical orbits may now be derived as a consequence of Newton's second law and the universal law of gravitation. An important feature of the gravitational force is that it is derivable from the gravitational potential $V(r) = -\alpha/r$

$$\mathbf{F} = -\frac{\alpha}{r^2}\hat{r} = -\nabla_{\mathbf{r}}\left(-\frac{\alpha}{r}\right) = -\nabla_{\mathbf{r}}V(r). \tag{3}$$

In obtaining the $1/r$ potential from Kepler's laws we have in effect solved an inverse problem, i.e., to deduce a potential from features of trajectories. More specifically, we deduced a potential from the period of oscillations that it supports. To solve such a problem in general is very difficult, and we (Newton and co.) are lucky to have succeeded in this case of central importance. Now let us address the direct problem of finding the orbits given the potential.

1.2 Conservation laws

• Now we wish to find the shapes of planetary orbits by solving Newton's second law of motion for a pair of gravitating masses $m_1 = m_e$, $m_2 = m_s$. To do this, it helps to obtain and use the conservation of energy. However, we need to take care of the fact that both the sun and earth can move. If we put $\alpha = Gm_e m_s$ and $V(r) = -\alpha/r$, Newton's second law for the earth ($\mathbf{r}_1$) and sun ($\mathbf{r}_2$) says

$$m_1\ddot{\mathbf{r}}_1 = \frac{\alpha}{r^2}\hat{r} = \nabla_{\mathbf{r}}V(r) \quad \text{and} \quad m_2\ddot{\mathbf{r}}_2 = -\frac{\alpha}{r^2}\hat{r} = -\nabla_{\mathbf{r}}V(r) \tag{4}$$

where $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$ is the radius vector from the sun to the Earth. It is also convenient to define the total mass $M = m_1 + m_2$ and center of mass coordinate $\mathbf{R}$.

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{M} \quad \text{and} \quad \mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1 \quad \Rightarrow \quad \mathbf{r}_1 = \mathbf{R} - \frac{m_2}{M}\mathbf{r} \quad \text{and} \quad \mathbf{r}_2 = \mathbf{R} + \frac{m_1}{M}\mathbf{r}. \tag{5}$$

infinitesimals, $\propto d\phi\, dr$.

It then follows that

$$\nabla_1 = -\nabla_r + \frac{m_1}{M}\nabla_R \quad \text{and} \quad \nabla_2 = \nabla_r + \frac{m_2}{M}\nabla_R \tag{6}$$

In particular, when acting on functions of r alone, such as $V(r)$,

$$\nabla_1 V(r) = -\nabla_r V(r) \quad \text{and} \quad \nabla_2 V(r) = +\nabla_r V(r) \tag{7}$$

We often abbreviate $\nabla_{\mathbf{r}} = \nabla$. Thus, Newton's second law for the sun and Earth may be written

$$\dot{\mathbf{p}}_1 = m_1\ddot{\mathbf{r}}_1 = \nabla_r V(r) = -\nabla_1 V(r) \quad \text{and} \quad \dot{\mathbf{p}}_2 = m_2\ddot{\mathbf{r}}_2 = -\nabla_r V(r) = -\nabla_2 V(r) \quad \text{where} \quad V(r) = -\frac{\alpha}{r}. \tag{8}$$

To obtain the conserved energy, we dot the first equation by the integrating factor $\dot{\mathbf{r}}_1$ and the second by $\dot{\mathbf{r}}_2$ to get

$$m_1\ddot{\mathbf{r}}_1 \cdot \dot{\mathbf{r}}_1 = \dot{\mathbf{r}}_1 \cdot \nabla_r V(r) \quad \text{and} \quad m_2\ddot{\mathbf{r}}_2 \cdot \dot{\mathbf{r}}_2 = -\dot{\mathbf{r}}_2 \cdot \nabla_r V(r) \tag{9}$$

Adding these two equations

$$\frac{d}{dt}\left(\frac{1}{2}m_1\dot{\mathbf{r}}_1^2 + \frac{1}{2}m_2\dot{\mathbf{r}}_2^2\right) = -\dot{\mathbf{r}} \cdot \nabla_r V(r) = -\frac{dV(r)}{dt}. \tag{10}$$

Total energy is thus conserved

$$E_{tot} = \frac{1}{2}m_1\dot{\mathbf{r}}_1^2 + \frac{1}{2}m_2\dot{\mathbf{r}}_2^2 - \frac{\alpha}{r}. \tag{11}$$

It is revealing to write this in terms of the centre of mass and relative coordinates. One finds

$$E_{tot} = E_{cm} + E \quad \text{where} \quad E_{cm} = \frac{1}{2}M\dot{\mathbf{R}}^2 \quad \text{and} \quad E = \frac{1}{2}m\dot{\mathbf{r}}^2 + V(r). \tag{12}$$

Simply by adding Newton's second law for the sun and earth one finds that $\ddot{\mathbf{R}} = 0$ so that E_{cm} is conserved. It follows that the energy of relative motion E is separately conserved. Subtracting the first from the second gives us the eom for $\mathbf{r}$:

$$\ddot{\mathbf{r}}_1 = \frac{1}{m_1}\nabla V \quad \text{and} \quad \ddot{\mathbf{r}}_2 = -\frac{1}{m_2}\nabla V \Rightarrow \ddot{\mathbf{r}} = \ddot{\mathbf{r}}_2 - \ddot{\mathbf{r}}_1 = -\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\nabla V \quad \Rightarrow \quad m\ddot{\mathbf{r}} \equiv \dot{\mathbf{p}} = -\nabla V. \tag{13}$$

Here we defined the reduced mass $m = m_1 m_2/M$ and the relative momentum $\mathbf{p} = m\dot{\mathbf{r}}$. Using this, one checks that the relative angular momentum $\mathbf{l} = \mathbf{r} \times \mathbf{p}$ is conserved since the force is central

$$\dot{\mathbf{l}} = \dot{\mathbf{r}} \times \mathbf{p} + \mathbf{r} \times \dot{\mathbf{p}} = \frac{1}{m}\mathbf{p} \times \mathbf{p} - \mathbf{r} \times \nabla_{\mathbf{r}} V(r) = 0. \tag{14}$$

The total angular momentum $\mathbf{l}_{tot} = \mathbf{r}_1 \times \mathbf{p}_1 + \mathbf{r}_2 \times \mathbf{p}_2$ is of course also conserved

$$\dot{\mathbf{l}}_{tot} = \mathbf{r}_1 \times \dot{\mathbf{p}}_1 + \mathbf{r}_2 \times \dot{\mathbf{p}}_2 = -(\mathbf{r}_2 - \mathbf{r}_1) \times \nabla V(r) = -\mathbf{r} \times \nabla V(r) = 0. \tag{15}$$

• Since $\dot{\mathbf{p}} = -\nabla V$, the relative momentum is not conserved (there is no translation invariance with respect to the relative coordinate). But the total momentum $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$ is conserved, indeed

$$\dot{\mathbf{P}} = \dot{\mathbf{p}}_1 + \dot{\mathbf{p}}_2 = \nabla V - \nabla V = 0. \tag{16}$$

• There is one more conserved quantity, the Laplace-Runge-Lenz vector which we will consider shortly.

1.3 Planetary orbits

• Since $\mathbf{l}$ is conserved, we choose $\hat{z}$ along $\mathbf{l}$, so that the orbits will be counter clockwise. The equation of an ellipse in plane polar coordinates is $\frac{\rho}{r} = 1 + \epsilon\cos\phi$ where $0 < \epsilon < 1$ is the eccentricity[2]. When $\epsilon = 0$ this is a circle of radius ρ. In cartesian coordinates $x = r\cos\phi, r = \sqrt{x^2+y^2}$ the equation takes the form

$$(1-\epsilon^2)x^2 + 2\rho\epsilon x + y^2 - \rho^2 = 0 \quad \text{or} \quad \frac{(1-\epsilon^2)^2}{\rho^2}\left(x + \frac{\rho\epsilon}{1-\epsilon^2}\right)^2 + \frac{(1-\epsilon^2)}{\rho^2}y^2 = 1. \tag{17}$$

This is now in the standard form $\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$. Half the latus rectum $\rho = a(1-\epsilon^2)$ is related to the length a of the semi-major axis, $b = \frac{\rho}{\sqrt{1-\epsilon^2}}$ is the semi-minor axis and $\epsilon = \sqrt{1 - \frac{b^2}{a^2}}$. When $\epsilon > 1$ the coefficients of x^2 and y^2 have opposite signs and we get a hyperbola. For $\epsilon = 1$ we get the parabola $y^2 = \rho^2 - 2\rho x$ opening out to the left.

• Conservation of relative energy and relative angular momentum allow us to establish the elliptical shape of planetary orbits. The 'relative energy' is expressed in terms of angular momentum

$$E = \frac{1}{2}m\dot{r}^2 + \frac{l^2}{2mr^2} - \frac{\alpha}{r} \quad \text{where} \quad \alpha = Gm_1m_2. \tag{18}$$

We get this from the square of relative angular momentum $\mathbf{l} = \mathbf{r}\times\mathbf{p}$, (we use $\hat{r}\cdot\mathbf{p} = m\dot{r}$ below)[3]

$$\mathbf{l}^2 = l^2 = (\mathbf{r}\times\mathbf{p})^2 = r^2p^2 - (\mathbf{r}\cdot\mathbf{p})^2 \quad \Rightarrow \quad \frac{\mathbf{p}^2}{2m} = \frac{(\hat{r}\cdot\mathbf{p})^2}{2m} + \frac{l^2}{2mr^2} \tag{19}$$

In polar coordinates, $l^2 = (mr^2)^2\left(\dot{\theta}^2 + \sin^2\theta\,\dot{\phi}^2\right)$ and for motion on the $\theta = \pi/2$ plane, $l = mr^2\dot{\phi}$.

• $V_{\text{eff}}(r) = \frac{l^2}{2mr^2} - \frac{\alpha}{r}$ is an effective potential that includes the repulsive 'centrifugal' angular momentum barrier. For fixed angular momentum $l \neq 0$, the minimum energy orbit is a circle of radius $r = \rho = \frac{l^2}{m\alpha}$ which is the minimum of the effective potential $V'_{\text{eff}}(r) = 0$. The planet executes uniform circular motion $\dot{r} = 0$ and $\dot{\phi} = \frac{l}{m\rho^2}$ with energy $E = -\frac{\alpha}{2\rho}$. If $0 > E > -\frac{\alpha}{2\rho}$, we expect the radial distance to oscillate about ρ with turning points at perihelion and aphelion. For $E \geq 0$ the orbit is unbound, though it has a turning point at perihelion, resulting in parabolic and hyperbolic orbits. Finally, if $l = 0$ there is no angular momentum barrier, we discuss this in a subsequent section. Now we obtain the shape of orbits.

• Energy conservation $E = \frac{1}{2}m\dot{r}^2 + V_{\text{eff}}(r)$ gives a 1st order equation. We could integrate it to find $t(r)$

$$\pm(t - t_0) = \sqrt{\frac{m}{2}}\int_{r_0}^{r}\frac{dr'}{\sqrt{E - V_{\text{eff}}(r')}} \tag{20}$$

[2]Perihelion $r = r_{min} = \frac{\rho}{1+\epsilon}$ when $\phi = 0$ and aphelion $r = r_{\max} = \frac{\rho}{1-\epsilon}$ when $\phi = \pi$. We have oriented and positioned the axes to ensure the semi-major axis is along $\hat{x}$ and there is a $y \to -y$ symmetry. The origin is at the right focus. A rotated ellipse results if we take $\frac{\rho}{r} = 1 + \epsilon\cos(\phi - \phi_0)$.

[3]One way to get this is to use the fact that the motion is on the $\theta = \pi/2$ plane and write $\mathbf{r} = (rc, rs)$, $\dot{\mathbf{r}} = (\dot{r}c - rs\dot{\phi}, \dot{r}s + rc\dot{\phi})$ where $c = \cos\phi, s = \sin\phi$, and thereby obtain $\dot{\mathbf{r}}\cdot\mathbf{r} = r\dot{r}$. The same works in spherical polar coordinates even for $\theta \neq \pi/2$.

and invert to find $r(t)$. Then we may use angular momentum conservation $l = mr^2\dot{\phi}$ to find $\phi(t)$

$$\phi - \phi_0 = \int_{t_0}^{t} \frac{l\, dt}{mr^2(t)} = \pm \frac{l}{\sqrt{2m}} \int_{r_0}^{r} \frac{dr}{r^2\sqrt{E - V_{\text{eff}}(r)}} \tag{21}$$

So the solution of the eom has been reduced to quadrature (integration).

• But if we are primarily interested in the shape of the orbit (rather than the time dependence), it is simpler to think of r as a function of ϕ. Then

$$\dot{r} = r'(\phi)\dot{\phi} = r'(\phi)\frac{l}{mr^2}. \tag{22}$$

Appearance of $\frac{r'}{r^2}$ suggests the substitution $u = 1/r$ in terms of which $\dot{r} = -\frac{l}{m}u'(\phi)$. The energy becomes

$$E = \frac{l^2}{2m}\left(u^2 + u'(\phi)^2\right) - \alpha u \tag{23}$$

Differentiating this gives us a simple 2nd order differential equation for the orbit

$$u'' + u = \frac{m\alpha}{l^2} \equiv \frac{1}{\rho} \quad \text{where} \quad \rho \quad \text{is the radius of the circular orbit for that } l. \tag{24}$$

This is the equation for a harmonic oscillator with constant driving force. A particular solution is $u_p = \frac{1}{\rho}$ and the general homogeneous solution is $u_h = N\cos(\phi - \phi_o)$. The first integration constant, the phase ϕ_o simply rotates the orbit and will be omitted. The second integration constant N has dimensions of inverse length and will be related to the energy (or eccentricity). Thus the equation for the orbit reduces to that of an ellipse

$$\frac{1}{r} = N\cos\phi + \frac{1}{\rho} \quad \text{or} \quad \frac{\rho}{r} = 1 + \epsilon\cos\phi \tag{25}$$

Here we defined the dimensionless constant $\epsilon = N\rho \geq 0$ which is the eccentricity. By substituting in the expression for energy we relate eccentricity to energy and ρ

$$E = -\frac{\alpha}{2\rho}\left(1 - \epsilon^2\right) = -\frac{\alpha}{2a} \quad \text{where} \quad \rho = \frac{l^2}{m\alpha}. \tag{26}$$

It is clear that for $E = -\alpha/2\rho$ eccentricity vanishes $\epsilon = 0$ and we get a circular orbit. For $-\alpha/2\rho < E < 0$ we have $0 < \epsilon < 1$ and we get elliptical planetary orbits. For $E = 0$, the eccentricity $\epsilon = 1$ and we have an unbound parabolic orbit $y^2 = \rho^2 - 2\rho x$. For $\epsilon > 1$, $E > 0$ and we have unbound hyperbolic orbits.

1.4 Period of elliptical orbits

• For $E < 0$, since orbits are closed curves (ellipses) motion is periodic. Why? After some time T, $\mathbf{r}$ returns to initial position $\mathbf{r}_0$ and energy is unchanged and so is potential energy (since it depends only on $|\mathbf{r}|$), so KE and speed must be unchanged. Direction of velocity is tangent to the same ellipse and is also unchanged. So both position and velocity return to their original values.

• There is a simple way to find the period of elliptical orbits. By the conservation of angular momentum, the areal speed is a constant $\frac{d\text{Ar}}{dt} = \frac{l}{2m}$ (Kepler's second law). Integrating over one

period, area of ellipse $\mathrm{Ar} = \frac{lT}{2m}$. But $\mathrm{Ar} = \pi ab = \frac{\pi\rho^2}{(1-e^2)^{3/2}}$ since $a = \frac{\rho}{(1-e^2)}$ and $b = \frac{\rho}{\sqrt{1-e^2}}$. Using this and $\rho = m^2/l\alpha$ to eliminate l and $m = m_1 m_2/M$ we get

$$T^2 = \frac{4m^2}{l^2}(\mathrm{Ar})^2 = \frac{4\pi^2 m}{\alpha}a^3 = \frac{4\pi^2}{GM}a^3 = \frac{a^3}{\tilde{K}}. \tag{27}$$

We have expressed the period in terms of the semi-major axis and $\tilde{K} = GM/4\pi^2$. We also recover Kepler's 3rd law (not just for circular orbits). Since $M = m_1 + m_2$, $\tilde{K}$ depends on the *sum* of solar and planetary masses. But since all planets are at least a 1000 times lighter than the Sun, $M \approx m_s$. Hence, $\tilde{K} \approx Gm_s/4\pi^2 = K$ reduces to Kepler's constant and is approximately the same for all planets.

1.5 LRL or eccentricity vector and relations among conserved quantities

• The $V(r) = -\alpha/r$ potential has the special feature that all bound trajectories are closed, leading to periodic motion. This is not generally true, of central potentials. For instance the central potential $V(r) = -\frac{\alpha}{r} - \frac{\alpha'}{r^2}$ for small[4] α' does have a closed trajectory, the circular one at the minimum of the effective potential. But not every bound trajectory is closed. For energy more than minimal, a typical trajectory fails to close and looks like a rosette or 'precessing ellipse'. It is clear from the effective potential that for fixed E and l, $r(t)$ is a periodic function of time, oscillating between turning points determined by $E = V_{\mathrm{eff}}(r_{\mathrm{min}}) = V_{\mathrm{eff}}(r_{\mathrm{max}})$. In particular, the perihelion and aphelion distances do not change with time. But the problem is that the period of r is not in general rationally related to the time it takes for the angle ϕ to go from zero to 2π. The change in ϕ as r goes from r_{min} (when $\phi = \phi_o$) to r_{max} and returns to r_{min} is

$$\phi - \phi_o = \frac{2l}{\sqrt{2m}}\int_{r_{min}}^{r_{\mathrm{max}}} \frac{dr}{r^2\sqrt{E - V_{\mathrm{eff}}(r)}}. \tag{28}$$

But this need not be a rational multiple of 2π. As a consequence the orbit is not closed. For such a rosette-shaped orbit, the vector from the origin to perihelion is not fixed, but rotates. Of course, this vector is only defined at discrete times when the planet is at perihelion, its length does not change since the distance to perihelion is fixed by the turning point r_{min} in V_{eff}. Among central potentials, only the $-\alpha/r$ and isotropic harmonic oscillator potentials $\frac{1}{2}m\omega^2 r^2$ are such that *every* bound orbit is closed.

• For the closed elliptical trajectories of the $-\alpha/r$ potential, the vector from the origin (focus) to the perihelion is a conserved vector. This explains the existence of the Laplace-Runge-Lenz conserved vector. One could try to guess what this vector is by trying out a linear combination of vectors $\mathbf{r}, \mathbf{p}$ and $\mathbf{p}\times\mathbf{l}$ that lie in the plane of the orbit. The combination that works is the LRL vector $\mathbf{A}$ (some authors divide the rhs by m)

$$\mathbf{A} = \mathbf{p}\times\mathbf{l} - m\alpha\hat{r}. \tag{29}$$

$\mathbf{A}\cdot\mathbf{l} = 0$ so $\mathbf{A}$ lies in the orbital plane. The 'eccentricity vector' is defined as (we will see that $|\epsilon| = \epsilon$),

$$\epsilon = \frac{\mathbf{A}}{m\alpha} = \frac{\mathbf{v}\times\mathbf{l}}{\alpha} - \hat{r}. \tag{30}$$

[4]We assume the conserved angular momentum is large enough for $l^2 > 2m\alpha'$. So there is an angular momentum barrier in the effective potential $V_{\mathrm{eff}} = \frac{l^2}{2mr^2} - \frac{\alpha}{r} - \frac{\alpha'}{r^2}$.

Let us first check that the LRL vector is conserved. Using $\dot{\mathbf{l}} = 0$ and $\dot{\mathbf{p}} = -\frac{\alpha \mathbf{r}}{r^3}$

$$\dot{\mathbf{A}} = \dot{\mathbf{p}} \times \mathbf{l} - m\alpha \frac{\dot{\mathbf{r}}}{r} + \frac{m\alpha\, \dot{r}\, \mathbf{r}}{r^2} = \dot{\mathbf{p}} \times (\mathbf{r} \times \mathbf{p}) - \frac{\alpha \mathbf{p}}{r} + \frac{\alpha(\mathbf{r}\cdot\mathbf{p})\mathbf{r}}{r^3} = \mathbf{r}(\dot{\mathbf{p}}\cdot\mathbf{p}) - \mathbf{p}(\dot{\mathbf{p}}\cdot\mathbf{r}) - \frac{\alpha \mathbf{p}}{r} + \frac{\alpha(\mathbf{r}\cdot\mathbf{p})\mathbf{r}}{r^3} = 0. \tag{31}$$

• Being a conserved vector we may find its direction at any time, say at perihelion. $\frac{\rho}{r} = 1 + \epsilon \cos\phi$. Since $\mathbf{l}$ is in the $\hat{z}$ direction, the motion is counterclockwise and perihelion occurs at $\phi = 0, r_{min} = \frac{\rho}{1+\epsilon}$. At perihelion, $\mathbf{r} = r\hat{x}$ and by the $y \to -y$ symmetry of the orbit, the tangent to the curve is in the $\hat{y}$ direction, $\mathbf{p} = p\hat{y}$. It follows that at perihelion[5]

$$\mathbf{A} = (lp - m\alpha)\hat{x} = m\alpha\epsilon\, \hat{x}. \tag{32}$$

Hence $\mathbf{A}$ points towards perihelion and has a magnitude $m\alpha\epsilon$. Thus, the eccentricity vector $\epsilon = \frac{\mathbf{A}}{m\alpha}$ has a length equal to the eccentricity. Both $\mathbf{A}$ and ϵ vanish for the circular orbits.

• Thus for motion in the potential $V(r) = -\alpha/r$ we have found 7 conserved quantities $E, \mathbf{l}$ and $\mathbf{A}$. But this system has only three degrees of freedom and requires 6 initial conditions $(\mathbf{r}(0), \dot{\mathbf{r}}(0))$ to determine time evolution. So the 7 conserved quantities cannot all be independently freely specified. We can have at most $2n-1$ independent conserved quantities for a system with n degrees of freedom. If there is such a maximal set of conserved quantities, and their values are specified, then they determine a curve in phase space, the trajectory parametrized by time. If there was another independent conserved quantity, it would force the trajectory to be a point.

• This implies there must be at least 2 relations among $E, \mathbf{l}$ and $\mathbf{A}$. One is obvious $\mathbf{A}\cdot\mathbf{l} = 0$. So we seek another scalar relation among the conserved quantities. The only scalars available to us are A^2 and l^2 so the relation must be of the form $f(E, A^2, l^2, m, \alpha) = 0$. To get an idea of what this relation may be, we recall the expressions for A, l, E for the orbits determined so far (i.e. for $l \neq 0$):

$$E = -\frac{\alpha}{2\rho}(1 - \epsilon^2), \quad A^2 = m^2\alpha^2\epsilon^2, \quad \text{and} \quad l^2 = m\alpha\rho. \tag{33}$$

Substituting for ρ and ϵ^2 in terms of l^2 and A^2 in E we arrive at the relation $A^2 = 2mEl^2 + m^2\alpha^2$. If a relation among conserved quantities holds for every solution of the equations of motion, then it must be generally true.

• To be sure, we may also obtain this scalar relation from the definition of $\mathbf{A}, \mathbf{l}, E$ (without using the solution of the Kepler problem) simply by computing the square of $\mathbf{A} = \mathbf{p}\times\mathbf{l} - m\alpha\hat{r}$ and using $p^2 = 2m(E + \alpha/r)$ and $\mathbf{p}\cdot\mathbf{l} = 0$,

$$\begin{aligned} \mathbf{A}^2 &= (\mathbf{p}\times\mathbf{l})^2 - 2m\alpha\hat{r}\cdot(\mathbf{p}\times\mathbf{l}) + m^2\alpha^2 = p^2l^2 - (\mathbf{p}\cdot\mathbf{l})^2 - \frac{2m\alpha}{r}\mathbf{l}\cdot(\mathbf{r}\times\mathbf{p}) + m^2\alpha^2 \\ &= 2mEl^2 + \frac{2m\alpha l^2}{r} - \frac{2m\alpha l^2}{r} + m^2\alpha^2 = 2mEl^2 + m^2\alpha^2. \end{aligned} \tag{34}$$

This relation only holds for a $1/r$ central potential. We may also view it as expressing the energy in terms of the squares of the conserved vectors $\mathbf{A}$ and $\mathbf{l}$:

$$E = \frac{A^2 - m^2\alpha^2}{2ml^2}. \tag{35}$$

[5] We found p at perihelion by writing $\frac{p^2}{2m} = E + \frac{\alpha}{r_{min}} = -\frac{\alpha}{2\rho}(1-\epsilon^2) + \frac{\alpha(1+\epsilon)}{\rho} \quad \Rightarrow \quad p = \sqrt{\frac{m\alpha}{\rho}}(1+\epsilon) = \frac{m\alpha}{l}(1+\epsilon)$.

It provides a simple way of obtaining the Bohr spectrum of the hydrogen atom $H = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{(4\pi\epsilon_o)r}$. For circular orbits $A^2 = 0$ and we identify $\alpha = \frac{e^2}{4\pi\epsilon_o}$. Quantization $l = n\hbar$ then gives the Bohr spectrum,

$$E_n = -\frac{me^4}{(4\pi\epsilon_o)^2 2n^2\hbar^2}. \tag{36}$$

Pauli got the Bohr spectrum by use of the LRL vector before the Schrödinger equation was formulated.

1.6 Collision of two gravitating point masses: collision time and universality

• In finding the orbits for the Kepler problem, we avoided the case $l = 0$ where there is no angular momentum barrier. We discuss it now. Consider two point masses m_1, m_2, subject only to their mutual gravitational force. Their center of mass moves in a straight line. Energy of relative motion is

$$E = \frac{1}{2}m\dot{\mathbf{r}}^2 - \frac{\alpha}{r} = \frac{1}{2}m\dot{r}^2 + \frac{l^2}{2mr^2} - \frac{\alpha}{r} \tag{37}$$

l is the magnitude of relative angular momentum. For a collision to occur, we need the relative angular momentum to be zero since it is conserved and is zero at the time of collision, the motion is purely radial and $E = \frac{1}{2}m\dot{r}^2 - \frac{\alpha}{r}$. In this case the effective potential is just $V = -\alpha/r$ and for $E < 0$ there is only one turning point at $r_{\max} = -\alpha/E$. For $E \geq 0$ there are no turning points and the motion can be unbounded.

• Suppose the particle is at $r = r_0$ at $t = 0$. There are two possibilities, (a) it is given a radially outward initial velocity or (b) it is given a radially inward initial velocity. In case (a) the particle will escape to $r = \infty$ if $E \geq 0$ or go out and return and collide if $E < 0$. In case (b) the particle will collide irrespective of its initial radially inward velocity. In case (a) with $E < 0$ the particle will return to r_0 with radially inward velocity and may be treated from thereon as in case (b). So we restrict to case (b) with radially inward initial velocity. In this case we know that $E \geq -\frac{\alpha}{r_0} \geq -\frac{\alpha}{r(t)}$ since kinetic energy is non-negative and $r(t) \leq r_0$ as the particle falls inward. Conservation of energy tells us that

$$\dot{r}^2 = \frac{2}{m}\left(E + \frac{\alpha}{r}\right) \tag{38}$$

During the motion $\dot{r} \leq 0$, as the particle is falling inward. So we take the negative square-root and get

$$\dot{r} = -\sqrt{\frac{2}{m}}\sqrt{E + \frac{\alpha}{r}} \quad \Rightarrow \quad -\int_0^t dt' = \int_{r_0}^{r} \frac{dr'}{\sqrt{\frac{2}{m}}\sqrt{E + \frac{\alpha}{r'}}} \tag{39}$$

Since the particle has to cover a finite distance and is speeding up, we expect a collision to happen in a finite time t_c when r reduces to zero. We assume the bodies are point-like, otherwise the collision will happen a little earlier.

$$t_c = \sqrt{\frac{m}{2}}\int_0^{r_0} \frac{dr}{\sqrt{E + \frac{\alpha}{r}}}. \tag{40}$$

Since the kinetic energy $E + \frac{\alpha}{r} > 0$ for $0 \leq r < r_0$, the integrand is finite for all $0 \leq r < r_0$. At $r = r_0$ the integrand is finite as long as the particle has non-zero initial velocity. Even if its

initial velocity is zero, the integrand has an integrable singularity. So the collision time is finite. We will find an expression for t_c shortly.

• It is also interesting to find the radial distance as a function of time, especially as the collision time is approached. For this we integrate from t to t_c

$$t_c - t = \sqrt{\frac{m}{2}} \int_0^r \frac{dr'}{\sqrt{E + \frac{\alpha}{r'}}}. \tag{41}$$

For $t \to t_c$, $r \to 0$ and the $\frac{\alpha}{r'}$ term dominates,

$$t_c - t \approx \sqrt{\frac{m}{2\alpha}} \int_0^r \sqrt{r'}\, dr' = \frac{2}{3}\sqrt{\frac{m}{2\alpha}}\, r^{3/2} \quad \Rightarrow \quad r(t) \approx \left(\frac{9\alpha}{2m}\right)^{1/3} (t_c - t)^{2/3} \quad \text{as} \quad t \to t_c. \tag{42}$$

We see that the behavior of radial distance just before the collision is independent of the energy E as well as the initial distance r_0. The power law $(t_c - t)^{2/3}$ is universal and $2/3$ is like a critical exponent. In fact, even if we had a third gravitating mass, it would not affect this result since its effects are negligible when the other two bodies approach each other. This power law may be regarded as a collisional version of Kepler's 3rd law which says that $R = K^{1/3}T^{2/3}$. Both these power laws are a reflection of the $1/r$ potential. They are related to a scaling symmetry ('mechanical similarity') of the $1/r$ potential.

• If $\mathbf{r}(t)$ is a solution of Newton's equation $m\ddot{\mathbf{r}} = -\frac{\alpha}{r^2}\hat{r}$, then so is $\mathbf{s}(t) = \lambda^{-2/3}\mathbf{r}(\lambda t)$, for any $\lambda > 0$ as one checks. In other words, $t \to \lambda t, \mathbf{r} \to \lambda^{-2/3}\mathbf{r}$ $(r \to \lambda^{-2/3}r, \phi \to \phi, \theta \to \theta)$ is a symmetry of the eom. To discover this symmetry, consider the transformation $t \to \lambda t, \mathbf{r}(\mathbf{t}) \to \lambda^\gamma \mathbf{r}(\lambda \mathbf{t})$, then $\dot{\mathbf{r}} \to \lambda^{\gamma+1}\dot{\mathbf{r}}$ and $\ddot{\mathbf{r}} \to \lambda^{\gamma+2}\ddot{\mathbf{r}}$ and $\frac{1}{r^2} \to \lambda^{-2\gamma}\frac{1}{r^2}$ and $\hat{r} \to \hat{r}$. Invariance of the eom tells us that $\lambda^{\gamma+2} = \lambda^{-2\gamma}$ or $\gamma = -2/3$.

• Finally, we find the collision time t_c for purely downward motion. There are two cases (1) $E \geq 0$ and (2) $-\frac{\alpha}{r_0} \leq E \leq 0$. (1) If $E > 0$ we get

$$t_c = \sqrt{\frac{m}{2\alpha}} \int_0^{r_0} \sqrt{\frac{r}{1 + \frac{Er}{\alpha}}}\, dr = \sqrt{\frac{m\alpha^2}{2E^3}}\, \tau_+ (Er_0/\alpha) \quad \text{where} \quad s = \frac{Er}{\alpha} \geq 0. \tag{43}$$

We defined the monotonically increasing function

$$\tau_+(s_0) = \int_0^{s_0} \sqrt{\frac{s}{1+s}}\, ds = \sqrt{s_0(1+s_0)} - \text{arcsinh}\sqrt{s_0} \quad \text{for} \quad s_0 \geq 0. \tag{44}$$

$$\tau_+(s_0) \to \frac{2}{3}s_0^{3/2} - \frac{s_0^{5/2}}{5} + \cdots \quad \text{as} \quad s_0 \to 0 \quad \text{and} \quad \tau_+(s_0) \to s_0 + \frac{1}{2} - \frac{1}{2}\log(4s_0) - \frac{3}{8s_0} + \cdots \quad \text{as} \quad s_0 \to \infty.$$

(2) For $-\frac{\alpha}{r_0} \leq E \leq 0$ we get by putting $u = -\frac{Er}{\alpha} > 0$ and $u_0 = -\frac{Er_0}{\alpha}$,

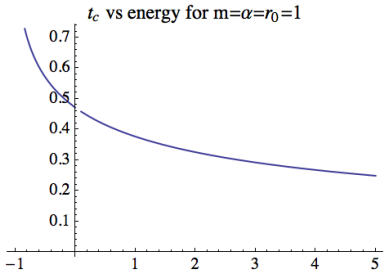
$$t_c = \sqrt{\frac{m\alpha^2}{2|E|^3}}\, \tau_- \left(-\frac{Er_0}{\alpha}\right) \quad \text{where} \quad \tau_-(u_0) = \int_0^{u_0} \sqrt{\frac{u}{1-u}}\, du = \arcsin\sqrt{u_0} - \sqrt{u_0(1-u_0)} \tag{45}$$

$\tau_-(u_0) \to (2/3)u_0^{3/2}$ as $u_0 \to 0$ and $\tau_-(1) = \pi/2$. Combining these two cases,

$$t_c = \sqrt{\frac{m\alpha^2}{2|E|^3}} \begin{cases} \left[\sqrt{\left(\frac{Er_0}{\alpha}\right)\left(1+\frac{Er_0}{\alpha}\right)} - \operatorname{arcsinh}\sqrt{\frac{Er_0}{\alpha}}\right] & \text{for} \quad E \geq 0 \\ \left[-\sqrt{\left(\frac{-Er_0}{\alpha}\right)\left(1+\frac{Er_0}{\alpha}\right)} + \arcsin\sqrt{\frac{-Er_0}{\alpha}}\right] & \text{for} \quad -\frac{\alpha}{r_0} \leq E \leq 0. \end{cases} \tag{46}$$

Though our formula for t_c is given in a piecewise manner, we checked that t_c and its derivatives with respect to E are continuous across $E = 0$, as the figure below partly indicates.

• If the body falls with zero initial speed (minimal energy $E = -\alpha/r_0$), then the collision time is maximal. Replacing $\alpha = Gm_1m_2$ and $m = m_1m_2/M$ so that $\frac{\alpha}{m} = GM$, we get $t_c = \frac{\pi}{2}\sqrt{\frac{r_0^3}{2GM}}$. It is reasonable that the time to impact increases with initial separation r_0 and decreases with increasing gravitational coupling and *total* mass. Imagine a ball falling onto the Earth. In this case, the reduced mass is approximately the ball's mass and the total mass is approximately the Earth's mass. Then we find that the time of descent from a fixed height is *universal*, (approximately independent of the ball's mass) as discovered by Galileo. Note that the collision time cannot be *exactly* independent of the mass of the ball. For, the collision time would then have to be independent of the mass of the earth as well (the process could be viewed as the earth rising up and colliding with the ball). But measurements show that objects would fall slower on a lighter planet. The above formula for t_c keeps its peace with Galileo's observation as well as this reciprocity requirement (Newton's 3rd law) by depending on the total mass rather than the individual masses separately. • As the energy grows, t_c monotonically decreases to zero.



If $E = 0$, then $t_c = \frac{2}{3}\sqrt{\frac{r_0^3}{2GM}}$. For high energies, the collision time goes to zero in a manner independent of α, as we'd expect (gravity may be ignored $E = \frac{1}{2}m\dot{r}^2$, and the particle covers a distance r_0 at the uniform speed $v = r_0/t_c$)

$$t_c \to \sqrt{\frac{mr_0^2}{2E}} \quad \text{as} \quad E \to \infty. \tag{47}$$

2 Conservative systems with one degree of freedom on a line

• Newton's 2nd law for a particle moving on a line is

$$m\ddot{x} = F. \tag{48}$$

If the force depends only on location $F = F(x)$ and not, say on velocity (as the magnetic Lorentz force does), then in one dimension, we may define a potential function such that $F(x) = -V'(x)$

or

$$V(x) = -\int_0^x F(x')\, dx'. \tag{49}$$

In one dimension, a force that is the derivative of a potential is called a conservative force. $V(x)$ is of course defined up to an additive constant which we fixed here by $V(0) = 0$. In this case, Newton's equation becomes $m\ddot{x} + V'(x) = 0$ and using the integrating factor $\dot{x}$, we find that energy $E = \frac{1}{2}m\dot{x}^2 + V(x)$ is conserved.

Time-reversal invariance. The equation $\ddot{x} = -V'(x)$ is time-reversal invariant in the sense that if $x(t)$ is a solution, then so is $x(-t)$. In other words, a movie of a solution played backwards is also an admissible motion. Under time reversal, for a conservative system, the familiar physical quantities transform as follows

$$t \to -t,\ \ x \to x,\ \ \dot{x} \to -\dot{x},\ \ \ddot{x} \to \ddot{x},\ \ F(x) \to F(x),\ \ V(x) \to V(x),\ \ E \to E. \tag{50}$$

• Of course, not every system is conservative. E.g. consider a particle that moves under the influence of both a conservative force as well as a frictional force proportional to its velocity

$$m\ddot{x} = -V'(x) - \gamma\dot{x} \quad \text{with} \quad \gamma > 0. \tag{51}$$

The friction term breaks the time-reversal invariance of this equation. In this case we may show that the above-defined energy is monotonically decreasing. Multiplying by $\dot{x}$ we get

$$\frac{d}{dt}\left(\frac{1}{2}m\dot{x}^2 + V(x)\right) = -\gamma\dot{x}^2 \leq 0. \tag{52}$$

The steady state solutions (time independent solutions $\dot{x} \equiv 0$) are at extrema of the potential $x = x_0$ where $V'(x_0) = 0$. For generic initial conditions (other than, for example, starting at rest at a maximum of V) the particle will execute damped oscillations and settle down at a local minimum of the potential.

2.1 Time period of oscillations between turning points

• Consider a particle moving on a line in a potential $V(x)$ that is differentiable, bounded below (say with global minimum $V = 0$), and tends to infinity as $x \to \pm\infty$. The equation of motion $m\ddot{x} = -V'(x)$ admits the conserved energy $E = \frac{1}{2}m\dot{x}^2 + V(x)$. For any fixed energy $E > 0$, the particle oscillates between a pair of adjacent turning points x_1, x_2 where $V(x_1) = E = V(x_2)$, i.e., kinetic energy vanishes[6]. There may be several such pairs of t.p.s. The solution of the eom reduces to quadrature. If the IC is $x(t_0) = x_0$

$$t - t_0 = \pm \int_{x(t_0)}^{x(t)} \frac{dx}{\sqrt{\left(\frac{2}{m}\right)(E - V(x))}}. \tag{53}$$

[6]At the left turning point $V'(x_1) < 0$ and at the right turning point $V'(x_2) > 0$. We do not include points x_* where V is an extremum $V'(x_*) = 0$ as turning points even if $E = V(x_*)$. So for x_* to be a t.p. we need $V'(x_*) \neq 0$. The reason is that the particle typically takes an infinite amount of time to reach an extremum of the potential and does not 'turn back' in finite time. In particular, we do not admit $\pm\infty$ as turning points. However, such extremal turning points may be treated as limiting cases

We must choose the + sign if the initial velocity is rightward and − sign if the initial velocity is leftward.

• The time to go from t.p. x_1 to x_2 and from x_2 to x_1 are equal (by time reversal invariance of Newton's equation or just by looking at the integrals below)

$$T_{x_1\to x_2} = \sqrt{\frac{m}{2}}\int_{x_1}^{x_2}\frac{dx}{\sqrt{E-V(x)}} \quad = \quad T_{x_2\to x_1} = -\sqrt{\frac{m}{2}}\int_{x_2}^{x_1}\frac{dx}{\sqrt{E-V(x)}} \tag{54}$$

Let us check that these times are finite. The range of integration is finite and the integrand is finite as long as $x \neq x_{1,2}$ as we are dividing by the square-root of the non-zero kinetic energy. The integrand diverges only at the t.p.s. Near the left turning point x_1, $V(x) = V(x_1) + V'(x_1)(x-x_1) + \cdots = E - |V'(x_1)|(x-x_1) + \cdots$ where $V'(x_1) < 0$. Thus, when $x \gtrsim x_1$, the integral behaves as

$$\sqrt{\frac{m}{2}}|V'(x_1)|\int_{x_1}^{*}(x-x_1)^{-1/2}dx \tag{55}$$

which is an integrable singularity. Thus the period of oscillation between t.p. x_1 and x_2 is finite and equal to

$$T(E;x_1,x_2) = \sqrt{2m}\int_{x_1}^{x_2}\frac{dx}{\sqrt{E-V(x)}}. \tag{56}$$

So a potential determines the function $T(E)$ for $E \geq \min_x V(x)$. $T(E)$ may be a multi-valued function for some values of E since there may be more than one pair of adjacent turning points for that E. A direct problem is to find $T(E)$ given $V(x)$, this has been reduced to quadrature.

• $T(E)$ may be evaluated explicitly for some potentials. The SHO $V(x) = \frac{1}{2}m\omega^2x^2$ is isochronous, $T(E) = \frac{2\pi}{\omega}\theta(E \geq 0)$ is independent of E and amplitude. See L & L for more examples.

2.2 Inverse problem: determination of potential from time period

• The inverse problem of deducing a potential with a given $T(E)$ is much harder[7]. The potential $V(x)$ may not be unique. For instance $V(x-x_0)$ has the same $T(E)$ as $V(x)$. We could avoid this non-uniqueness by requiring $V(0) = 0$ with suitable shifts of x and V. But V could be non-unique in more non-trivial ways. L & L give an example.

• Besides, we have seen that $T(E)$ is not even single-valued if the potential supports more than one type of oscillation for a fixed energy (a double well potential for instance). For simplicity, suppose we seek only those potentials $V(x)$ which are convex, having a single minimum, say $V(0) = 0$ and $V(x) \to \infty$ for $x \to \pm\infty$. Then $T(E)$ is single-valued and related to $V(x)$ via energy conservation

$$T(E) = \sqrt{2m}\int_{x_1}^{x_2}\frac{dx}{\sqrt{E-V(x)}}. \tag{57}$$

Here $V(x_1) = V(x_2) = E$ are adjacent turning points. We may regard this as a non-linear integral equation for the unknown function $V(x)$, given $T(E)$.

[7] A problem of a related sort was solved in going from Kepler's 3rd law to Newton's law of gravitation.

• For simplicity, suppose we only look for a potential that is symmetric $V(x) = V(-x)$[8]. In this case

$$T(E) = 2\sqrt{2m}\int_0^{x_0} \frac{dx}{\sqrt{E - V(x)}}, \quad \text{where} \quad V(x_0) = E \quad \text{and} \quad x_0 > 0. \tag{58}$$

• Interestingly, the above non-linear integral equation can be turned into a linear integral equation for $x'(V)$ if we regard x as a function of V. Then $dx = x'(V)\,dV$ and $x = 0 \Rightarrow V = 0$ while $x = x_0$ implies $V = E$:

$$2\sqrt{2m}\int_0^{E} \frac{x'(V)\,dV}{\sqrt{E - V}} = T(E). \tag{59}$$

This is now an inhomogeneous linear integral equation for $f(V) = x'(V)$[9]. If we are able to solve this equation, then we may integrate to find $x(V) = \int_0^V x'(W)dW$. The non-linear part of the problem is then to invert $x(V)$ to find $V(x)$. This could be done graphically for instance.

• Remarkably, the above linear integral equation can be solved for $x'(V)$. The idea to extract $x'(V)$ is to multiply either side by a suitable power of $(W - E)$ and integrate over E. We try $(W - E)^{-1/2}$,

$$2\sqrt{2m}\int_0^{W} dE \int_0^{E} dV \frac{x'(V)}{\sqrt{(E - V)(W - E)}} = \int_0^{W} dE \frac{T(E)}{\sqrt{W - E}}. \tag{62}$$

Changing the order of integrals, noting that $V \le E \le W$ and that $V \ge 0$ and $V \le W$, we get

$$2\sqrt{2m}\int_0^{W} dV\; x'(V) \int_V^{W} \frac{dE}{\sqrt{(E - V)(W - E)}} = \int_0^{W} dE \frac{T(E)}{\sqrt{W - E}}. \tag{63}$$

The inner integral is just π (independent of W, V!) upon making the substitution $y = \sqrt{\frac{W-E}{E-V}}$. Thus

$$x(V) = \frac{1}{2\pi\sqrt{2m}}\int_0^{V} \frac{T(E)\,dE}{\sqrt{V - E}}. \tag{64}$$

So the determination of $x(V)$ has been reduced to calculating a certain integral transform of the period function $T(E)$. Finally, we must invert $x(V)$ to find $V(x)$.

• As a simple illustration, let us 'discover' the SHO potential from its isochronous property, namely $T(E)$ is independent of E. Suppose $T(E) = \frac{2\pi}{\omega}$ for some constant angular frequency ω. In this case $\int_0^V \frac{dE}{\sqrt{V-E}} = 2\sqrt{V}$. Thus

$$x(V) = \frac{1}{2\pi}\frac{1}{\sqrt{2m}}\frac{2\pi}{\omega}2\sqrt{V} \quad \Rightarrow \quad V(x) = \frac{1}{2}m\omega^2 x^2. \tag{65}$$

[8]It turns out that with this condition $V(x)$ is unique, though there are infinitely many non-symmetric convex $V(x)$ with the same $T(E)$. See L & L.

[9]The integral kernel that appears above $K(E, V) = (E - V)^{-1/2}$ is translation invariant, depending only on $E - V$:

$$2\sqrt{2m}\int_0^{E} K(E - V)x'(V)\,dV = T(E). \tag{60}$$

Compare with the case of Fourier transform and inverse Fourier transform where the kernel is $K(x, k) = e^{ikx}$:

$$f(x) = \int \tilde{f}(k)e^{ikx}\frac{dk}{2\pi} \;\Rightarrow \int f(x)e^{-ilx}dx = \int \frac{dk}{2\pi}\tilde{f}(k)\int dx\; e^{ikx-ilx} = \tilde{f}(l). \tag{61}$$

2.3 Time delay and (abbreviated) action shift

• So far we considered oscillations or 'bound states' where the particle's energy is such that it is confined within the potential. Let us briefly consider a case where the particle can escape to infinity, i.e., a 'scattering state'. For simplicity consider a potential that tends to zero as $x \to \pm\infty$. Most physically occurring conservative forces arise from such potentials, there are no forces far from the region of interest. Particularly simple special cases are (1) a 'repulsive' potential $V(x) > 0$, shaped like a speed breaker on a road and (2) an 'attractive' potential $V(x) < 0$, shaped like a depression/trough on a road. A famous example of such a potential is $V(x) = \pm V_0 \text{sech}^2(x/l)$ for $V_0 > 0, l > 0$. Of course, energy $E = \frac{1}{2}m\dot{x}^2 + V(x)$ is conserved. Here the term 'repulsive potential' for $V(x) > 0$ is meant to intuitively convey that the scattering region is like a barrier, it repels particles that try to approach it from either side. Calculate the force for $V(x) = V_0 \text{sech}^2(x/l)$ and show that this is the case for $V_0 > 0$.

• We will be interested in situations where the particle comes in from $x = -\infty$ and escapes to $x = \infty$. So we must have $E > 0$. In fact, we will assume $E > \max_x V$, so that it does not hit a barrier and rebound. For lower energies, the potential may also support oscillations in some local minima, as discussed in the previous section.

• A plausible concept that replaces the time period of oscillations is the time it takes for the particle to go from $-\infty$ to $+\infty$. But typically, this is infinite. In fact, even a free particle with any finite velocity takes infinitely long to go from $-\infty$ to $+\infty$. So a better concept is the time delay, the excess time it takes the particle to traverse this distance relative to a free particle. We will see that this is finite as long as the potential falls off sufficiently fast at $\pm\infty$.

• So we first consider the time taken to go from $-a$ to $+a$ with and without a potential

$$T_V(a) = \sqrt{\frac{m}{2}} \int_{-a}^{a} \frac{dx}{\sqrt{E - V(x)}} \quad \text{and} \quad T_0(a) = \sqrt{\frac{m}{2}} \int_{-a}^{a} \frac{dx}{\sqrt{E}}. \tag{66}$$

Define the (regularized) time delay

$$\Delta T(a) = T_V(a) - T_0(a) = \sqrt{\frac{m}{2}} \int_{-a}^{a} \left(\frac{1}{\sqrt{E - V(x)}} - \frac{1}{\sqrt{E}} \right) dx. \tag{67}$$

The time delay is then the limit as $a \to \infty$

$$\Delta T = \lim_{a \to \infty} \Delta T(a) = \sqrt{\frac{m}{2}} \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{E - V(x)}} - \frac{1}{\sqrt{E}} \right) dx. \tag{68}$$

Though the individual times are both infinite, we will show that the difference is finite, if for large $|x|$, the particle in potential V behaves nearly like a free particle. Let us examine the behavior of the integrand for large $|x|$ using the fact that $V \to 0$ as $|x| \to \infty$. Since $E > 0$, $|V/E| < 1$ for sufficiently large $|x|$, and

$$(E-V)^{-1/2} - E^{-1/2} = \frac{(1 - V/E)^{-1/2}}{\sqrt{E}} - \frac{1}{\sqrt{E}} = \frac{1}{\sqrt{E}} \left(1 + \frac{V}{2E} + \cdots \right) - \frac{1}{\sqrt{E}} \to \frac{V}{2E^{3/2}} + \cdots \quad \text{as} \quad |x| \to \infty. \tag{69}$$

In other words, for large $|x|$, the integrand is simply proportional to V. So the time delay will be finite if $V(x)$ is integrable, i.e., if $\int_{-\infty}^{\infty} V \, dx < \infty$. This will be the case for instance if $V(x)$ is bounded and decays exponentially fast as $|x| \to \infty$. In fact, it is sufficient that the

potential decay as a power law $1/|x|^{1+\epsilon}$ for any $\epsilon > 0$. The Coulomb/Newton potential where $E = \frac{1}{2}m\dot{r}^2 + \frac{l^2}{2mr^2} - \frac{\alpha}{r}$ is on the border-line.

• Notice that the time delay is positive for a purely repulsive potential ($V(x) > 0$). Suppose the particle comes in from $-\infty$ with speed v_∞. Then its speed at x is

$$v(x) = \sqrt{\frac{2}{m}(E - V)} = \sqrt{v_\infty^2 - \frac{2V(x)}{m}}. \tag{70}$$

So in a purely positive potential, $v(x) \leq v_\infty$. Under the influence of the potential, the particle slows down compared to a free particle. So it will take longer to reach $+\infty$. On the other hand, in a purely attractive potential $V(x) < 0$, the time delay is negative. The particle speeds up compared to the free particle and arrives in advance.

• As in the previous section, one may study the inverse problem of determination of scattering potential from knowledge of time delay $\Delta T(E)$. This too is a problem of solving an analogous non-linear integral equation, though we do not pursue it here.

• Relation of time delay to action shift: A quantity of some importance in mechanics (e.g. it appears in the Bohr-Sommerfeld quantization condition) is the *abbreviated* action, which may be evaluated for a trajectory between fixed times t_1 and t_2, when the particle is at x_1 and x_2.

$$\mathscr{s} = \int_{t_1}^{t_2} p\, \dot{x}\, dt = \int_{x_1}^{x_2} p(x)\, dx = \int_{x_1}^{x_2} \sqrt{2m(E - V(x))}\, dx. \tag{71}$$

As before, we assume $E > \max_x V$. Holding x_1, x_2 fixed, it is evident that the derivative of the abbreviated action is equal to the time it takes the particle to go from x_1 to x_2.

$$\frac{d\mathscr{s}}{dE} = \sqrt{\frac{m}{2}} \int_{x_1}^{x_2} \frac{dx}{\sqrt{E - V(x)}} = T_{x_1 \to x_2}. \tag{72}$$

This relation between abbreviated action and duration of trajectory also holds for oscillatory motion.

• As with the total time, $\mathscr{s}$ is infinite for a 'full' trajectory between $x = \pm\infty$. So it makes sense to consider the (abbreviated) action shift

$$\Delta\mathscr{s} = \int_{-\infty}^{\infty} \left(\sqrt{2m(E - V)} - \sqrt{2mE} \right)\, dx \tag{73}$$

Then the time delay is $\Delta T = \frac{d\Delta\mathscr{s}}{dE}$.

3 From Newtonian to Lagrangian mechanics

3.1 Configuration space, Newton's laws, phase space, dynamical variables

• Based on the examples studied, we collect some terminology and facts. A point particle moving in a central force field has three degrees of freedom, we need three coordinates to specify the location of the particle. The Earth-moon system considered in isolation has six degrees of freedom. The number of degrees of freedom does not depend on the nature of forces. A fluid in a container has a very large number of degrees of freedom, say the locations of the molecules,

it is often treated as a system with infinitely many degrees of freedom. An instantaneous configuration of the earth-moon system is any possible location of the earth and moon. The set of all instantaneous configurations of a mechanical system is called its configuration space $\mathcal{Q}$. For a pair of point particles, $\mathcal{Q}$ is the manifold $\mathbb{R}^6$ with coordinates given (say) by the cartesian components of the radius vectors of each of the particles $\mathbf{r}_1^i, \mathbf{r}_2^j$ for $i, j = 1, 2, 3$. The number of degrees of freedom is the dimension of the configuration space.

• The zeroth law of classical mechanics can be regarded as saying that the trajectory $\mathbf{r}(t)$ of a particle is a (twice) differentiable function of time. This is a law that applies to planets, pendulums etc. But it fails for Brownian motion (movement of pollen grains in water). It also fails for electrons in an atom treated quantum mechanically. The quantum mechanical analogue of this zeroth law of classical mechanics is that the wave function or propagator (time evolution operator) is a (once) differentiable function of time. Newton formulated three laws of classical mechanics in the Principia.

• Newton's 1st law says that "Every body persists in its state of being at rest or of moving uniformly straight forward, except insofar as it is compelled to change its state by force impressed." [Isaac Newton, The Principia, A new translation by I.B. Cohen and A. Whitman, University of California press, Berkeley 1999.]. The quantum mechanical analogue of this law is that the propagator (time evolution operator) of a free particle is a gaussian. Gaussian propagators replace straight lines in the quantum theory.

$$U(\mathbf{r}, t; \mathbf{r}', t') = \left(\frac{m}{ih(t-t')}\right)^{3/2} \exp\left[\frac{im|\mathbf{r}-\mathbf{r}'|^2}{2\hbar(t-t')}\right]. \tag{74}$$

• The departure from rest or straight line motion is caused by forces. Newton's 2nd law says that the rate of change of momentum is equal to the impressed force, and is in the direction in which the force acts. For a single particle, the trajectory $\mathbf{r}(t) = (x^1, x^2, x^3) = (x, y, z)$ in *cartesian coordinates*, satisfies

$$m\ddot{\mathbf{r}} = \mathbf{F} \quad \text{or} \quad \dot{\mathbf{p}} = \mathbf{F}, \quad \text{or} \quad m\ddot{x}^i = F^i. \tag{75}$$

Here the momentum $\mathbf{p} = m\mathbf{v} = m\dot{\mathbf{r}}$. Velocities are tangent vectors to the configuration space. The form of Newton's equation changes in curvilinear coordinates. Many interesting forces (such as gravity) arise as gradients of potential functions, $\mathbf{F} = -\nabla V(\mathbf{r})$. For such 'conservative' forces, energy $E = \frac{1}{2}m\dot{\mathbf{r}}^2 + V(\mathbf{r})$ is conserved along trajectories $\dot{E} = 0$.

• The quantum mechanical analogue of Newton's second law is Schrodinger's equation for the time evolution of the propagator. Forces enter through the potential in the hamiltonian, eg. $H = \frac{p^2}{2m} + V$:

$$i\hbar\frac{\partial U(t,t')}{\partial t} = HU(t,t'). \tag{76}$$

Recall that the propagator evolves the wave function forward in time $U(t,t')|\psi(t')\rangle = |\psi(t)\rangle$.

• Newton's 3rd law says that to every action there is always opposed an equal reaction.

• Being 2nd order in time, Newton's equation requires both the initial position $\mathbf{r}$ and velocity/momentum $\mathbf{p}$ as initial conditions. Knowledge of current position and momentum determines the trajectory via Newton's 2nd law. The *state* of the particle is specified by giving its instantaneous position *and* momentum. The set of possible instantaneous states of the particle

is called its phase space manifold M. For a particle moving in 3D space, its configuration space is $\mathbb{R}^3$ and its phase space is $\mathbb{R}^6$ (locations and momenta).

• The path of the particle $\mathbf{r}(t)$ (satisfying Newton's equation and initial conditions) in configuration space is called its trajectory. Also of interest is the trajectory in phase space $(\vec{x}(t), \vec{p}(t))$. Consider the phase plane trajectories for a free particle with one degree of freedom. Since energy is conserved, phase space trajectories must lie inside level sets of energy $E = p^2/2m$. But in general, an energy level set is a union of trajectories. For the free particle, the energy level curves are horizontal straight lines of fixed p which is conserved. Trajectories come with a direction, the arrow of time. Draw the phase portrait.

• The components of position, momentum, angular momentum $\mathbf{l} = \mathbf{r} \times \mathbf{p}$ and Energy $E = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r})$ are interesting physical quantities associated with the dynamics of a particle. They are examples of dynamical variables or observables. In general, a dynamical variable is a (usually smooth) function on phase space. For a single particle dynamical variables may be regarded as functions $f(\mathbf{r}, \mathbf{p})$. The potential $V(\mathbf{r})$ is a function on configuration space and so also a function on phase space. x^i are called coordinate functions on configuration space. x^i, p_j are called coordinate functions of phase space. Conserved quantities are dynamical variables that are constant along *every* trajectory. Of course, the value of a conserved quantity may differ from trajectory to trajectory.

3.2 Lagrangian formulation and principle of extremal action

• The principle of extremal action provides a powerful reformulation of Newton's 2nd law, especially for systems with conservative forces. It leads to Lagrange's equations of motion, which are equivalent to Newton's 2nd law. One advantage of Lagrange's equations is that they retain the same form in all systems of coordinates on configuration space.

• The idea of the action principle is as follows. A static solution (time independent trajectory) of Newton's equation for a particle in a potential $m\ddot{x} = -V'(x)$ occurs when the particle is located at an extremum of the potential. The action principle gives a way of identifying (possibly) time-dependent trajectories as extrema of an action function. However, unlike the potential, the action is *not* a function on configuration space. It is a function on the *space of paths* on configuration space. Suppose $q^i(t)$ for $t_i \leq t \leq t_f$ is a path on $\mathcal{Q}$. It is common to use q^i (instead of x^i) for coordinates on configuration space. q^i need not be cartesian coordinates of particles, any system of coordinates will work. Then the action is typically a functional of the form

$$S[q] = \int_{t_i}^{t_f} L(q^i, \dot{q}^i)\, dt. \tag{77}$$

Here $L(q^i, \dot{q}^i)$ is called the Lagrangian of the system, a function of coordinates and velocities. For a suitable L (invariably the difference between kinetic and potential energies, $L = T - V$) Newtonian trajectories are extrema of S.

• In other words, we consider the problem of determining the classical trajectory that a particle must take if it is at q_i at t_i and q_f at t_f. Instead of specifying the initial velocity, we give the initial and final positions at these times. Which among all the paths that connect these points solve Newton's equation? The action (variational) principle says that classical trajectories are extrema of S. Note that unlike the initial value problem where $q^j(t_i), \dot{q}^j(t_i)$ are specified,

this initial-final value problem (where $q^j(t_i)$ and $q^j(t_f)$) are specified, may not have a unique solution. The action may have more than one extremum. Give an example!

• To understand this idea, we need to determine the conditions for S to be extremal. These conditions are called Euler-Lagrange equations. In the static case, the condition for $V(x)$ to be extremal is that its change under an infinitesimal shift δx of x must vanish to first order in δx, this turns out to be the condition $V'(x) = 0$.

• The Euler-Lagrange equations are got by computing the infinitesimal change in action δS under a small change in path $q^i(t) \to q^i(t) + \delta q^i(t)$ while holding the initial and final locations $q^i(t_i), q^i(t_f)$ unchanged. Assuming the variation in the path is such that $\frac{d\delta q(t)}{dt} = \delta\dot{q}$, we get

$$\begin{aligned} \delta S &= \sum_{i=1}^{n} \int_{t_i}^{t_f} dt' \left\{ \frac{\partial L}{\partial q^i} \delta q^i(t') + \frac{\partial L}{\partial \dot{q}^i} \delta \dot{q}^i(t') \right\} + \mathcal{O}(\delta q)^2 \\ &= \int_{t_i}^{t_f} \delta q^i(t') \left(\frac{\partial L}{\partial q^i} - \frac{d}{dt'} \frac{\partial L}{\partial \dot{q}^i} \right) dt' + \delta q^i(t_f) \frac{\partial L}{\partial \dot{q}^i(t_f)} - \delta q^i(t_i) \frac{\partial L}{\partial q^i(t_f)} + \mathcal{O}(\delta q)^2 \end{aligned} \quad (78)$$

We integrated by parts to isolate the coefficient of δq. The last two 'boundary terms' are zero due to the initial and final conditions and so the condition $\delta S = 0$ can be reduced to a condition that must hold at each time, since $\delta q^i(t')$ are arbitrary at each intermediate time. So choosing, roughly, $\delta q^i(t') = 0$ except for a specific time $t' = t$ we get the Euler-Lagrange (EL) (or just Lagranges's) equations

$$\frac{\partial L}{\partial q^i(t)} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i(t)} = 0, \quad i = 1, 2, \ldots n. \quad (79)$$

• Now let us see how the principle of extremal action implies Newton's equation of motion for a particle in a potential, by a suitable choice of L. Comparing $m\ddot{q} = -V'(q)$ with the EL equation $\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q}$ we notice that if we choose $L = \frac{1}{2}m\dot{q}^2 - V(q)$, then

$$\frac{\partial L}{\partial \dot{q}} = m\dot{q} \quad \text{and} \quad \frac{\partial L}{\partial q} = -V'(q) \quad (80)$$

and the EL equation reduces to Newton's equation.

3.3 Conjugate momentum and its geometric meaning, cyclic coordinates

• The momentum p_i conjugate to the coordinate q^i is defined as

$$p_i = \frac{\partial L}{\partial \dot{q}^i} \quad (81)$$

In general conjugate momenta do not have the dimensions MLT^{-1}, just as generalized coordinates q^i do not necessarily have dimensions of length. Conjugate momentum is a useful concept. The momentum p_j conjugate to a coordinate q^j that does not appear in the Lagrangian is automatically conserved.

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}^j(t)} = \frac{\partial L}{\partial q^j(t)} = 0. \quad (82)$$

Such a coordinate is called a cyclic coordinate. For example for a free particle moving on line $L = \frac{1}{2}m\dot{x}^2$ has the cyclic coordinate x leading to the conservation of the conjugate momentum $p_x = m\dot{x},\ \dot{p}_x = 0$.

• Geometrically, the trajectory $q^i(t)$ is a curve on configuration space. At any instant of time $\dot{q}^i(t)$ is a tangent vector to this curve. In general, the generalized velocities are tangent vectors to the configuration space. On the other hand, the generalized momenta p_i are called co-tangent vectors, they are elements of the vector space dual to the tangent space. Tangent and cotangent vectors *at the same point of the configuration space* may be contracted to get a number, for instance $p_i\dot{q}^i$ is a number at each point of configuration space. This number is independent of what coordinate system we use on configuration space.

• Not every conserved quantity may arise as the momentum conjugate to a cyclic coordinate. For example, if we use cartesian coordinates for the particle in a central potential on a plane, $L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) - V(\sqrt{x^2 + y^2})$, then neither coordinate is cyclic and neither of the momenta $(p_x = m\dot{x}, p_y = m\dot{y})$ are conserved. But as we see below the momentum conjugate to the cyclic angular coordinate is conserved. So some physical insight/cleverness/luck may be needed in choosing coordinate systems in which one or more coordinate is cyclic.

3.4 Coordinate invariance of the form of Lagrange's equations

• For a particle on a plane in a central potential, in polar coordinates we may obtain the kinetic energy from the square of Euclidean line element $ds^2 = dr^2 + r^2 d\phi^2$. So the square of velocity is $(ds/dt)^2 = \dot{r}^2 + r^2\dot{\phi}^2$. Hence,

$$L = T - V = \frac{m}{2}(\dot{r}^2 + r^2\dot{\phi}^2) - V(r) \tag{83}$$

The momenta conjugate to (r, ϕ) are

$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r} \quad \text{and} \quad p_\phi = \frac{\partial L}{\partial \dot{\phi}} = mr^2\dot{\phi}. \tag{84}$$

They coincide with the radial component of linear momentum and the z-component of angular momentum. The first of Lagrange's equations is

$$\dot{p}_r = m\ddot{r} = \frac{\partial L}{\partial r} = mr\dot{\phi}^2 - V'(r). \tag{85}$$

This is the balance of radial acceleration, centripetal acceleration and central force. On the other hand, ϕ is a cyclic coordinate and so p_ϕ is conserved:

$$\dot{p}_\phi = \frac{d}{dt}(mr^2\dot{\phi}) = \frac{\partial L}{\partial \phi} = 0 \quad \Rightarrow \quad mr\ddot{\phi} = -2m\dot{r}\dot{\phi}. \tag{86}$$

This states the conservation of angular momentum, and involves the so-called Coriolis term on the rhs when written out. Note that Newton's equations do not take the same form in all systems of coordinates. There is no force in the $\hat{\phi}$ direction, yet the naive 'angular acceleration' $m\ddot{\phi}$ is non-zero. On the other hand, Lagrange's equations $\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} = \frac{\partial L}{\partial q^i}$ are valid in all systems of coordinates. We obtained them from the action principle without making any assumption about what the q^i are. So q^i could be Cartesian or polar or any other coordinates.

• Let us illustrate the coordinate invariance of the form of Lagrange's equations and the non-invariance of the form of Newton's equations. Consider a free particle on the positive half line $q > 0$ with Lagrangian $L(q, \dot{q}) = \frac{1}{2}m\dot{q}^2$. In this case Lagrange's equation reduces to $\ddot{q} = 0$.

Now let us choose a different coordinate system on configuration space, defined by $Q = q^2$. If Newton's equation $\mathbf{F} = m\ddot{\mathbf{r}}$ were coordinate invariant then we would guess that the equation of motion for Q must be $m\ddot{Q} = 0$ since there is no force. But this is not the correct equation of motion. The correct equation of motion may be obtained by making the change of variable $q \to Q$ in $\ddot{q} = 0$. Using $\dot{Q} = 2q\dot{q}$ and $\ddot{Q} = 2q\ddot{q} + 2\dot{q}^2$ one arrives at

$$2Q\ddot{Q} - \dot{Q}^2 = 0. \tag{87}$$

This is the equation of motion written in terms of Q. Notice that it *doesn't* have the same form as Newton's equation for q.

• On the other hand, let us find the Lagrangian as a function of Q and $\dot{Q}$ and the resulting Lagrange equations to see if they give the correct result found above. First we express the Lagrange function in terms of the new coordinate

$$L(q, \dot{q}) = \frac{1}{2}m\dot{q}^2 = \frac{m\dot{Q}^2}{8Q} = \tilde{L}(Q, \dot{Q}). \tag{88}$$

If the form of Lagrange's equations are the same in the Q coordinate system we must have

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{Q}} = \frac{\partial L}{\partial Q} \quad \text{or} \quad \frac{m\ddot{Q}}{4Q} - \frac{m\dot{Q}^2}{4Q^2} = -\frac{m\dot{Q}^2}{8Q^2} \tag{89}$$

Simplifying, we see that Lagrange's equation agrees with the transformed version of Newton's equation $2Q\ddot{Q} - \dot{Q}^2 = 0$. So we verified that Lagrange's equations take the same form in both the q and Q coordinates. As mentioned above, this is generally true for any choice of coordinates on configuration space.

• It may be noted that the equations of motion $\ddot{q} = 0$ and $\frac{2\ddot{Q}}{Q} = \frac{\dot{Q}^2}{Q^2}$ are not of the same form, though they are equivalent. What we found is that the eom, *when expressed in terms of the respective Lagrange functions* take the same form: $\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q}$ and $\frac{d}{dt}\frac{\partial \tilde{L}}{\partial \dot{Q}} = \frac{\partial \tilde{L}}{\partial Q}$.

3.5 Hamiltonian and its conservation

• Besides the momenta conjugate to cyclic coordinates, the Lagrangian formulation leads automatically to another conserved quantity, the hamiltonian. For a moment suppose the Lagrangian depends explicitly on time $L = L(q(t), \dot{q}(t), t)$. Then

$$\frac{dL}{dt} = \frac{\partial L}{\partial q}\dot{q} + \frac{\partial L}{\partial \dot{q}}\ddot{q} + \frac{\partial L}{\partial t} = \dot{p}\dot{q} + p\ddot{q} + \frac{\partial L}{\partial t} = \frac{d(p\dot{q})}{dt} + \frac{\partial L}{\partial t} \quad \Rightarrow \quad \frac{d(p\dot{q} - L)}{dt} = -\frac{\partial L}{\partial t}. \tag{90}$$

So if we define the hamiltonian $H = p\dot{q} - L$, then $\dot{H} = -\frac{\partial L}{\partial t}$. So if the Lagrangian does not depend explicitly on time, then H is conserved.

• For many of the systems we study, the hamiltonian coincides with energy. Suppose we consider a system with potential energy $V(q)$ and kinetic energy $T = \frac{1}{2}g_{ij}(q)\dot{q}^i\dot{q}^j$ and total energy $E = T + V$. Here $g_{ij} = g_{ji}$ may be taken to be a symmetric tensor, it is a sort of position dependent mass matrix, usually a positive matrix. For example, even for a free particle on the plane in polar coordinates (r, θ), $g_{ij} = m\begin{pmatrix} 1 & 0 \\ 0 & r^2 \end{pmatrix}$ is a position dependent matrix. For

such systems, the kinetic energy defines a Riemannian metric on configuration space. Suppose the Lagrangian is

$$L = T - V = \frac{1}{2} g_{ij}(q)\dot{q}^i\dot{q}^j - V(q) \tag{91}$$

Then one finds that the conjugate momenta are $p_k = g_{ki}\dot{q}^i$ and the hamiltonian coincides with energy

$$H = p_k\dot{q}^k - L = g_{ki}\dot{q}^i\dot{q}^k - \frac{1}{2} g_{ij}\dot{q}^i\dot{q}^j + V = \frac{1}{2} g_{ij}(q)\dot{q}^i\dot{q}^j + V(q) = E. \tag{92}$$

Here we regard the hamiltonian as a function of coordinates and generalized velocities. Later on when we discuss the Hamiltonian formulation of mechanics, we will eliminate $\dot{q}^i$ in favor of momenta and regard the hamiltonian as a function of coordinates and momenta.

• If the Lagrangian is not bilinear in velocities, (say quadrilinear $T = g_{ij}\dot{q}^i\dot{q}^j + h_{ijkl}\dot{q}^i\dot{q}^j\dot{q}^k\dot{q}^l$), then the hamiltonian may not coincide with energy defined as $T + V$. While the hamiltonian is always conserved (provided $\frac{\partial L}{\partial t} = 0$), $E = T + V$ may not be conserved and may not be a particularly interesting physical quantity.

3.6 Non-uniqueness of Lagrangian

• A Lagrangian for a given system of equations is not uniquely defined. For instance, we may add a constant to $L(q, \dot{q}, t)$ without affecting the EL equations. We may also multiply the Lagrangian by a constant. Another source of non-uniqueness arises from the freedom to add the total time derivative of any (differentiable) function $F(q, t)$ to the Lagrangian. The change in the action is

$$L \to L + \dot{F} \;\; \Rightarrow \;\; S \to S + \int_{t_i}^{t_f} \frac{dF}{dt} dt = F(q(t_f), t_f) - F(q(t_i), t_i) \tag{93}$$

But this quantity has zero variation since $t_i, t_f, q(t_i), q(t_f)$ are all held fixed as the path is varied. So the addition of $\dot{F}$ to L does not affect the EL equations. Notice that we could not allow F to depend on $\dot{q}$ since $\delta\dot{q}(t_i), \delta\dot{q}(t_f) \neq 0$ in general and such an F would modify the EL equations. There is no restriction on the initial and final velocities of the perturbed paths.

3.7 From symmetries to conserved quantities: Noether's theorem on invariant variational principles

• Newton/Lagrange equations of classical mechanics have been formulated as conditions for the action $S = \int L\, dt$ to be extremal. Many concepts (such as symmetries) may be formulated more simply in terms of the action/Lagrangian than in terms of the equations of motion.

• If a coordinate q^j is absent in the Lagrangian (q^j *is a cyclic coordinate*), then the corresponding conjugate momentum $p_j = \frac{\partial L}{\partial \dot{q}^j}$ is conserved in time. This follows from Lagrange's equation $\dot{p}_j = \frac{\partial L}{\partial q^j}$. If the Lagrangian is independent of a coordinate, then in particular, it is unchanged when this coordinate is varied $\delta L = 0$ under $q^j \to q^j + \delta q^j$. We say that translations of q^j are a symmetry of the Lagrangian. This relation between symmetries and conserved quantities is deeper, it goes beyond mere translations of a coordinate.

• A transformation of coordinates $q^i \to \tilde{q}^i$ is a symmetry of the equations of motion (eom) if it leaves them unaltered: i.e., the eom for $\tilde{q}$ is the same as that for q. Symmetries usually allow

us to produce new solutions from known ones. For example, the free particle equation $m\ddot{q} = 0$ is left unchanged by a translation of the coordinate $q \to \tilde{q} = q + a$ for any constant length a. Now $q = 0$ is one static solution. We may use the symmetry under translations to produce other static solutions, namely $q = a$ for any a, i.e., the particle is at rest at location with coordinate a rather than at the origin. Incidentally, the momentum of a free particle is conserved in time. We will see that such symmetries are associated with conserved quantities. On the other hand, the equation of motion of a particle attached to a spring $m\ddot{q} = -kq$ is non-trivially modified by a translation of the coordinate $q \to \tilde{q} = q+a$ since $\tilde{q}$ satisfies a different equation $m\ddot{\tilde{q}} = -k\tilde{q}+ka$. Moreover, $p = m\dot{q}$ is not (in general) conserved for a particle executing simple harmonic motion, the momentum is zero at the turning points and maximal at the point of equilibrium.

• It is important to note that not every transformation of q qualifies as a symmetry of the equations of motion. We have already argued that every transformation of coordinates leaves the form of Lagrange's equations invariant. So here, when we say leaves the eom invariant we are not referring to the form of Lagranges equations i.e., $\frac{\partial}{\partial t}\frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q}$ but to the differential equations written out explicitly (without any Lagrange function present).

• A symmetry of the Lagrangian is a transformation that leaves L unchanged. E.g. the free particle $L = \frac{1}{2}m\dot{q}^2$ is unchanged under the shift $q \to q + a$. It follows that the action $S[q] = \int_{t_1}^{t_2} \frac{1}{2}m\dot{q}^2\, dt$ is unchanged under the shift $q \to q + a$. Since the eom are the conditions for S to be stationary, a symmetry of the Lagrangian must also be a symmetry of Lagrange's equations. Noether's theorem constructs a conserved quantity associated to each infinitesimal symmetry of the Lagrangian[10]. Let us see how. Suppose the infinitesimal change $q^i \to q^i + \delta q^i$ leaves the Lagrangian unchanged to linear order in δq. Then it is automatically an infinitesimal symmetry of the action. Let us explicitly calculate the first variation of the action for paths between the times t_1 and t_2, $S[q + \delta q] = S[q] + \delta S[q]$. Up to terms of order $(\delta q)^2$ we get

$$\begin{aligned} \delta S &= \int_{t_1}^{t_2} \left[\delta q^i \frac{\partial L}{\partial q^i} + \delta \dot{q}^i \frac{\partial L}{\partial \dot{q}^i}\right] dt = \int_{t_1}^{t_2} \left[\delta q^i \frac{\partial L}{\partial q^i} + \frac{d}{dt}\left(\delta q^i \frac{\partial L}{\partial \dot{q}^i}\right) - \delta q^i \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right] dt \\ &= \delta q^i(t_2)\frac{\partial L}{\partial \dot{q}^i}(t_2) - \delta q^i(t_2)\frac{\partial L}{\partial \dot{q}^i}(t_1) + \int_{t_1}^{t_2} \delta q^i \left[\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right] dt \end{aligned} \tag{94}$$

So far, this is true for any path and for any infinitesimal change δq^i. Let us now specialize to infinitesimal changes about a trajectory, so that $q^i(t)$ satisfies Lagrange's equations and the last term vanishes. Further more, we assume that the transformation is an infinitesimal symmetry of the Lagrangian, so that $\delta S = 0$:

$$0 = \delta S = \delta q^i(t_2)\frac{\partial L}{\partial \dot{q}^i}(t_2) - \delta q^i(t_2)\frac{\partial L}{\partial \dot{q}^i}(t_1). \tag{95}$$

Since t_1, t_2 are arbitrary, the quantity $\delta q^i \frac{\partial L}{\partial \dot{q}^i}$ must be constant along a trajectory. In other words, an infinitesimal symmetry $q \to q + \delta q$ of the Lagrangian implies that the quantity $Q = p_i(t)\delta q^i(t) = \vec{p}\cdot\delta\vec{q}$ is a constant of the motion, i.e. the dynamical variable Q has the same value at all points along a trajectory.

• E.g. 1: We already saw that the free particle Lagrangian is translation invariant with $\delta q^i = a^i$ where a^i are the components of an arbitrary infinitesimal vector. It follows that $Q = a^i p_i =$

[10]There is a generalization to the case where the Lagrangian changes by a total time derivative, which we will discuss.

$\vec{p} \cdot \vec{a}$ is a conserved quantity. In other words, the component of momentum in *any* direction is conserved.

• E.g. 2: Now consider a particle in a central potential $V(\mathbf{q}^2)$ so that the Lagrangian is

$$L(\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2} m \dot{\mathbf{q}} \cdot \dot{\mathbf{q}} - V(\mathbf{q} \cdot \mathbf{q}) \tag{96}$$

Let us first show that L is invariant under rotations of three dimensional space $\vec{q} \to R\vec{q}$ where R is any $SO(3)$ rotation matrix ($R^t R = I, \det R = 1$). Recall that the dot product is defined as $\mathbf{a} \cdot \mathbf{b} = \mathbf{a}^t \mathbf{b}$ for any column vectors $\mathbf{a}, \mathbf{b}$ and that $(R\mathbf{a})^t = \mathbf{a}^t R^t$ for any matrix R and ^{t} denotes transposition. Thus

$$L(R\mathbf{q}, R\dot{\mathbf{q}}) = \frac{1}{2} m \dot{\mathbf{q}} R^t R \dot{\mathbf{q}} - V(\mathbf{q}^t R^t R \mathbf{q}) = \frac{1}{2} m \dot{\mathbf{q}}^t \dot{\mathbf{q}} - V(\mathbf{q}^t \mathbf{q}) = L(\mathbf{q}, \dot{\mathbf{q}}). \tag{97}$$

So the Lagrangian is invariant under rotations. Noether's theorem, however, refers to infinitesimal transformations, rotations in this case. So let us find a formula for an infinitesimal rotation.

• Suppose we make an infinitesimal rotation of the vector $\mathbf{q}$ about the axis $\hat{n}$ by a small angle θ counter-clockwise. Then the vector $\mathbf{q}$ sweeps out a sector of a cone. Suppose $\mathbf{q}$ makes an angle ϕ with respect $\hat{n}$, so that the opening angle of the cone is ϕ. Then the rotated vector $\tilde{\mathbf{q}}$ also makes an angle ϕ with respect to the axis $\hat{n}$. Let $\delta\mathbf{q} = \tilde{\mathbf{q}} - \mathbf{q}$ be the infinitesimal change in $\mathbf{q}$. By looking at the base of this cone, we find that it is a sector of a circle with radius $q \sin\phi$ and opening angle θ. So we find that $|\delta\mathbf{q}| = \theta q \sin\phi$. Moreover δq points in the direction of $\hat{n} \times \mathbf{q}$. Thus, under a counter-clockwise rotation about the axis $\hat{n}$ by a small angle θ, the change in $\mathbf{q}$ is

$$\delta\mathbf{q} = \theta\, \hat{n} \times \mathbf{q} \qquad \text{and} \qquad \delta\dot{\mathbf{q}} = \theta\, \hat{n} \times \dot{\mathbf{q}} \tag{98}$$

In particular, we see that $\delta\mathbf{q}$ and $\delta\dot{\mathbf{q}}$ are orthogonal to $\mathbf{q}$ and $\dot{\mathbf{q}}$ respectively.

• Now let us check that the Lagrangian is invariant under infinitesimal rotations:

$$L(\mathbf{q} + \delta\mathbf{q}, \dot{\mathbf{q}} + \delta\dot{\mathbf{q}}) \approx \frac{1}{2} m \dot{\mathbf{q}}^2 + \frac{1}{2} m \dot{\mathbf{q}} \cdot \delta\dot{\mathbf{q}} + \frac{1}{2} m \delta\dot{\mathbf{q}} \cdot \dot{\mathbf{q}} - V(\mathbf{q}^2 + \mathbf{q} \cdot \delta\mathbf{q} + \delta\mathbf{q} \cdot \mathbf{q}) = L(\mathbf{q}, \dot{\mathbf{q}}) \tag{99}$$

The last equality follows on account of the orthogonality properties just mentioned. Thus the Lagrangian (and action) are invariant under infinitesimal rotations. The resulting conserved quantity from Noether's theorem is

$$Q = \vec{p} \cdot \theta\ (\hat{n} \times \vec{q}) = \theta\, \hat{n} \cdot (\vec{q} \times \vec{p}) = \theta\, \vec{L} \cdot \hat{n}. \tag{100}$$

Since Q is conserved for any small angle θ and for any axis of rotation $\hat{n}$, we conclude that the component of angular momentum in *any* direction is conserved. So the angular momentum vector is a constant of motion $\frac{d\vec{L}}{dt} = 0$, a fact we are familiar with from the Kepler problem for the $1/r$ central potential. We also knew this since the torque $\vec{r} \times \vec{F}$ on such a particle about the force centre vanishes: the moment arm and force both point radially.

3.8 Generalization of Noether's theorem when Lagrangian changes by a total time derivative

• As before, consider an infinitesimal transformation $q \to q + \delta q$ which is a symmetry of the equations of motion. In other words, if $q(t)$ is a solution of the eom, then so is $q + \delta q$ for small

δq. Interestingly, even if the Lagrangian is not invariant under this transformation, but changes by a total time derivative $\delta L = \frac{dK}{dt}$, then we have a conserved quantity

$$Q = p_i \, \delta q^i - K. \tag{101}$$

Let us see why this is the case. Consider the action for a path between times t_1 and t_2. As before we may compute the change in action due to an infinitesimal variation of path δq

$$\delta S = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right] dt = \int_{t_1}^{t_2} \left[\left(\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right) \delta q + \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \delta q \right) \right] \tag{102}$$

Now suppose the path happened to be a trajectory satisfying Lagrange's equations, then the first term vanishes and the change in action under the above transformation is

$$\delta S = (p \, \delta q)(t_2) - (p \, \delta q)(t_1). \tag{103}$$

Note that in general, the action will not be invariant under this transformation. It is also important to bear in mind that the variation δq need not vanish at t_1 and t_2. The infinitesimal change δq knows nothing about t_1, t_2, it is not the type of variation one considers while deriving the EL equations.

• Now we have another way of computing the infinitesimal change in action around a trajectory, due to the above transformation,

$$\delta S = \int_{t_1}^{t_2} \delta L \, dt = \int_{t_1}^{t_2} \frac{dK}{dt} dt = K(t_2) - K(t_1). \tag{104}$$

Equating these two expressions for δS we find

$$p_i(t_2) \, \delta q^i(t_2) - K(t_2) = p_i(t_1) \, \delta q^i(t_1) - K(t_1). \tag{105}$$

Since t_1, t_2 are arbitrary, we conclude that the quantity $Q(t) = p_i \delta q^i - K$ is a constant of motion, $\dot{Q} = 0$.

• Let us illustrate with the example of a Galilean boost for a free particle. Consider a free particle in 1D with Lagrangian $L = \frac{1}{2} m \dot{x}^2$ and equation of motion $m\ddot{x} = 0$. Define the infinitesimal Galilean boost

$$x \to \tilde{x} = x + \delta x = x + ct \tag{106}$$

where c is a small speed. Then

$$\delta x = ct, \quad \delta \dot{x} = c, \quad \text{and} \quad \delta \ddot{x} = 0. \tag{107}$$

It follows that the transformation leaves the equation of motion unchanged since $m\ddot{\tilde{x}} = m\ddot{x} = 0$. So a Galilean boost is a symmetry of the equation of motion. The corresponding change in the Lagrangian is a total time derivative

$$\delta L = m\dot{x} \, \delta \dot{x} = mc\dot{x} = \frac{d}{dt}(mcx). \tag{108}$$

So we may take $K = mcx$ (K is defined up to an additive constant). The above theorem asserts that

$$Q = p \, \delta x - K = p \, \delta x - mcx = c(pt - mx) \tag{109}$$

is a constant of motion. Since c is an arbitrary small constant, we drop it and take $Q = pt - mx$. We check using the equation of motion ($\dot{p} = 0$) that Q is indeed conserved:

$$\dot{Q} = \dot{p}t + p - m\dot{x} = p - p = 0. \tag{110}$$

A Galilean boost is a symmetry also for a particle subject to a constant force, where $V(x) = V_0 x$ is linear. But it is not a symmetry of the equation of motion $m\ddot{x} + V'(x) = 0$ for a particle in a more general potential. Though $\delta\ddot{x} = 0$, $\delta V'(x) = V''(x)ct \neq 0$ in general. A simple harmonic oscillator potential, for instance, breaks Galilean invariance, just as it breaks translation invariance.

3.9 Hamilton's equations & relation to geodesics for free particle

• We introduced the hamiltonian $H = p_i\dot{q}^i - L(q, \dot{q})$ as an interesting conserved quantity implied by Lagrange's equations. Here $p_i = \frac{\partial L}{\partial \dot{q}^i}$. To understand H better, let us compute its differential using Lagrange's equations

$$dH = p_i d\dot{q}^i + \dot{q}^i dp_i - \frac{\partial L}{\partial q^i}dq^i - \frac{\partial L}{\partial \dot{q}^i}d\dot{q}^i = p_i d\dot{q}^i + \dot{q}^i dp_i - \dot{p}_i dq^i - p_i d\dot{q}^i = -\dot{p}_i dq^i + \dot{q}^i dp_i \tag{111}$$

This reveals that the independent variables in H are the generalized coordinates q^i and the generalized momenta p_i, the terms involving the differentials of velocities cancelled out. So we should think of H as $H(q, p)$. Now by the definition of partial derivatives,

$$dH = \frac{\partial H}{\partial q^i}dq^i + \frac{\partial H}{\partial p_i}dp_i. \tag{112}$$

Comparing, we find that the time derivatives of coordinates and momenta may be expressed in terms of partial derivatives of the Hamiltonian

$$\dot{q}^i = \frac{\partial H}{\partial p_i} \quad \text{and} \quad \dot{p}_i = -\frac{\partial H}{\partial q^i} \tag{113}$$

• These first order ODEs are called Hamilton's equations. They give us yet another way of expressing the equations of time evolution. To make sense of these equations we are first supposed to express $H = p_i\dot{q}^i - L(q^i, \dot{q}^i)$ as a function of q^j and p_j. This is done by eliminating $\dot{q}^i$ in favor of q, p using the definition of conjugate momenta $p_j = \frac{\partial L}{\partial \dot{q}^j}$.

• If the L and H depend explicitly on time, then the differential of the hamiltonian is

$$dH = \dot{q}dp - \dot{p}dq - \frac{\partial L}{\partial t}dt \quad \text{and} \quad dH = \frac{\partial H}{\partial q}dq + \frac{\partial H}{\partial p}dp + \frac{\partial H}{\partial t}dt. \tag{114}$$

Comparing, we get

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q} \quad \text{and} \quad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}. \tag{115}$$

So even for a time-dependent H, hamilton's equations for coordinates and momenta take the same form.

• E.g. particle in a 1D potential. Then $L = \frac{1}{2}m\dot{q}^2 - V(q)$ and $p = m\dot{q}$ so $\dot{q} = p/m$. Then $H = p\dot{q} - L = pp/m - p^2/2m + V(q) = p^2/2m + V(q)$. Hamilton's equations are $\dot{q} = \frac{\partial H}{\partial p} = p/m$

which recovers the definition of conjugate momentum and $\dot{p} = -\frac{\partial H}{\partial q} = -V'(q)$ which is Newton's second law.

• More generally, suppose $L = \frac{1}{2} g_{ij} \dot{x}^i \dot{x}^j - V(x)$ where g_{ij} is a symmetric positive (and hence invertible) matrix field on $\mathcal{Q}$. Then we find $p_i = g_{ij} \dot{x}^i$. Solving for the velocities we get $\dot{x}^i = g^{ij} p_j$ where g^{ij} is the inverse of the metric, $g_{ij} g^{jk} = \delta_i^k$. Then

$$H = p_i \dot{x}^i - L = p_i g^{ij} p_j - \frac{1}{2} g_{ij} g^{ik} p_k g^{jl} p_l + V(x) = \frac{1}{2} g^{ij} p_i p_j + V(x). \tag{116}$$

Hamilton's equations then read

$$\dot{x}^i = \frac{\partial H}{\partial p_i} = g^{ij} x_j \quad \text{and} \quad \dot{p}_i = -\frac{\partial H}{\partial x^i} = -\frac{1}{2} p_k p_l \frac{\partial g^{kl}}{\partial x^i} - \frac{\partial V}{\partial x^i} \tag{117}$$

To explore the geometric and physical meaning of Hamilton's equations, let us consider the case $V = 0$ where there is no external force. Then Newton's 1st law applies and the trajectories must be straight lines on configuration space. Of course, $\mathcal{Q}$ is in general, a curved manifold. So straight lines must be interpreted as geodesics with respect to the metric g_{ij}. Hamilton's (and Lagrange's) equations must reduce to the geodesic equation for the coordinates $(\ddot{x}^l + \Gamma^l{}_{ij} \dot{x}^i \dot{x}^j = 0)$. Let us see whether this is the case. Since we want second order equations for x we look at Lagrange's equations:

$$\dot{p}_k = \frac{\partial L}{\partial x^k} = \frac{1}{2} g_{ij,k} \dot{x}^i \dot{x}^j \tag{118}$$

where $,k$ denotes partial differentiation $\frac{\partial}{\partial x^k}$. Now $p_k = g_{kj} \dot{x}^j$, so

$$\dot{p}_k = g_{kj,i} \dot{x}^i \dot{x}^j + g_{kj} \ddot{x}^j \tag{119}$$

Thus the equations of motion are

$$g_{kj} \ddot{x}^j = \left[\frac{1}{2} g_{ij,k} - g_{kj,i} \right] \dot{x}^i \dot{x}^j. \tag{120}$$

Multiplying by the inverse metric g^{lk} and summing on k,

$$\ddot{x}^l = g^{lk} \left[\frac{1}{2} g_{ij,k} - g_{kj,i} \right] \dot{x}^i \dot{x}^j = \frac{1}{2} g^{lk} \left[g_{ij,k} - g_{kj,i} - g_{ki,j} \right] \dot{x}^i \dot{x}^j. \tag{121}$$

Here we used the symmetry of $\dot{x}^i \dot{x}^j$ to write $g_{kj,i} = \frac{1}{2}(g_{kj,i} + g_{ki,j})$. Thus Lagrange's equations reduce to the geodesic equation

$$\ddot{x}^l + \Gamma^l_{ij} \dot{x}^i \dot{x}^j = 0 \quad \text{where} \quad \Gamma^l{}_{ij} = \frac{1}{2} g^{lk} \left[g_{ki,j} + g_{kj,i} - g_{ij,k} \right] \tag{122}$$

are the Christoffel symbols.

3.10 Hamiltonian from Legendre transform of Lagrangian

• The Legendre transform gives a way of summarizing the passage from Lagrangian to Hamiltonian. Notice that the definition of conjugate momentum $p = \frac{\partial L}{\partial \dot{q}}$ is the condition for $p\dot{q} - L$ to

be extremal with respect to small variations in $\dot{q}$. Moreover, the extremal value of this function is the hamiltonian $H(q,p)$. Thus, we may write

$$H(q,p) = \text{ext}_{\dot{q}} \left[p_i \dot{q}^i - L(q,\dot{q}) \right] \tag{123}$$

The extremization is carried out with respect to all the generalized velocities. The key step in the Legendre transform is to solve for the velocities in terms of the momenta and coordinates using $p_i = \frac{\partial L}{\partial \dot{q}^i}$. This is not always possible. It could happen that there is none or more than one solution $\dot{q}$ for given q, p. Then H would not be a single-valued function of coordinates and momenta. A condition that guarantees that the Legendre transform exists as a single-valued function is convexity (or concavity) of the Lagrangian as a twice differentiable function of $\dot{q}$. L is convex provided the 2^{nd} derivative (hessian) matrix $\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}$ is a positive matrix everywhere on $\mathcal{Q}$. This condition is satisfied by $L = \frac{1}{2} m \dot{q}^2$ if $m > 0$. Here $p\dot{q} - L$ is a quadratic function of $\dot{q}$ and has a unique extremum for any p. More generally if $L = \frac{1}{2} g_{ij}(q) \dot{q}^i \dot{q}^j + V(q)$, then the hessian is just the metric tensor $g_{ij}(q)$. So positivity of the kinetic energy metric on $\mathcal{Q}$ ensures convexity of the Lagrangian. We have already seen that in this case the Hamiltonian may be obtained as a single valued function of coordinates and momenta $H = \frac{1}{2} g^{ij} p_i p_j + V(q)$.

• On the other hand, let us attempt to compute the Legendre transform of $L = \frac{1}{4}\dot{q}^4 - \frac{1}{2}\dot{q}^2$. We expect to run into trouble. Indeed, there is often more than one solution $\dot{q}$ for a given p when we try to solve for $\dot{q}$ in $p = \frac{\partial L}{\partial \dot{q}} = \dot{q}^3 - \dot{q}$. In this case, the Legendre transform H is not single-valued.

• When the Legendre transform is defined, the Lagrangian can be re-obtained from $H(q,p)$ by an (inverse) Legendre transform

$$L(q,\dot{q}) = \text{ext}_p \left[p\dot{q} - H(q,p) \right]. \tag{124}$$

4 Simple pendulum

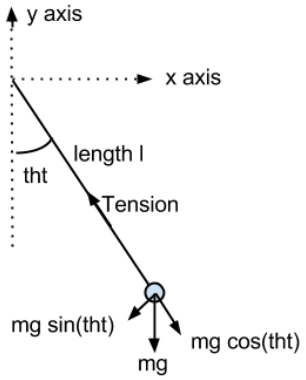
• Consider a bob of mass m suspended from a massless rigid rod of length l clamped at a pivot. The bob is free to move in a vertical plane subject to Earth's gravitational force. This system is an idealized simple pendulum, it is used in clocks. A heavy pendulum bob (wrecking ball) may be used to demolish buildings!

• From our experience we know that the pendulum is in stable equilibrium when hanging vertically downward, the downward gravitational force being balanced by the upward tension force in the rod. A small push makes the bob-oscillate through small angles, always remaining close to the equilibrium position. The pendulum is also in equilibrium when it is balanced vertically upwards. But this is unstable equilibrium, a small push in either direction will take the bob far from the point of equilibrium.

• We are aware of two distinctive types of motion of a pendulum. (1) **Libration:** Oscillations between a pair of turning points around the vertical. In a sense, the bob is *bound* or trapped near its point of stable equilibrium. (2) **Rotation:** if the 'energy' or 'initial speed' of the pendulum is above a specific value, the bob may rotate around the pivot, in general at a non-uniform rate (slower at the top and faster and the bottom). The bob is not trapped near its point of stable equilibrium and the motion does not have any turning points. This is in a sense an unbound or 'scattering' orbit, though the bob cannot escape since the length of the rod is held fixed.

4.1 Newton's second law and equation of motion

• Let us denote the counter-clockwise angle of deflection from the stable equilibrium position by θ. We use a Cartesian coordinate system with y vertically upwards, x to the right.



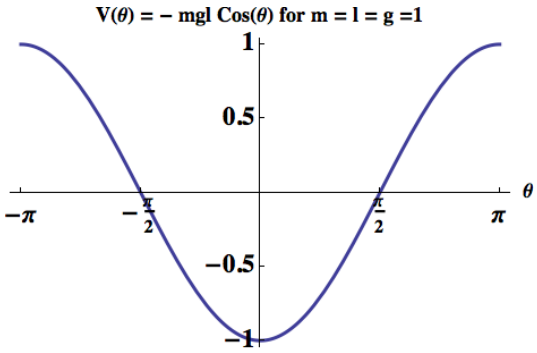


Figure 1: Simple pendulum with bob of mass m suspended from a fixed support with massless rod of length l.

• The vertically downward force due to gravity mg is resolved into a radial component $mg\cos\theta$ and a tangential component $mg\sin\theta$. The bob is at fixed radial distance l from the pivot, so it undergoes no radial acceleration. The radial component of the gravitational force is balanced by the tension in the rod and the centripetal force $ml\dot{\theta}^2$. The tangential component of the gravitational force tends to reduce the angle of deflection and causes the bob to accelerate towards its equilibrium position. Suppose $s = l\theta$ is the arc length corresponding to deflection angle θ. Then the tangential velocity of the bob is $\frac{ds}{dt} = \dot{s} = l\dot{\theta}$ and its acceleration is $l\ddot{\theta}$. Newton's second law then says that

$$\vec{F} = m\vec{a} \quad \Rightarrow \quad -mg\sin\theta = ml\ddot{\theta}. \tag{125}$$

From this we find the equation of motion of a simple pendulum

$$\ddot{\theta} = -\frac{g}{l}\,\sin\theta. \tag{126}$$

• The mass of the bob cancelled out, so the time dependence of θ, and the motion of the pendulum is independent of m! In particular, the time period of oscillation (which we will determine) is independent of the mass. This was discovered experimentally by Galileo around 1602. The equation of motion is second order in time but very non-linear. Even before trying to solve it, we may determine many qualitative features of the motion.

4.2 Energy, Lagrangian, angular momentum

• Energy is conserved during the motion. Multiplying the equation by $\dot{\theta}$, we get

$$\dot{\theta}\ddot{\theta} = -\omega^2\sin\theta\,\dot{\theta} \quad \Rightarrow \quad \frac{1}{2}\frac{d}{dt}\dot{\theta}^2 = \omega^2\frac{d}{dt}\cos\theta \quad \Rightarrow \quad \frac{d}{dt}\left[\frac{1}{2}\dot{\theta}^2 - \omega^2\cos\theta\right] = 0. \tag{127}$$

Multiplying by ml^2 for dimensional reasons, we get the conserved quantity

$$E = \frac{1}{2}ml^2\dot{\theta}^2 - mgl\cos\theta \tag{128}$$

E may be interpreted as the total energy of the system. Recall that the kinetic energy is

$$\text{KE} = \frac{1}{2}mv^2 = \frac{1}{2}m\dot{s}^2 = \frac{1}{2}ml^2\dot{\theta}^2 \quad \text{and the potential energy PE} \quad = V(\theta) = -mgl\cos\theta. \quad (129)$$

We have chosen the potential energy to be zero at the level of the pivot. So the potential energy is $-mgl$ when the pendulum is hanging downwards and equal to mgl when pointing vertically upwards.

• The extrema of the potential energy $V(\theta) = -mgl\cos\theta$ are equilibrium positions where the pendulum is stationary. Now $V'(\theta) = mgl\sin\theta = 0$ when $\theta = 0, \pi$, corresponding to the bob pointing vertically downwards and vertically upwards. The former is a local minimum of the potential (stable equilibrium). The latter is a local maximum of the potential (unstable equilibrium).

• The pendulum admits a Lagrangian description. If we put

$$L = T - V = \frac{1}{2}ml^2\dot{\theta}^2 + mgl\cos\theta. \quad (130)$$

Then we see that the momentum conjugate to θ is $p_\theta = ml^2\dot{\theta}$ and Lagrange's equation reduces to Newton's second law

$$\dot{p}_\theta = -mgl\sin\theta \quad \Rightarrow \quad \ddot{\theta} = -\frac{g}{l}\sin\theta. \quad (131)$$

• p_θ is the z-component of angular momentum about the pivot. Let $\mathbf{r}$ be the radius vector of the bob with pivot as the origin and $\mathbf{p}$ its linear momentum, then angular momentum is

$$\mathbf{L} = \mathbf{r}\times\mathbf{p} = mvr\hat{z} = ml^2\dot{\theta}\,\hat{z} \equiv p_\theta\hat{z} \quad \text{where} \quad p_\theta = ml^2\dot{\theta}. \quad (132)$$

Angular momentum is *not conserved* since there is a non-zero torque $\mathbf{r}\times\mathbf{F}$ about the pivot. The force on the bob is the resultant of the radially inward tension and vertically downward force of gravity, but only gravity provides a non-zero torque that tends to restore the pendulum to its equilibrium position.

$$\vec{\tau} = \mathbf{r}\times\mathbf{F} = -lmg\sin\theta\,\hat{z} \quad (133)$$

Thus angular momentum varies according to the differential equation

$$\frac{d\mathbf{L}}{dt} = \vec{\tau} \quad \Longrightarrow \quad \frac{dp_\theta}{dt} = -mgl\sin\theta. \quad (134)$$

If we use $p_\theta = ml^2\dot{\theta}$, this is the same equation as Newton's second law.

• Though angular momentum is not conserved in general, it becomes a 'better conserved quantity' as the energy increases. In the limit of high energies $E \gg mgl$, where most of the energy is kinetic $\frac{1}{2}ml^2\dot{\theta}^2 \gg mgl$, we may ignore the small gravitational force and it produces a negligible torque. Angular momentum p_θ is conserved in this limit and the pendulum executes uniform circular motion at high angular speed $\dot{\theta} \gg \omega$.

4.3 Hamilton's equations and phase portrait

• The simple pendulum also admits a hamiltonian formulation. The phase space variables are θ and p_θ and the hamiltonian is

$$H(\theta, p_\theta) = \text{ext}_{\dot{\theta}}\left[p_\theta\dot{\theta} - L\right] = \frac{p_\theta^2}{2ml^2} - mgl\cos\theta. \quad (135)$$

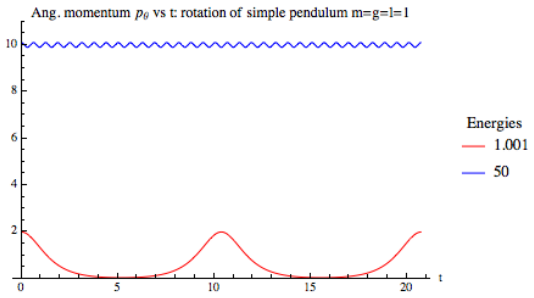


Figure 2: Angular momentum vs time for simple pendulum rotational motion $m = l = g = 1$ and low and high energies. Notice that it becomes a better conserved quantity at high energies.

Hamilton's equations are a pair of first order differential equations, they contain the same information as Newton's 2nd order equation,

$$\frac{d\theta}{dt} = \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{ml^2} \quad \text{and} \quad \frac{dp_\theta}{dt} = -\frac{\partial H}{\partial \theta} = -mgl\sin\theta. \tag{136}$$

The phase space variables θ, p_θ completely characterize the current state of the pendulum and their values along with this pair of equations determine the future motion of the pendulum.

• The set of possible values of (θ, p_θ) comprise the phase space. θ can take any value from $-\pi$ to π. $\pm\pi$ both correspond to a pendulum that is vertically upward at the instant considered. So the possible orientations of the pendulum are parametrized by points on a circle S^1.

• Angular momentum $p_\theta = ml^2\dot{\theta}$ can take any real value (positive or negative). If $p_\theta = 0$, the pendulum has zero angular velocity, as when it is at rest in equilibrium. A positive value of p_θ corresponds to a bob that rotates counter clockwise, the faster it goes round the pivot, the higher p_θ is. If $p_\theta < 0$, the bob rotates clockwise.

• The instantaneous state of a pendulum is determined by a point in the cartesian product $\mathbb{S}^1 \times \mathbb{R}$, i.e., an infinite cylinder which is the phase space of a simple pendulum. The motion of the pendulum defines a curve (trajectory) $(\theta(t), p_\theta(t))$ on phase space. It is instructive to plot the trajectories on phase space. Since the Hamiltonian is a constant of motion, it is constant along trajectories. So each level curve of the hamiltonian is either a trajectory or a union of trajectories.

• The trajectory with least energy is the one where the bob is permanently at rest at $\theta = 0, p_\theta = 0$. As the bob is supplied with more energy, it oscillates about its stable equilibrium point. Conservation of energy allows us to find the maximum angle of deflection $\theta_{\max}$ at which the bob comes instantaneously to rest (turning point)

$$E = -mgl\cos\theta_{\max} \quad \Rightarrow \quad \theta_{\max} = \arccos\left(-\frac{E}{mgl}\right). \tag{137}$$

We see that energy is an increasing function of $\theta_{\max}$. Energy goes from $-mgl$ to mgl as $\theta_{\max}$ is raised from 0 to π. When $E = mgl$ we have an unstable equilibrium at the phase point $\theta = \pm\pi, p_\theta = 0$. When $E > mgl$, the bob goes round and round the pivot and there is no turning point or maximum angle of deflection. The phase portrait is shown in fig 3. Notice the separatrix that separates the librational trajectories from the rotational ones. The separatrices consist of the limiting trajectories with energy $E \uparrow mgl$ where the bob just makes it to the

top, either clockwise or counter clockwise. Librational trajectories are contractible curves on the cylindrical phase space while rotational trajectories are not contractible, they wind around the cylinder.

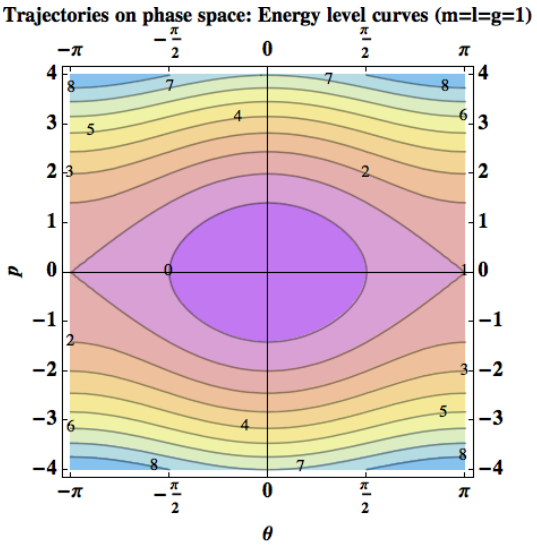


Figure 3: Trajectories on cylindrical phase space of simple pendulum. The right $\theta = \pi$ and left $\theta = -\pi$ edges of the diagram are to be identified, thus producing a cylinder with vertical axis parametrized by p_θ. The value of energy on the level curves is also indicated for $m = g = l = 1$.

4.4 Divergence of period as E approaches mgl from below

- The time period of librational motion is determined using conservation of energy

$$E = \frac{1}{2}ml^2\dot{\theta}^2 - mgl\cos\theta \quad \Rightarrow \quad dt = \pm\sqrt{\frac{ml^2}{2}}\frac{d\theta}{\sqrt{E + mgl\cos\theta}} \tag{138}$$

The maximum angle of deflection is $\theta_{\max} = \arccos\left(-\frac{E}{mgl}\right)$. Using the fact that E is an even function of both θ and $\dot{\theta}$, the period is four times the time taken for the bob to go from $\theta = 0$ to $\theta_{\max}$:

$$T(E) = 4\int_0^{\theta_{\max}} \frac{d\theta}{\sqrt{\frac{2}{ml^2}(E + mgl\cos\theta)}} = \frac{2\sqrt{2}}{\omega}\int_0^{\theta_{\max}} \frac{d\theta}{\sqrt{\epsilon + \cos\theta}} \tag{139}$$

where we introduced the dimensionless energy $\epsilon = \frac{E}{mgl}$. For libration $-mgl \le E < mgl$ so $-1 \le \epsilon < 1$.

- Now, when E approaches mgl from below, $\theta_{\max} \to 1^-$ and

$$\lim_{\epsilon\to 1^-} T(\epsilon) = \frac{2\sqrt{2}}{\omega}\int_0^{\pi} \frac{d\theta}{\sqrt{1 + \cos\theta}}. \tag{140}$$

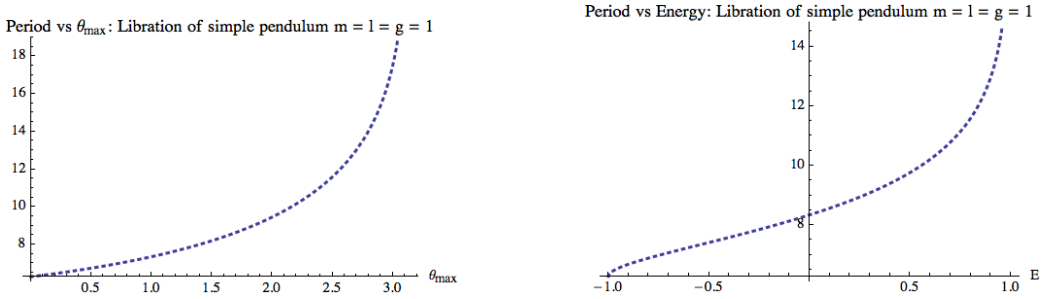
This integral diverges. The integrand has a non-integrable singularity at $\theta = \pi$. Indeed, if we put $\theta = \pi - x$, then $\cos(\pi - x) = -\cos x = -1 + \frac{1}{2}x^2 - \cdots$. So the integrand has a simple pole

$\sim \frac{1}{x}$ at $x = 0$ and the integral diverges. In other words, as the energy approaches mgl, the bob takes an infinite amount of time to reach the vertically upward position.

• With some more effort one may show that the time period diverges logarithmically as $E \to mgl^-$:

$$T(\epsilon) = -\frac{2}{\omega} \log\left[\frac{1-\epsilon}{32}\right] + \mathcal{O}(1-\epsilon) \quad \text{as} \quad \epsilon = \frac{E}{mgl} \to 1^-. \tag{141}$$

So the time period diverges, but does so rather slowly. Contrast this with the power-law divergence of the time period $T(E) \sim (-E)^{-3/2}$ in the Kepler problem and $T(E) \sim (-E)^{-1/2}$ for the sech^2 potential. The time period as a function of $\theta_{\max}$ as well as energy is plotted in the figure, showing the slow divergence as $\theta_{\max} \to \pi$. As $\theta_{\max} \to 0$, the period approaches $2\pi\sqrt{l/g}$.



4.5 Oscillation through small angles: simple harmonic motion

If the pendulum always remains close to its point of equilibrium, (small oscillations about its stable equilibrium position), then $|\theta| \ll \pi/2$ and we may approximate $\sin\theta \approx \theta$. The eom $\ddot{\theta} = -\omega^2 \sin\theta$ may be approximated by the linear equation $\ddot{\theta} = -\omega^2\theta$. The general solution is

$$\theta(t) = A\cos\omega t + B\sin\omega t. \tag{142}$$

A, B are dimensionless constants of integration. They are related to the initial angle and initial angular velocity by $\theta(0) = A$ and $\dot{\theta}(0) = B\omega$. Putting $A = \theta_{\max}\cos\phi$ and $B = \theta_{\max}\sin\phi$, the solution is

$$\theta(t) = \theta_{\max}\sin(\omega t + \phi) \quad \text{with} \quad \theta(0) = \theta_{\max}\sin\phi \quad \text{and} \quad \dot{\theta}(0) = \omega\theta_{\max}\cos\phi. \tag{143}$$

It is clear that the angle is a sinusoidally oscillating function of time, with a maximum angle of deflection $\theta_{\max}$, called the amplitude. Of course, for the small angle approximation to hold, $\theta_{\max}$ must be small compared to $\pi/2$. Such motion is called simple harmonic oscillation. An important feature of simple harmonic oscillation is that the angle is a periodic function of time. The period of oscillation here is

$$T = 2\pi/\omega = 2\pi\sqrt{l/g} \tag{144}$$

The period is the minimum time taken for the pendulum to return to its initial location with its initial angular velocity (including sign). As mentioned, the period is independent of the bob's mass. Just as remarkably, the period is independent of the amplitude $\theta_{\max}$. We say that a pendulum executing small oscillations is isochronous, as discovered experimentally by Galileo. This is a feature that allowed pendulums to be used as the most accurate clocks ('chronometers')

from the mid 1600s (Huygens, 1656) to the early 20th century. The best pendulum clocks had an accuracy of about a second per day. They were replaced by clocks based on quartz crystal oscillators which are still in use and have an accuracy of as much as one second in 30 years. Atomic clocks based on the frequency of EM waves emitted in atomic transitions are now the most accurate clocks. The finest are correct to better than one second in 30 million years.

• Pendulums were also used as gravimeters, to measure the variation of the acceleration due to gravity over the surface of the earth. Indeed it was found that pendulums of the same length lose time near the equator and gain time at high latitudes, so g is smaller near the equator and grows with latitude. This is explained by the fact that the earth bulges out near the equator and is flattened at the poles.

• It was also found empirically that even if the oscillations are not small, the motion is still periodic, but the time period grows with amplitude $\theta_{\max}$. However, the eom $\ddot{\theta} = -\omega^2 \sin\theta$ cannot be solved in general using elementary functions like polynomials and trigonometric functions of time. We need elliptic functions.

4.6 Brief introduction to Jacobi elliptic functions

• The time dependence of the deflection angle of a simple pendulum may be expressed in terms of the Jacobi elliptic function sn. One way to motivate the Jacobi elliptic functions in via the differential equations they satisfy. Recall that circular functions may be defined by a pair of trigonometric evolution equations. They are the following ODEs and initial conditions (primes here denote differentiation in u)

$$\sin' u = \cos u, \quad \cos' u = -\sin u \quad \text{with} \quad \sin 0 = 0, \quad \cos 0 = 1. \tag{145}$$

The Jacobi elliptic functions (they also arose in finding the arc length of an ellipse) are defined via a system of 3 ODEs inspired by Euler's equations for the components of angular momentum in the principal axis co-rotating frame of a rigid body subject to no external torque. Recall that $\dot{\mathbf{L}} + \boldsymbol{\Omega} \times \mathbf{L} = 0$ where $\mathbf{L} = I\boldsymbol{\Omega}$. The inertia tensor $I = \mathrm{diag}(I_1, I_2, I_3)$ in the principal axis frame. Eliminating $\boldsymbol{\Omega}$ we get

$$\begin{aligned}
&\dot{L}_1 + a_{23} L_2 L_3 = 0 \quad \text{where} \quad a_{23} = \frac{1}{I_2} - \frac{1}{I_3} \\
&\dot{L}_2 + a_{31} L_3 L_1 = 0 \quad \text{where} \quad a_{31} = \frac{1}{I_3} - \frac{1}{I_1} \\
&\dot{L}_3 + a_{12} L_1 L_2 = 0 \quad \text{where} \quad a_{12} = \frac{1}{I_1} - \frac{1}{I_2}.
\end{aligned} \tag{146}$$

Motivated by these equations, we consider three ODEs for the 3 Jacobi elliptic functions $\mathrm{sn}(u,k)$, $\mathrm{cn}(u,k)$ and $\mathrm{dn}(u,k)$, which are functions of a re-scaled time variable u and the elliptic modulus k[11]

$$\mathrm{sn}'(u,k) = \mathrm{cn}(u,k)\,\mathrm{dn}(u,k), \quad \mathrm{cn}'(u,k) = -\mathrm{sn}(u,k)\,\mathrm{dn}(u,k) \quad \text{and} \quad \mathrm{dn}'(u,k) = -k^2\,\mathrm{sn}(u,k)\,\mathrm{cn}(u,k).$$

[11] For the rigid body, $k^2 = \frac{a_{12}}{a_{23}} \frac{\left(2E - \frac{L^2}{I_3}\right)}{\left(\frac{L^2}{I_1} - 2E\right)}$ is related to the constants a_{ij} depending on the moments of inertia, conserved energy $E = \frac{L_1^2}{2I_1} + \frac{L_2^2}{2I_2} + \frac{L_3^2}{2I_3}$ and conserved angular momentum $L^2 = L_1^2 + L_2^2 + L_3^2$.

Here $0 \le k \le 1$. Primes denote differentiation in u. These are supplemented by initial conditions

$$\mathrm{sn}(0,k) = 0, \quad \mathrm{cn}(0,k) = 1, \quad \text{and} \quad \mathrm{dn}(0,k) = 1. \tag{147}$$

Just as $\sin^2 u + \cos^2 u = 1$ is a constant of motion for the trigonometric evolution, we have some constants of motion for the evolution of elliptic functions

$$\mathrm{sn}^2 + \mathrm{cn}^2 = 1, \quad k^2\,\mathrm{sn}^2 + \mathrm{dn}^2 = 1 \quad \text{and} \quad \mathrm{dn}^2 - k^2\,\mathrm{cn}^2 = 1 - k^2. \tag{148}$$

These quadratic relations are established by explicit differentiation and use of initial conditions.

• We may use these quadratic relations to eliminate cn and dn from the system of ODEs and get a single ODE for sn with elliptic modulus $0 \le k \le 1$ appearing as a parameter

$$\mathrm{sn}' = \mathrm{cn}\,\mathrm{dn} \;\Rightarrow\; (\mathrm{sn}')^2 = (1 - \mathrm{sn}^2)(1 - k^2\,\mathrm{sn}^2) \;\Rightarrow\; du = \frac{ds}{\sqrt{(1-s^2)(1-k^2s^2)}} \tag{149}$$

Integrating from 0 to u and using the fact that $\mathrm{sn}(0) = 0$ we express the solution via quadrature

$$u(s) = \int_0^s \frac{dt}{\sqrt{(1-t^2)(1-k^2t^2)}} \tag{150}$$

This is called an *incomplete elliptic integral*, and inverting it gives another way (different from, but equivalent to the 3 ODEs we began with) of defining the Jacobi elliptic function $s = \mathrm{sn}(u)$. Elliptic functions may also be defined using power series expansions (they are complex analytic functions of both u and k) as well as via more geometric constructions.

• To compare with how inverse trigonometric functions are defined, we let $k \to 0$ and see that the equation for dn becomes $\mathrm{dn}'(u,0) = 0$ so that $\mathrm{dn}(u,0) = 1$ and

$$\mathrm{sn}'(u,0) = \mathrm{cn}(u,0) \quad \text{and} \quad \mathrm{cn}'(u,0) = -\,\mathrm{sn}(u,0) \tag{151}$$

with initial conditions $\mathrm{sn}(0,0) = 0$ and $\mathrm{cn}(0,0) = 1$. So the elliptic functions reduce to trigonometric functions when the modulus k vanishes

$$\mathrm{sn}(u,0) = \sin(u), \quad \mathrm{cn}(u,0) = \cos(u) \quad \text{and} \quad \mathrm{dn}(u,0) = 1. \tag{152}$$

The differential equation becomes

$$\sin' u = \sqrt{1 - \sin^2 u} \;\Rightarrow\; \frac{ds}{\sqrt{1-s^2}} = du \;\Rightarrow\; u = \int_0^s \frac{dt}{\sqrt{1-t^2}} = \arcsin(s) \;\Rightarrow\; s = \sin u. \tag{153}$$

• Symmetry under reflection $u \to -u$. We notice that $-\,\mathrm{sn}(-u,k)$, $\mathrm{cn}(-u,k)$ and $\mathrm{dn}(-u,k)$ satisfy the same ODEs and initial conditions as $\mathrm{sn}(u,k)$, $\mathrm{cn}(u,k)$ and $\mathrm{dn}(u,k)$. Assuming a unique solution to the initial value problem we find that sn is an odd function of u while cn, dn are even

$$\mathrm{sn}(-u,k) = -\,\mathrm{sn}(u,k), \quad \mathrm{cn}(-u,k) = \mathrm{cn}(u,k) \quad \text{and} \quad \mathrm{dn}(-u,k) = \mathrm{dn}(u,k). \tag{154}$$

• For use in the pendulum problem, it is convenient to re-write the incomplete elliptic integral using the fairly natural change of variable $kt = \sin\frac{\theta}{2}$. Then one finds that the elliptic function $s = \mathrm{sn}(u,k)$ results from inverting the incomplete elliptic integral

$$u(s,k) = \frac{1}{2}\int_0^{2\arcsin ks} \frac{d\theta}{\sqrt{k^2 - \sin^2\frac{\theta}{2}}} = \frac{1}{\sqrt{2}}\int_0^{2\arcsin(ks)} \frac{d\theta}{\sqrt{2k^2 - 1 + \cos\theta}}. \tag{155}$$

• The complete elliptic integral is defined as $u(1,k)$, obtained by letting the upper limit of integration be maximal. We will see that the period of a pendulum may be expressed in terms of $K(k)$, the complete elliptic integral of the first kind, defined for $0 \le k \le 1$ by

$$K(k) = \int_0^1 \frac{dt}{\sqrt{(1-t^2)(1-k^2t^2)}} = \frac{1}{2}\int_0^{2\arcsin k} \frac{d\theta}{\sqrt{k^2 - \sin^2\left(\frac{\theta}{2}\right)}} = \frac{1}{\sqrt{2}}\int_0^{2\arcsin k} \frac{d\theta}{\sqrt{2k^2 - 1 + \cos\theta}}. \tag{156}$$

When the modulus k vanishes, $K(0) = \arcsin 1 = \pi/2$.

4.7 Time dependence of pendulum in terms of elliptic functions

• The solution of the eom was reduced to quadrature using the constancy of energy

$$\dot\theta = \sqrt{\frac{2}{ml^2}}\sqrt{E + mgl\cos\theta} \quad \Rightarrow \quad t - t_o = \int_{\theta(t_o)}^{\theta(t)} \frac{d\theta'}{\sqrt{\frac{2}{ml^2}[E + mgl\cos\theta']}}. \tag{157}$$

When $E < mgl$ the bob oscillates with a maximum angle of deflection $\theta_{\max} = \arccos(-E/mgl)$. A phase plot of level curves of energy shows that the motion is periodic with a period given by

$$T = 4\int_0^{\theta_{\max}} \frac{d\theta}{\sqrt{\frac{2}{ml^2}[E + mgl\cos\theta]}}. \tag{158}$$

• Now let us solve for trajectories of energy E and initial deflection $\theta(0) = 0$ in terms of elliptic functions. First we pass to dimensionless energy and time variables by defining $\epsilon = E/mgl$ and $\tau = \omega t$ where $\omega = \sqrt{g/l}$ is the angular frequency of small oscillations. Then

$$\tau = \omega t = \frac{1}{\sqrt{2}}\int_0^{\theta} \frac{d\theta'}{\sqrt{\epsilon + \cos\theta'}} \tag{159}$$

Comparing with the incomplete elliptic integral for $s = \operatorname{sn}(u,k)$,

$$u = \frac{1}{\sqrt{2}}\int_0^{2\arcsin ks} \frac{d\theta'}{\sqrt{2k^2 - 1 + \cos\theta'}} \tag{160}$$

we read off $u = \tau$, $k = \sqrt{\frac{1}{2}(\epsilon+1)}$ and $\theta = 2\arcsin ks$. Thus the time dependence of librational trajectories of a simple pendulum with initial condition $\theta(0) = 0$ is given by

$$\theta(t) = 2\arcsin\left[k\,\operatorname{sn}(\omega t, k)\right]. \tag{161}$$

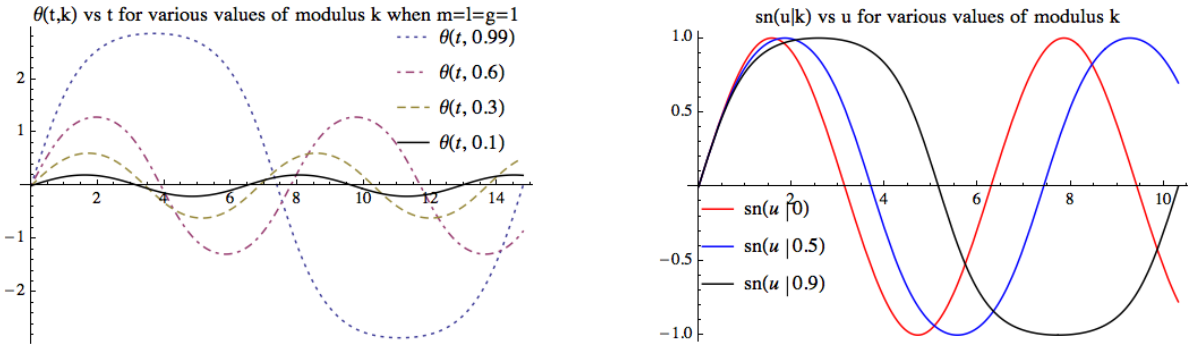
• We check that this reduces to the known sinusoidal trajectory for low energies. If $E \gtrsim -mgl$ then $k \gtrsim 0$ and the argument of the arcsin is small ($|\operatorname{sn}| \le 1$ since $\operatorname{sn}^2 + \operatorname{cn}^2 = 1$), and we may replace $\arcsin(k\operatorname{sn})$ by $k\operatorname{sn}$. Moreover, for small k, $\operatorname{sn}(u,k) \approx \sin u$, so

$$\theta(t) \approx 2k\sin(\omega t) \tag{162}$$

recovering the small amplitude sinusoidal oscillations of the deflection angle $\theta(t)$.

• Notice that the elliptic modulus k is a monotonically increasing function of energy. As E goes from $-mgl$ to mgl, ϵ increases from -1 to 1, k increases from 0 to 1 corresponding to

an amplitude $\theta_{\max}$ increasing from 0 to π. We plot the angle as a function of time in the figure for various values of energy holding m, g, l fixed. The increase in period and amplitude with energy or elliptic modulus k is evident. Also visible is the manner in which for small k the angle approaches a sine function. As the energy increases, the bob spends more and more time around the vertically upward position ($|\theta| \lesssim \pi$).



• We already argued that $\theta(t)$ is periodic with period T. Let us express T as a complete elliptic integral

$$T = \frac{4}{\omega\sqrt{2}} \int_0^{\theta_{\max}} \frac{d\theta}{\sqrt{\epsilon + \cos\theta}} = \frac{4}{\omega\sqrt{2(1+\epsilon)}} \int_0^{\theta_{\max}} \frac{d\theta}{\sqrt{1-s^2}} = \frac{4}{\omega} \int_0^1 \frac{ds}{\sqrt{(1-s^2)(1-k^2s^2)}} = \frac{4}{\omega} K(k)$$

As before, $ks = \sin(\theta/2)$ and at the upper limit, $\cos\theta_{\max} = -\epsilon$ implies $s_{\max} = 1$.

• The period is a monotonically increasing function of energy E or $k = \sin(\theta_{\max}/2)$, since the factor $(1 - k^2s^2)$ in the denominator decreases as k grows from 0 to 1. This is also evident from the series expansion since all the coefficients are positive (see Problem set 8)

$$T = 2\pi\sqrt{\frac{l}{g}} \left[1 + \left(\frac{1}{2}\right)^2 k^2 + \left(\frac{1.3}{2.4}\right)^2 k^4 + \left(\frac{1.3.5}{2.4.6}\right)^2 k^6 + \cdots\right]. \tag{163}$$

We have already shown that the period of librational motion $T(k)$ diverges as $k \to 1^-$.

• Since $\theta(t) = 2\arcsin[k\,\mathrm{sn}(\omega t, k)]$, it follows that the Jacobi elliptic function $\mathrm{sn}(u, k)$ is periodic with period $\omega T = 4K(k)$.

• For $\epsilon = E/mgl > 1$ we have rotational motion around the pivot, with the bob slowing down near the top. The motion is again periodic and the period is again given in terms of the complete elliptic integral of the first kind

$$T_{\mathrm{rot}} = \frac{1}{\omega} \int_0^{2\pi} \frac{d\theta}{\sqrt{2\,(\epsilon + \cos\theta)}} \quad \text{for} \quad \epsilon > 1. \tag{164}$$

The angle as a function of time for rotational motion may be obtained by inverting an incomplete elliptic integral of the first kind. Assuming $\theta(t = 0) = 0$ and putting $k = \sqrt{\frac{1+\epsilon}{2}}$,

$$t = \frac{1}{\omega} \int_0^{\theta} \frac{d\phi}{\sqrt{2(\epsilon + \cos\phi)}}. \tag{165}$$

5 Hamiltonian mechanics

• We previously defined the hamiltonian $H = p\dot{q} - L$ in terms of the Lagrangian, and expressed the eom as 1st order equations using the hamiltonian. Now we begin a deeper study of hamiltonian mechanics.

5.1 Poisson brackets

• Consider a particle (or system of particles) with configuration space R^n with generalized coordinates q_i and generalized momenta $p_i = \frac{\partial L}{\partial \dot{q}^i}$. To motivate the idea of Poisson brackets, let us use Hamilton's equations ($\dot{q}^i = \frac{\partial H}{\partial p_i}$ and $\dot{p}_i = -\frac{\partial H}{\partial q^i}$) to find the time evolution of any dynamical variable $f(q, p; t)$. f is in general a function on phase space, which could depend explicitly on time.

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q^i}\frac{dq^i}{dt} + \frac{\partial f}{\partial p_i}\frac{dp_i}{dt} \right) = \frac{\partial f}{\partial t} + \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q^i}\frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial H}{\partial q^i} \right) = \frac{\partial f}{\partial t} + \{f, H\}. \quad (166)$$

Here we introduced Poisson's bracket of f with the hamiltonian. More generally, the p.b. of two dynamical variables gives another dynamical variable defined as[12]

$$\{f, g\} = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q^i} \right). \quad (167)$$

So the time derivative of any observable is given by its Poisson bracket with the hamiltonian (aside from any explicit time-dependence). From here on, we will restrict to observables that are not explicitly time-dependent (i.e. depend on time only via $q(t)$ and $p(t)$), unless otherwise stated. Hamilton's equations for time evolution may now be written

$$\dot{q}^i = \{q^i, H\} \quad \text{and} \quad \dot{p}_j = \{p_j, H\}. \quad (168)$$

If H isn't explicitly dependent on time, then time does not appear explicitly on the RHS of hamilton's equations. In this case, we say that the ODEs for q and p are an autonomous system.

• One advantage of Poisson brackets is that the time evolution of any observable $f(q, p)$ is given by an equation of the same sort $\dot{f} = \{f, H\}$. We say that the hamiltonian generates infinitesimal time evolution via the Poisson bracket (more on this later).

$$f(q(t + \delta t), p(t + \delta t)) = f(q(t), p(t)) + (\delta t)\ \{f, H\} + \mathcal{O}((\delta t)^2). \quad (169)$$

• If $\{f, g\} = 0$ we say that f 'Poisson commutes' with g. In particular, f is a constant of motion iff it Poisson commutes with the hamiltonian, $\dot{f} = 0 \Leftrightarrow \{f, H\} = 0$. We begin to see the utility of the Poisson bracket in the study of conserved quantities.

• The Poisson bracket has some notable properties. The p.b. of any dynamical variable with a constant is zero. The Poisson bracket is **linear** in each entry. Verify that $\{f, cg\} = c\{f, g\}$ and $\{f, g + h\} = \{f, g\} + \{f, h\}$ etc. where c is a real constant.

[12] Some authors (e.g. Landau & Lifshitz) define the p.b. with an overall minus sign relative to our definition.

• The Poisson bracket is **anti-symmetric** in the dynamical variables $\{f, g\} = -\{g, f\}$. In particular, the p.b. of any observable with itself vanishes $\{h, h\} = 0$. A special case of this encodes the conservation of energy. Assuming H isn't explicitly dependent on time,

$$\frac{dH}{dt} = \{H, H\} = 0. \tag{170}$$

• Since the above formula for the p.b. involves only first order derivatives of f, the p.b. satisfies the **Leibnitz/product rule** of differential calculus. Check that

$$\{fg, h\} = f\{g, h\} + \{f, h\}g \quad \text{and} \quad \{f, gh\} = \{f, g\}h + g\{f, h\}. \tag{171}$$

In the Poisson bracket $\{f, g\}$ we refer to f as the function in the first slot or entry and g as occupying the second. Anti-symmetry ensures that the Leibnitz rule applies to the second entry as well. We say that the p.b. is a **derivation** in either entry.

• The **fundamental Poisson brackets** are between the basic dynamical variables, namely coordinates and momenta. The above formulae give for one degree of freedom

$$\{q, p\} = 1 \quad \text{or} \quad \{p, q\} = -1, \quad \text{while} \quad \{q, q\} = 0 \quad \text{and} \quad \{p, p\} = 0. \tag{172}$$

The last two equations are in fact trivial consequences of the anti-symmetry of the p.b. For n-degrees of freedom we have the fundamental p.b. among the coordinates and momenta

$$\{q^i, p_j\} = \delta^i_j, \quad \text{and} \quad \{q^i, q^j\} = \{p_i, p_j\} = 0 \quad \text{for } 1 \leq i, j \leq n\,. \tag{173}$$

These are sometimes called the canonical ('standard') Poisson bracket relations between coordinates and conjugate momenta. The noun *canon* and the adjective *canonical* refer to something that is standard or conventional.

• **Poisson's theorem:** Perhaps the most remarkable feature of the Poisson bracket is that it can be used to produce new conserved quantities from a pair of existing ones. Poisson's theorem states that if f and g are conserved, then so is $\{f, g\}$. Let us first illustrate this with a couple of examples. For a free particle moving on a plane we know that p_x and p_y are both conserved. Their Poisson bracket is $\{p_x, p_y\} = 0$, which is of course a trivially conserved quantity. As a second example, consider a particle moving in three dimensions under the influence of a central potential. We know that $L_x = yp_z - zp_y$ and $L_y = zp_x - xp_z$ are both conserved. We compute $\{L_x, L_y\}$ by using bi-linearity, the Leibnitz rule and other properties of the p.b. and find $\{L_x, L_y\} = L_z$. And indeed, we know that L_z is also a conserved quantity. Similarly we check that

$$\{L_x, L_y\} = L_z, \quad \{L_y, L_z\} = L_x \quad \text{and} \quad \{L_z, L_z\} = L_y. \tag{174}$$

• **Jacobi identity:** More generally, Poisson's theorem is a consequence of the Jacobi identity. For any three dynamical variables f, g and h, the following cyclic sum of 'double' Poisson brackets vanishes:

$$\{f, \{g, h\}\} + \{h, \{f, g\}\} + \{g, \{h, f\}\} = 0. \tag{175}$$

Using anti-symmetry we could write the Jacobi identity also as

$$\{\{f, g\}, h\} + \{\{g, h\}, f\} + \{\{h, f\}, g\} = 0. \tag{176}$$

Before we prove the Jacobi identity, let us use it to establish Poisson's theorem. Suppose f, g are conserved so that each of them Poisson commutes with the hamiltonian $h = H$, i.e., $\{f, h\} = \{g, h\} = 0$. Then the Jacobi identity implies that

$$\{\{f, g\}, H\} = 0 \quad \Rightarrow \quad \frac{d}{dt}\{f, g\} = 0. \tag{177}$$

So the p.b. of two conserved quantities is again a conserved quantity.

• **Poisson tensor:** To prove the Jacobi identity, it is convenient to introduce a compact notation. Let us combine the coordinates and momenta into a $2n$-component 'grand' coordinate ξ on phase space. We regard ξ as a coordinate on *phase space* and write its components with upper indices:

$$\vec{\xi} = (\xi^1, \xi^2 \cdots, \xi^n, \xi^{n+1}, \cdots, \xi^{2n}) = (\vec{q}, \vec{p}) = (q^1, \cdots, q^n, p_1, \cdots, p_n) \tag{178}$$

Then check the fundamental Poisson bracket relations may be expressed in terms of ξ^i

$$\{\xi^i, \xi^j\} = r^{ij} \quad \text{where} \quad r^{\text{row column}} = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \tag{179}$$

Here r is a $2n \times 2n$ block matrix with $n \times n$ blocks consisting of the identity and zero matrices as indicated. The constant matrix r^{ij} is sometimes called the Poisson 'tensor' of the canonical p.b. relations.

• The p.b. of any pair of observables may now be written in terms of the 'fundamental' p.b. between coordinates and momenta. Show that

$$\{f, g\} = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q^i} \right) = \sum_{i,j=1}^{2n} \frac{\partial f}{\partial \xi^i}\frac{\partial g}{\partial \xi^j}\{\xi^i, \xi^j\} = \sum_{i,j=1}^{2n} r^{ij}\partial_i f \partial_j g. \tag{180}$$

Here we used subscripts on f, g to denote partial differentiation, $\frac{\partial f}{\partial \xi^i} \equiv f_i$. All properties of the canonical Poisson brackets are encoded in the Poisson tensor. Of particular importance to us is the anti-symmetry of r^{ij} (equivalent to antisymmetry of the p.b.) and the constancy of the components r^{ij}.

• Let us now prove the Jacobi identity. We wish to evaluate the cyclic sum

$$J = \{\{f, g\}, h\} + \{\{g, h\}, f\} + \{\{h, f\}, g\}. \tag{181}$$

We use the Poisson tensor and the Leibnitz rule to write the first term of J as

$$\{\{f, g\}, h\} = \left(f_i g_j r^{ij}\right)_k h_l r^{kl} = \left[f_{ik} g_j h_l + f_i g_{jk} h_l\right] r^{ij} r^{kl} \tag{182}$$

Adding its cyclic permutations,

$$J = \left[f_{ik} g_j h_l + f_i g_{jk} h_l + g_{ik} h_j f_l + g_i h_{jk} f_l + h_{ik} f_j g_l + h_i f_{jk} g_l\right] r^{ij} r^{kl}. \tag{183}$$

If J has to vanish for any smooth functions f, g, h on phase space, then the terms involving 2nd derivatives of f must mutually cancel as must those involving 2nd derivatives of g or h. So let us consider the two terms involving second derivatives of f, and call the sum J_f. We find

$$J_f \;\; = \;\; f_{ik} g_j h_l r^{ij} r^{kl} + f_{jk} g_l h_i r^{ij} r^{kl} = f_{ik} g_j h_l r^{ij} r^{kl} + f_{ik} g_l h_j r^{ji} r^{kl}$$

$$
\begin{aligned}
&= f_{ik}g_j h_l r^{ij}r^{kl} + f_{ik}g_j h_l r^{li}r^{kj} = f_{ik}g_j h_l r^{ij}r^{kl} + f_{ki}g_j h_l r^{lk}r^{ij} \\
&= f_{ik}g_j h_l r^{ij}r^{kl} - f_{ik}g_j h_l r^{ij}r^{kl} = 0. \qquad (184)
\end{aligned}
$$

We relabeled indices of summation $i \leftrightarrow j$, $j \leftrightarrow l$ and $i \leftrightarrow k$ in the three successive equalities and finally used the equality of mixed partial derivatives $\frac{\partial^2 f}{\partial \xi^i \xi^k} = \frac{\partial^2 f}{\partial \xi^k \xi^i}$ and antisymmetry of the Poisson tensor $r^{kl} = -r^{lk}$. Thus we have shown that $J_f = 0$ and by cyclic symmetry, $J_g = J_h = 0$. Thus $J = 0$ and the Jacobi identity has been established. As a corollary we obtain Poisson's theorem on conservation of p.b. of conserved quantities.

5.2 Variational principles for Hamilton's equations

• We seek an extremum principle for Hamilton's equations, just as we had one for Lagrange's equations: $S[q] = \int L\, dt$ and $\delta S = 0$. Hamilton's variational principle for his equations is given by the functional of a path on *phase space* $(q^i(t), p_j(t))$

$$
S[q,p] = \int_{t_i}^{t_f} \left[p_i \dot{q}^i - H(q,p) \right]\, dt. \qquad (185)
$$

Recall that $L(q,\dot{q}) = \mathrm{ext}_p(p\dot{q} - H(q,p))$, which motivates the formula for $S[q,p]$. Note that $S[q]$ is a functional of a path on configuration space, while $S[q,p]$ is a functional of a path on phase space. They are not the same, though we denote both by S and call both 'action'. We ask that this functional $S[q,p]$ be stationary with respect to small variations in the phase path $(q(t), p(t))$ while holding $\delta q(t_i) = 0$ and $\delta q(t_f) = 0$. Note that we do not constrain $\delta p(t_i)$ or $\delta p(t_f)$. That would be an over specification[13]. Now

$$
\delta S = \int_{t_i}^{t_f} \left[\delta p_i\, \dot{q}^i + p_i \delta \dot{q}^i - \frac{\partial H}{\partial q^i}\delta q^i - \frac{\partial H}{\partial p_i}\delta p_i \right]\, dt + \ldots \qquad (186)
$$

We find upon integrating by parts in the second term and using $\delta q(t_{i,f}) = 0$,

$$
S[q+\delta q, p+\delta p] = S[q,p] + \int_{t_i}^{t_f} \left[\dot{q}^i \delta p_i - \dot{p}_i \delta q^i - \frac{\partial H}{\partial q^i}\delta q^i - \frac{\partial H}{\partial p_i}\delta p_i \right] dt + \ldots . \qquad (187)
$$

The action must be stationary with respect to arbitrary infinitesimal independent variations δp, δq subject to $\delta q(t_i) = \delta q(t_f) = 0$. So the coefficients of δp and δq must individually vanish. Thus we recover Hamilton's equations at all times $t_i < t < t_f$:

$$
\dot{q}^i = \frac{\partial H}{\partial p_i} \quad \text{and} \quad \dot{p}_i = -\frac{\partial H}{\partial q^i}. \qquad (188)
$$

Hamilton's equations treat position and momentum on an equal footing except for a sign. But the above boundary conditions treat them asymmetrically. This is a clue that there is another variational principle for Hamilton's equations. Consider the functional of a path on phase space

$$
\tilde{S}[q,p] = \int_{t_i}^{t_f} \left[-q^j \dot{p}_j - H(q,p) \right] dt \qquad (189)
$$

[13] There would in general not be *any* trajectory joining specified values of q *and* p at *both* t_i and t_f. Demonstrate this in the case of a free particle.

which we extremize with respect to small variations $\delta q, \delta p$ while holding $\delta p_j(t_i) = \delta p_j(t_f) = 0$. Then integrating by parts,

$$\delta\tilde{S} = \int_{t_i}^{t_f} \left[-\dot{p}_j \delta q^j - q^j \delta\dot{p}_j - \frac{\partial H}{\partial q^j}\delta q^j - \frac{\partial H}{\partial p_j}\delta p_j \right] dt = \int_{t_i}^{t_f} \left[\left(\dot{p}_j + \frac{\partial H}{\partial q^j} \right) \delta q^j + \left(\dot{q}^j - \frac{\partial H}{\partial p_j} \right) \delta p_j \right] dt \tag{190}$$

So $\delta\tilde{S} = 0$ also implies Hamilton's equations. We will exploit both these variational principles while studying canonical transformations.

5.3 Lagrange's and Hamilton's equations take same form in all systems of coordinates on $\mathcal{Q}$

• One of the advantages of having a variational principle is that it allows us to show that the equations of motion *expressed in terms of the hamiltonian*, take the same form in any system of coordinates on configuration space $\mathcal{Q}$. We first recall why this is the case for Lagrange's equations.

• We begin by observing that the condition for a function to be stationary is independent of choice of coordinates, as long as we make non-singular changes of coordinates[14]. Consider $f(x)$, it is extremal when $f'(x) = 0$. Now change to a new coordinate $X(x)$ (e.g. $X(x) = 2x$). Then $f(x) = f(x(X)) \equiv \tilde{f}(X)$. Moreover, by the chain rule, $f'(x) = \tilde{f}'(X)\frac{dX}{dx}$. If the change of variables is non-singular, $\frac{dX}{dx} \neq 0$. It follows that $f'(x) = 0 \Leftrightarrow \tilde{f}'(X) = 0$. For several variables, a real-valued function $f(x)$ is extremal at a point if $\frac{\partial f}{\partial x^i} = 0$ for all i. Under a change of coordinates $x^i \mapsto X^i(x)$, $\frac{\partial f}{\partial x^i} = \frac{\partial f}{\partial X^j} J^j_i$ where the Jacobian matrix $J^j_i = \frac{\partial X^j}{\partial x^i}$. Now the condition for any function f to be extremal is independent of coordinates provided the Jacobian matrix does not have kernel (i.e. has trivial null space), which is the same as being non-singular or having non-zero determinant at the relevant point.

• Recall that Lagrange's equations are the conditions for stationarity of the action $S[q] = \int L(q, \dot{q})\, dt$. Now suppose we make a non-singular change of coordinates $q \to Q(q)$ on $\mathcal{Q}$. We work with 1 degree of freedom though the same applies to several degrees of freedom. We define a new Lagrange function by expressing the old coordinates and velocities in terms of the new ones

$$S[q] = \int L(q, \dot{q})\, dt = \int \tilde{L}(Q, \dot{Q})\, dt \equiv \tilde{S}[Q] \quad \text{where} \quad L(q, \dot{q}) = \tilde{L}(Q(q), \dot{Q}(q, \dot{q})). \tag{191}$$

As before, the conditions for stationarity under infinitesimal variations are the same: $\delta S[q] = 0$ iff $\delta\tilde{S}[Q] = 0$. Thus, Lagrange's equations must take the same form in the q and Q coordinates:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q} \quad \Leftrightarrow \quad \frac{d}{dt}\frac{\partial \tilde{L}}{\partial \dot{Q}} = \frac{\partial \tilde{L}}{\partial Q}. \tag{192}$$

• We apply the same sort of reasoning to argue that hamilton's equations take the same form in all systems of coordinates on $\mathcal{Q}$. Suppose we change from $q \to Q$. Then we get a new Lagrange function $\tilde{L}(Q, \dot{Q})$. We also get a new conjugate momentum $P = \frac{\partial \tilde{L}}{\partial \dot{Q}}$ while $p = \frac{\partial L}{\partial \dot{q}}$.

[14] A change of variables $q^i \to Q^i$ is said to be non-singular if it is a smooth and invertible change of variables (*with smooth inverse*). The change is non-singular in some neighbourhood of the point $\vec{q}_0$ if the matrix of first partials (Jacobian matrix) $J^i_j = \frac{\partial Q^i}{\partial q^j}$ is a non-singular matrix (i.e. has non-zero determinant) at $\vec{q} = \vec{q}_0$.

In general, $Q = Q(q)$ but P will be a function of both q and p. Hamilton's equations are the conditions for the action functional $S[q,p] = \int [p\dot{q} - H(q,p)]\, dt$ to be extremal with respect to infinitesimal variations in the phase path $\delta S = 0$. We also have a new hamiltonian $\tilde{H}(Q,P) = H(q(Q), p(Q,P))$ and new action functional

$$\tilde{S}[Q,P] = \int [P\dot{Q} - \tilde{H}(Q,P)]\, dt \quad \text{while} \quad S[q,p] = \int [p\dot{q} - H(q,p)]\, dt. \tag{193}$$

As before, the conditions $\delta S = 0$ imply the conditions $\delta \tilde{S} = 0$ so that Hamilton's equations take the same form in both systems of coordinates on configuration space.

• Though we changed coordinates on $\mathcal{Q}$, we didn't change the momenta in an arbitrary way. Instead, here the change in momenta was induced by the change in coordinates via the formula $P = \frac{\partial \tilde{L}}{\partial \dot{Q}}$ where $\tilde{L}(Q,\dot{Q})$ is the Lagrangian expressed in terms of the new coordinates and velocities. So far, we used the Lagrangian as a walking stick to define the momenta. But Hamilton's equations treat coordinates and momenta on a fairly equal footing. Leaving behind the walking stick of the Lagrange function, one wonders if Hamilton's equations take the same form in a larger class of coordinate systems on *phase space* as opposed to just *configuration space*. Remarkably, Hamilton's equations *do* take the same form in a slightly larger class of coordinate systems on phase space, namely those that are *canonically* related to q, p. It is possible to see this using the variational principle, but we first develop an alternative viewpoint involving Poisson brackets.

5.4 Canonical transformations

• Recall that the space of generalised coordinates and momenta is called phase space. Hamilton's equations $\dot{q}^i = \frac{\partial H}{\partial p_i}, \dot{p}_i = -\frac{\partial H}{\partial q^i}$ may be easier to solve (or understand qualitatively) in some systems of coordinates and momenta compared to others. For instance, there may be more cyclic coordinates in one system. E.g., for a particle in a central potential $V(r)$ on the plane, the eom are simpler to handle in polar coordinates r, θ than in Cartesian coordinates x, y. From the Lagrangian

$$L(x,y,\dot{x},\dot{y}) = \frac{1}{2}m\left(\dot{x}^2 + \dot{y}^2\right) - V\left(\sqrt{x^2+y^2}\right) = \frac{1}{2}m\left(\dot{r}^2 + r^2\dot{\theta}^2\right) - V(r) = \tilde{L}(r,\theta,\dot{r},\dot{\theta}), \tag{194}$$

θ is a cyclic coordinate and its conjugate momentum $L_z = p_\theta = mr^2\dot{\theta}$ is conserved. On the other hand, neither p_x nor p_y is conserved. One checks that Hamilton's equations take the same form in cartesian and polar coordinates (as guaranteed by the preceding section's argument):

$$\begin{aligned} &\dot{x} = \frac{\partial H}{\partial p_x},\ \dot{y} = \frac{\partial H}{\partial p_y},\ \dot{p}_x = -\frac{\partial H}{\partial x},\ \dot{p}_y = -\frac{\partial H}{\partial y} \quad \text{where} \quad p_x = \frac{\partial L}{\partial \dot{x}} \ \text{ and } \ p_y = \frac{\partial L}{\partial \dot{y}} \\ \Leftrightarrow \quad &\dot{r} = \frac{\partial H}{\partial p_r},\ \dot{\theta} = \frac{\partial H}{\partial p_\theta},\ \dot{p}_r = -\frac{\partial H}{\partial r},\ \dot{p}_\theta = -\frac{\partial H}{\partial \theta} \quad \text{where} \quad p_r = \frac{\partial L}{\partial \dot{r}} \ \text{ and } \ p_\theta = \frac{\partial L}{\partial \dot{\theta}}. \end{aligned} \tag{195}$$

We say that the transformation from cartesian coordinates and conjugate momenta (x, y, p_x, p_y) to polar coordinates and conjugate momenta $(r, \theta, p_r, p_\theta)$ is a canonical transformation. We also check (problem set 10) that the fundamental Poisson brackets among coordinates and momenta are preserved

$$\{x, p_x\} = \{y, p_y\} = 1, \qquad \{x, p_y\} = \{y, p_x\} = \{x, y\} = \{p_x, p_y\} = 0$$

$$\text{and} \qquad \{r, p_r\} = \{\theta, p_\theta\} = 1, \qquad \{r, p_\theta\} = \{\theta, p_r\} = \{r, \theta\} = \{p_r, p_\theta\} = 0. \tag{196}$$

• Suppose we start with a system of coordinates q^i and conjugate momenta p_i, in which Hamilton's equations take the standard form $\dot{q} = \frac{\partial H}{\partial p}, \dot{p} = -\frac{\partial H}{\partial q}$. A canonical transformation (CT) of coordinates and momenta from old ones (q^i, p_i) to new ones (Q^i, P_i) is one that preserves the form of Hamilton's equations. At the very least, if we make a change of variables that is canonical, we do not need to re-derive the equations of motion, they are guaranteed to take the Hamiltonian form.

• But not every choice of coordinates and momenta is canonical. For example, we notice that Hamilton's equations treat coordinates and momenta on a nearly equal footing. So suppose we simply exchange coordinates and momenta by defining $Q = p$ and $P = q$. Then the hamiltonian may be written in terms of the new variables $H(q, p) = H(P, Q) \equiv \tilde{H}(Q, P)$. We find that

$$\dot{Q} = \dot{p} = -\frac{\partial H}{\partial q} = -\frac{\partial \tilde{H}}{\partial P} \quad \text{and} \quad \dot{P} = \dot{q} = \frac{\partial H}{\partial p} = \frac{\partial \tilde{H}}{\partial Q}. \tag{197}$$

So the eom in the new variables *do not* have the form of Hamilton's equations, they are off by a sign. So $(q, p) \mapsto (p, q)$ is *not* a canonical transformation. We may also check that the transformation *does not* preserve the fundamental p.b.

$$\{q, p\} = 1 \quad \text{while} \quad \{Q, P\} = \{p, q\} = -1 \tag{198}$$

• In the last section we saw that any change of coordinates alone ('point transformation') $q^i \to Q^i$, with the associated 'induced' change in momenta $P_i = \frac{\partial \tilde{L}}{\partial \dot{Q}^i}$ is automatically canonical. An example of such a canonical transformation is the one from cartesian to polar coordinates for a particle on a plane. The interesting thing is that there are canonical transformations that are *more general* than those resulting from changes of coordinates (point transformations) on $\mathcal{Q}$. Perhaps the simplest such examples are (1) $Q = p, P = -q$ and (2) $Q = -p, P = q$ which mix coordinates and momenta for one degree of freedom. Check that Hamilton's equations retain their form, as do the fundamental Poisson brackets.

• In the above examples of CTs, along with Hamilton's equations, the fundamental p.b. among coordinates and momenta were also preserved. This is true in general as we now argue.

5.4.1 Form of Hamilton's equations are preserved iff fundamental Poisson brackets are preserved

• It is worth noting that a transformation is canonical irrespective of what the hamiltonian is. The form of Hamilton's equations must be unchanged for *any* smooth $H(q, p)$. This suggests it should be possible to state the condition of canonicity without reference to the hamiltonian. We will show now (for 1 degree of freedom, for simplicity) that a transformation preserves the form of Hamilton's equations iff it preserves the fundamental Poisson brackets.

• **Proof:** Suppose we make a smooth invertible change of coordinates and momenta $q \mapsto Q = Q(q, p)$ and $p \mapsto P = P(q, p)$. The inverse transformation expresses the old coordinates and momenta in terms of the new ones $q = q(Q, P)$ and $p = p(Q, P)$. The old coordinates satisfy canonical Poisson brackets $\{q, p\} = 1$, $\{q, q\} = \{p, p\} = 0$. Under this change, the old hamiltonian $H(q, p)$ transforms into a new hamiltonian $\tilde{H}(Q, P) = H(q(Q, P), p(Q, P))$.

Suppose the above transformation preserves the form of Hamilton's equations. Denoting partial derivatives by subscripts,

$$\dot{q} = H_p \quad \text{and} \quad \dot{p} = -H_q \quad \text{while} \quad \dot{Q} = \tilde{H}_P \quad \text{and} \quad \dot{P} = -\tilde{H}_Q. \tag{199}$$

Then we'll show that $\{Q, P\} = 1$. The other two p.b. $\{Q, Q\}$ and $\{P, P\}$ vanish by anti-symmetry.

• By hamilton's equations and the chain rule, $\dot{Q} = \tilde{H}_P = H_q q_P + H_p p_P = -\dot{p} q_P + \dot{q} p_P$. We also know that $\dot{Q} = Q_q \dot{q} + Q_p \dot{p}$. We want to equate these two expressions and extract information about the p.b. $\{Q, P\} = Q_q P_p - Q_p P_q$. As it is the partial derivatives of Q and P that appear in this p.b., it is of interest to express q_P, p_P etc in terms of partial derivatives of Q and P using the following Lemma.

• **Lemma:** $q_P = -Q_p \{Q, P\}$, $p_P = Q_q \{Q, P\}$, $p_Q = -\frac{P_q}{\{Q,P\}}$, and $q_Q = \frac{P_p}{\{Q,P\}}$.

• **Proof:** Recall that for an invertible map of one variable, $x \to X(x) = f(x)$ with inverse $x = x(X) = f^{-1}(X)$ the derivatives are reciprocally related $\frac{dX}{dx} = \left(\frac{dx}{dX}\right)^{-1}$. This arises from differentiating the identity $(f \circ f^{-1})(X) = f(f^{-1}(X)) = X$ with respect to X. We get $f'(x)x'(X) = 1$ or $X'(x)x'(X) = 1$.

• What is the analogous formula for the map $F : x^i = (q, p) \mapsto X^i = (Q, P)$? Here

$$F : \mathbb{R}^2 \to \mathbb{R}^2, \quad F(q, p) = (Q, P) \quad \text{and} \quad F^{-1} : \mathbb{R}^2 \to \mathbb{R}^2, \quad F^{-1}(Q, P) = (q, p). \tag{200}$$

In other words, $F^{-1}(\vec{X}) = \vec{x}$ or $F^i(\vec{x}) = X^i$. As before, $F \circ F^{-1}$ is the identity, so

$$F(F^{-1}(\vec{X})) = \vec{X} \quad \Rightarrow \quad F^i(\vec{x}(\vec{X})) = X^i, \quad \text{and differentiating,} \quad \frac{\partial F^i}{\partial x^j} \frac{\partial x^j}{\partial X^k} = \delta^i_k. \tag{201}$$

Here the matrices of first partials are

$$\frac{\partial F^i}{\partial x^j} = \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} \end{pmatrix} \quad \text{and} \quad \frac{\partial x^j}{\partial X^k} = \begin{pmatrix} \frac{\partial q}{\partial Q} & \frac{\partial q}{\partial P} \\ \frac{\partial p}{\partial Q} & \frac{\partial p}{\partial P} \end{pmatrix}. \tag{202}$$

The above condition says that the matrix product must be the identity

$$\begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} \end{pmatrix} \begin{pmatrix} \frac{\partial q}{\partial Q} & \frac{\partial q}{\partial P} \\ \frac{\partial p}{\partial Q} & \frac{\partial p}{\partial P} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{203}$$

We get a system of four equations for the four 'unknowns' q_Q, q_P, p_Q, p_P

$$Q_q q_P = -Q_p p_P, \quad P_q q_P + P_p p_P = 1, \quad P_q q_Q = -P_p p_Q, \quad \text{and} \quad Q_q q_Q + Q_p p_Q = 1. \tag{204}$$

These are, in fact, two pairs of linear equations in two unknowns. They are easily solved for the partials of the old variables (e.g. by matrix inversion). The solution involves the reciprocal of the determinant of the coefficient matrix, which is just the p.b. $\{Q, P\} = Q_q P_p - Q_p P_q$:

$$q_P = -\frac{Q_p}{\{Q, P\}}, \quad p_P = \frac{Q_q}{\{Q, P\}}, \quad p_Q = -\frac{P_q}{\{Q, P\}}, \quad q_Q = \frac{P_p}{\{Q, P\}}. \tag{205}$$

• Armed with this lemma, we return to the fact that the eom retains its form in the new variables:

$$\dot{Q} = \tilde{H}_P = \frac{[\dot{p} Q_p + \dot{q} Q_q]}{\{Q, P\}} = \frac{\dot{Q}}{\{Q, P\}}. \tag{206}$$

For this equation to be satisfied we must have $\{Q,P\}=1$. Similarly,

$$\dot{P}=-\tilde{H}_Q=-H_qq_Q-H_pp_Q=\dot{p}\frac{P_p}{\{Q,P\}}+\dot{q}\frac{P_q}{\{Q,P\}}=\frac{1}{\{Q,P\}}\left[P_q\dot{q}+P_p\dot{p}\right]=\frac{\dot{P}}{\{Q,P\}}. \quad (207)$$

For this to hold, again we need $\{Q,P\}=1$. Thus we have shown that if Hamilton's equations retain their form in the new coordinates, then the transformation also preserves the form of the fundamental p.b.

• Let us now prove the converse, namely, if the transformation $(q,p)\mapsto(Q,P)$ preserves the form of the p.b., i.e., if $\{Q,P\}=1$, then it must preserve the form of Hamilton's equations. So we must show that $\frac{\partial\tilde{H}}{\partial P}=\dot{Q}$ and $-\frac{\partial\tilde{H}}{\partial Q}=\dot{P}$. Let us compute

$$\frac{\partial\tilde{H}}{\partial P}=\frac{\partial H}{\partial q}q_P+\frac{\partial H}{\partial p}p_P=-\dot{p}q_P+\dot{q}p_P=\dot{p}Q_p+\dot{q}Q_q=\dot{Q}. \quad (208)$$

In the penultimate equality we used a result from the lemma and the assumption that $\{Q,P\}=1$. So the first of Hamilton's equations holds in the new variables! Similarly, we show that the second of Hamilton's equations also holds in the new variables

$$\frac{\partial\tilde{H}}{\partial Q}=\frac{\partial H}{\partial q}\frac{\partial q}{\partial Q}+\frac{\partial H}{\partial p}\frac{\partial p}{\partial Q}=-\dot{p}q_Q+\dot{q}p_Q=-\dot{p}P_p-\dot{q}P_q=-\dot{P}. \quad (209)$$

So we showed that if the transformation preserves the p.b., then it is canonical (i.e., preserves the form of Hamilton's equations). A similar result also holds for several degrees of freedom, though we do not discuss it here. So the new coordinates and momenta are said to be canonical provided

$$\dot{Q}^i=\frac{\partial\tilde{H}}{\partial P_i}\ \text{ and }\ \dot{P}_i=-\frac{\partial\tilde{H}}{\partial Q^i}\ \text{ or equivalently }\ \{Q^i,P_j\}=\delta_{ij}\ \text{ and }\ \{Q^i,Q^j\}=\{P_i,P_j\}=0. \quad (210)$$

• Time evolution by any hamiltonian gives us examples of canonical transformations. Recall that (we will prove this shortly) the equal time Poisson brackets of coordinates and momenta

$$\{q^i(t),p_j(t)\}=\delta^i_j \quad \text{and} \quad \{q^i(t),q^j(t)\}=\{p_i(t),p_j(t)\}=0 \quad (211)$$

are valid at all times. So the map from $(q^i(t_1),p_i(t_1))$ to $(q^i(t_2),p_i(t_2))$ which is a map from phase space to itself, is canonical for any times t_1,t_2. So hamiltonian evolution gives us a 1-parameter family of canonical transformations.

• It may be noted that unequal-time Poisson brackets contain dynamical information and depend on the hamiltonian. Equal-time Poisson brackets do not depend on the hamiltonian and are in a sense kinematical. Unequal time p.b. $\{f(q(0),p(0)),g(q(t),p(t))\}$ may be reduced to equal time p.b. by solving the equations of motion and expressing $g(q(t),p(t))$ in terms of initial values $q(0)$ and $p(0)$.

5.4.2 Brief comparison of classical and quantum mechanical formalisms

• This is a good opportunity to compare certain features of classical and quantum mechanics.

1. In CM, the space of (pure) states is the phase space. In QM it is the quantum mechanical Hilbert space (vector space $\mathcal{H}$ with inner product $\langle \cdot, \cdot \rangle$).

2. In CM, observables are smooth real-valued functions on phase space. In QM, observables (A, B etc) are self-adjoint (hermitian) operators on Hilbert space. Self-adjointness is the analogue of reality, both of which ensure that results of measurements are real numbers.

3. The Poisson bracket of observables in CM is replaced by the commutator of operators (upto a factor of $i\hbar$) in QM, e.g. $\{x, p\} = 1 \longrightarrow \frac{1}{i\hbar}[x, p] = 1$. Both operations map a pair of observables to a new observable.

4. In CM, time evolution is a 1-parameter family of canonical transformations. In QM, time evolution is a 1-parameter family of unitary transformations $U(t) = e^{-iHt/\hbar}$.

5. Unitary transformations ($|\psi\rangle \to |\psi'\rangle = U|\psi\rangle$ and $A \to A' = UAU^\dagger$ with $U^\dagger U = I$) are quantum analogs of canonical transformations. Both preserve the structure of the formalism. CTs preserve the fundamental p.b. while unitary transformations preserve the Heisenberg canonical commutation relations, since $[A', B'] = U[A, B]U^\dagger$ and in particular $[q', p'] = U[q, p]U^\dagger = U(i\hbar)U^\dagger = i\hbar$. Unitary transformations also preserve inner products $\langle U\phi|U\psi\rangle = \langle \phi|U^\dagger U\psi\rangle = \langle \phi|\psi\rangle$.

5.4.3 Canonical transformations for one degree of freedom: Area preserving maps

• To better understand the concept, let us focus on canonical transformations for systems with one degree of freedom. So we have just one coordinate q and one canonically conjugate momentum p which together parametrize phase space and satisfy canonical p.b. relations $\{q, p\} = 1$. Suppose we transform to a new pair of coordinates and momenta $Q(q, p)$ and $P(q, p)$. Then what does it mean for the transformation to be canonical? It means the new variables satisfy the same p.b., i.e.,

$$1 = \{Q, P\} = \frac{\partial Q}{\partial q}\frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial P}{\partial q} \tag{212}$$

The quantity that appears above is in fact the determinant of the Jacobian matrix of 1st partials

$$\det J = \det \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} \end{pmatrix} = \frac{\partial Q}{\partial q}\frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial P}{\partial q}. \tag{213}$$

Both (q, p) and (Q, P) provide coordinate systems on phase space. We recall from calculus that the Jacobian determinant is the factor relating oriented area elements on phase space

$$dQ\ dP = (\det J)\ dq\ dp \tag{214}$$

So a canonical transformation for a system with one degree of freedom is simply a transformation that preserves the *signed* area element on phase space. Such a transformation is called area preserving.

• Pictorially, what is an area preserving map? The map $F : \mathbb{R}^2 \to \mathbb{R}^2$ specified by $q \to Q(q, p)$ and $p \to P(q, p)$ maps points on the plane to points on the plane. E.g. it could be the translation map $q \to q + 1, p \to p + 2$ or a rotation etc. Under such a transformation, any domain $D \subset \mathbb{R}^2$

will be mapped to a new region $D' = F(D)$. The map is area preserving if for any D with finite area, $\mathrm{Ar}(D) = \mathrm{Ar}(D')$ i.e., $\iint_D dqdp = \iint_{D'} dqdp$. The above condition guarantees this, since

$$\mathrm{Ar}(D) = \iint_D dqdp = \int_{F(D)} \frac{dQdP}{\det J} = \iint_{F(D)} dQdP = \iint_{D'} dqdp = \mathrm{Ar}(D'). \tag{215}$$

In the first equality we changed variables of integration and in the second we used $\det J = 1$ and relabeled the dummy variables of integration $Q \to q$ and $P \to p$.

• Area preserving maps of the phase plane are all the canonical transformations for one degree of freedom. These include (but are not restricted to) rigid motions like translations and rotations of the *phase plane*. For example, time evolution by a generic hamiltonian is a CT which in general will morph a nice looking disk on the phase plane into a complicated region having the same area. For several degrees of freedom, it can be shown that a transformation of coordinates and momenta is canonical provided it preserves the area elements in *every* two dimensional tangent plane through each point in phase space.

5.4.4 CTs preserve Poisson tensor and formula for p.b. of any pair of observables

• We showed that CTs preserve the fundamental p.b. between coordinates and momenta. What about the p.b. between arbitrary observables f, g? In the old coordinates,

$$\{f, g\} \equiv \{f, g\}_{q,p} = \sum_i \left(\frac{\partial f}{\partial q^i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q^i} \right). \tag{216}$$

It turns out that if $(q, p) \to (Q, P)$ is canonical (i.e., preserves the fundamental p.b.) then (and only then), the formula for $\{f, g\}$ may also be expressed as[15]

$$\{f, g\} = \sum_i \left(\frac{\partial f}{\partial Q^i} \frac{\partial g}{\partial P_i} - \frac{\partial f}{\partial P_i} \frac{\partial g}{\partial Q^i} \right). \tag{217}$$

Let us show this for one degree of freedom (though the same calculation also works for n degrees of freedom by putting in the indices.) Now by definition and the chain rule and rearranging terms,

$$\begin{aligned} \{f, g\} &= f_q g_p - f_p g_q = (f_Q Q_q + f_P P_q)(g_Q Q_p + g_P P_p) - (f_Q Q_p + f_P P_p)(g_Q Q_q + g_P P_q) \\ &= f_Q g_P (Q_q P_p - Q_p P_q) + f_P g_Q (P_q Q_p - P_p Q_q) + f_Q g_Q (Q_q Q_p - Q_p Q_q) + f_P g_P (P_q P_p - P_p P_q) \\ &= (f_Q g_P - f_P g_Q)\{Q, P\} + f_Q g_Q \{Q, Q\} + f_P g_P \{P, P\}. \end{aligned} \tag{218}$$

Of course, the last two terms are identically zero by anti-symmetry of p.b., but we displayed them as they help in writing the corresponding formula for n degrees of freedom:

$$\{f, g\} = \left(f_{Q^i} g_{P_j} - f_{P_j} g_{Q^i}\right)\{Q^i, P_j\} + f_{Q^i} g_{Q^j} \{Q^i, Q^j\} + f_{P_i} g_{P_j} \{P_i, P_j\}. \tag{219}$$

Now we see that

$$\{f, g\} = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial Q^i} \frac{\partial g}{\partial P_i} - \frac{\partial f}{\partial P_i} \frac{\partial g}{\partial Q^i} \right) = \{f, g\}_{Q,P}. \tag{220}$$

[15] We are being a bit sloppy with notation here. When we differentiate in Q, P we are regarding $f = f(q(Q, P), p(Q, P))$.

iff the new coordinates and momenta satisfy canonical p.b. relations, i.e., if

$$\{Q^i, P_j\} = \delta^i_j, \quad \text{and} \quad \{Q^i, Q^j\} = 0 = \{P_i, P_j\}. \tag{221}$$

Thus a transformation is canonical if the p.b. of any pair of observables is given by the same sort of formula whether computed using the old or new variables:

$$(q,p) \mapsto (Q,P) \quad \text{is a canonical transformation iff} \quad \{f,g\}_{q,p} = \{f,g\}_{Q,P} \quad \forall \ f,g. \tag{222}$$

• Yet another way of stating the canonicity of a transformation is that it preserves the Poisson tensor. Suppose $\vec{\xi} = (\vec{q}, \vec{p})$ is the grand coordinate on phase space in the old variable and $\vec{\Xi} = (\vec{Q}, \vec{P})$ is the new one[16]. Then the preservation of fundamental p.b means

$$\{\xi^i, \xi^j\} = r^{ij} = \{\Xi^i, \Xi^j\}. \tag{223}$$

In other words, a CT is one that leaves the Poisson tensor invariant, component-wise, just as an isometry is one that leaves a metric tensor invariant. By the foregoing,

$$\{f,g\} = \{f,g\}_{q,p} = \sum_{ij} \frac{\partial f}{\partial \xi^i} \frac{\partial g}{\partial \xi^j} r^{ij} = \sum_{ij} \frac{\partial f}{\partial \Xi^i} \frac{\partial g}{\partial \Xi^j} r^{ij} = \{f,g\}_{Q,P} \tag{224}$$

where the *same* Poisson tensor r^{ij} appears in both expressions, though the differentiation is with respect to old variables in the first expression and with respect to new variables in the second expression.

5.4.5 Generating function for infinitesimal canonical transformations

• The condition for a transformation from canonical coordinates and momenta (q_i, p_i) to new ones (Q^i, P_i) to be canonical is that the Poisson brackets must be preserved. It would be nice to find an explicit way of producing canonical transformations. Let us address this question for infinitesimal canonical transformations, those that depart from the identity transformation by a small amount. It turns out that any such canonical transformation can be expressed in terms of a single 'generating' function on phase space. In other words, we consider transformations of the form

$$Q^i = q^i + \delta q^i(q,p) \quad \text{and} \quad P_i = p_i + \delta p_i(q,p) \quad \text{where} \quad \delta q^i, \delta p_i \quad \text{are small.} \tag{225}$$

Note that we do not expand $\delta q, \delta p$ in powers of q and p, we are not assuming that q, p are small. Now we impose the conditions that the new coordinates and momenta satisfy canonical p.b. up to terms quadratic in δq^i and δp_i for $1 \leq i, j \leq n$.

$$\begin{aligned}
0 = \{Q^i, Q^j\} = \{q^i + \delta q^i, q^j + \delta q^j\} \approx \{q^i, \delta q^j\} + \{\delta q^i, q^j\} \quad &\Rightarrow \quad \frac{\partial \delta q^j}{\partial p_i} - \frac{\partial \delta q^i}{\partial p_j} = 0. \\
0 = \{P_i, P_j\} \approx \{p_i, \delta p_j\} + \{\delta p_i, p_j\} \quad &\Rightarrow \quad \frac{\partial \delta p_j}{\partial q^i} - \frac{\partial \delta p_i}{\partial q^j} = 0. \\
\delta_{ij} = \{Q^i, P_j\} \approx \{q^i, p_j\} + \{q^i, \delta p_j\} + \{\delta q^i, p_j\} \quad &\Rightarrow \quad \frac{\partial \delta p_j}{\partial p_i} + \frac{\partial \delta q^i}{\partial q^j} = 0.
\end{aligned} \tag{226}$$

[16] Ξ is the capital Greek letter, pronounced Xi.

Thus we have re-written the conditions for an infinitesimal transformation to be canonical as a system of homogeneous linear partial differential equations for the small changes in coordinates and momenta $\delta q^i(q,p)$ and $\delta p_i(q,p)$. They look formidable, in fact there are apparently more equations than unknowns for $n \geq 2$. Accounting for antisymmetry, $\{Q^i, Q^j\} = 0$ gives one condition for each $n \geq i > j \geq 1$, which makes $\frac{n^2-n}{2}$ equations, and the same number for $\{P_i, P_j\} = 0$. $\{Q^i, P_j\} = \delta^i_j$ gives n^2 more conditions. So we have $n^2 - n + n^2 = 2n^2 - n$ equations for $2n$ unknown functions δq^i and δp_i. However, the equations are not all independent and they admit an infinite dimensional family of solutions! The key is to notice that the last set of equations, even for 1 degree of freedom $\frac{\partial \delta p}{\partial p} + \frac{\partial \delta q}{\partial q} = 0$ look like the condition for the divergence of a vector field on the plane $\vec{B} = (\delta q, \delta p)$ to vanish. Recall that the divergence-free condition $\nabla \cdot \mathbf{B}$ on a magnetic field may be solved identically by introducing a vector potential $\vec{B} = \nabla \times \mathbf{A}$. This suggests we seek solutions in the form $\delta q = \frac{\partial f}{\partial p}, \delta p = -\frac{\partial f}{\partial q}$. On the other hand, the first two systems of equations look like the conditions for the curl of a vector field on the plane to vanish. If $E = (E_x, E_y)$ is an electric field on a plane, then $\nabla \times E = (\partial_x E_y - \partial_y E_x)\hat{z}$. Recall that if the curl of a vector field on the plane vanishes $\nabla \times E = 0$, then we can express the vector field as the gradient of a scalar function $E = -\nabla\phi = (-\partial_x\phi, -\partial_y\phi)$. All this motivates us to express δq^i and δp_j as derivatives of a scalar function f. Check that the above equations are identically satisfied if we put

$$\delta q^i = \frac{\partial f}{\partial p_i} = \{q^i, f\} \quad \text{and} \quad \delta p_i = -\frac{\partial f}{\partial q^i} = \{p_i, f\} \tag{227}$$

for an arbitrary twice differentiable function $f(q,p)$ on phase space. We say that f is an infinitesimal generator for the above infinitesimal CT. The small quantity f generates the infinitesimal CT via the Poisson bracket, it is determined up to an additive constant. This ambiguity is the analogue of the invariance of electric and magnetic fields under gauge transformations. In the case of $\mathbb{R}^{2n}$ phase space, all infinitesimal CTs may be obtained through appropriate choices of generators $f(q,p)$. It is also possible to build up finite CTs by composing a succession of infinitesimal ones (see problem set 12). We will say more about finite CTs later.

• We may of course compose CTs $(q,p) \to (Q,P) \to (\tilde{Q}, \tilde{P})$ to make new CTs and also invert a CT. Check that $-f$ generates the inverse of the infinitesimal CT generated by f. $f = 0$ generates the identity CT. Arbitrary smooth generating functions $f(q,p)$ parametrize the neighborhood of the group identity, i.e. the Lie algebra. Since we need infinitely many real parameters to specify a function $f(q,p)$ (such as all its Taylor coefficients), the Lie algebra and group of CTs is infinite dimensional. To first approximation, check that $f + g$ generates the CT consisting of the composition of the infinitesimal CTs generated by f and g, in *either* order. But this approximation is a bit crude, the order does matter since the group of CTs is non-abelian. The non-abelian nature is encoded in the Lie bracket, which is just the p.b. of infinitesimal generators $\{f, g\}$ (see problem set 11).

• We already noted that hamiltonian time evolution over any time interval is a CT since it preserves the p.b. among the q's and p's. The above result allows us to interpret infinitesimal time evolution as an infinitesimal CT and identify the corresponding generating function. Hamilton's equations for evolution over a small time δt give, to leading order in δt,

$$Q^i \equiv q^i(t + \delta t) = q^i(t) + \delta t \frac{\partial H}{\partial p_i} \quad \text{and} \quad P_i \equiv p_i(t + \delta t) - \delta t \frac{\partial H}{\partial q^i}. \tag{228}$$

In this case the small change in coordinates and momenta are

$$\delta q^i = \frac{\partial(H\ \delta t)}{\partial p_i} = \{q^i, H\ \delta t\} \quad \text{and} \quad \delta p_i = -\frac{\partial(H\ \delta t)}{\partial q^i} = \{p_i, H\ \delta t\}. \tag{229}$$

From these equations we read off the infinitesimal generator of time evolution over a small time δt as $f = H(q,p)\ \delta t$. Notice that f is indeed a small quantity. We say that the hamiltonian generates the infinitesimal CT corresponding to infinitesimal time evolution via the Poisson bracket.

• Just like the hamiltonian, every observable $f(q,p)$ generates an infinitesimal CT. E.g. what infinitesimal CT does the angular momentum component ϵL_z generate? One finds

$$\delta x = -\epsilon y, \delta y = \epsilon x, \delta z = 0 \quad \text{and} \quad \delta p_x = -\epsilon p_y, \delta p_y = \epsilon p_x, \delta p_z = 0. \tag{230}$$

This CT is a counter clockwise rotation in the $x-y$ plane and $p_x - p_y$ plane by the small angle ϵ. Contrast it with the infinitesimal CT generated by $f = x^2 + p_x^2$.

• It is also interesting to have an expression for the infinitesimal change in a given observable $g(q,p)$ due to a canonical transformation generated by $f(q,p)$:

$$\delta g = \frac{\partial g}{\partial q^i}\delta q^i + \frac{\partial g}{\partial p_i}\delta p_i = \frac{\partial g}{\partial q^i}\frac{\partial f}{\partial p_i} - \frac{\partial g}{\partial p_i}\frac{\partial f}{\partial q^i} = \{g, f\}. \tag{231}$$

So the change in any observable is given by its p.b. with the infinitesimal generator.

5.4.6 Symmetries & Noether's theorem in the hamiltonian framework

• In the hamiltonian formalism, it is natural to define a symmetry transformation as a canonical transformation $(q^i, p_i) \to (Q^i, P_i)$ that leaves the hamiltonian invariant. The former condition ensures that a symmetry preserves the p.b. This requirement allows us to obtain a conserved quantity from an infinitesimal symmetry. This is expected from Noether's theorem, which we proved in the Lagrangian framework. Symmetries of the hamiltonian that aren't CTs, generally do not lead to conserved quantities.

• E.g., if the hamiltonian is independent of a coordinate q, then it is invariant under translations of q, $H(q,p) = H(q+a,p)$. These are implemented by the CT $q \to q + a, p \to p$. q is then a cyclic coordinate and the conjugate momentum is conserved $\dot{p} = -\frac{\partial H}{\partial q} = 0$. More generally a transformation is said to leave the hamiltonian invariant if $H(q,p) = H(Q(q,p), P(q,p))$. It is important to distinguish between an invariant function and just a scalar function. A scalar function on a manifold is one whose value at a physical location does not depend on the coordinate address we give for the location. A scalar function satisfies $\phi(q,p) = \phi(q(Q,P), p(Q,P))$ for all $q(Q,P), p(Q,P)$. I.e, its value at a point whose coordinates in the old system are (q,p) does not change if we express q, p in terms of some other arbitrarily chosen coordinates. The hamiltonian of any system is a scalar function on phase space. An invariant function is a scalar function with the *additional property* that its value does not change if we *change the physical location* at which it is evaluated by a symmetry transformation, i.e., $H(q,p) = H(Q(q,p), P(q,p))$ where $(q,p) \to (Q,P)$ is not an arbitrary transformation, but a symmetry transformation.

• Symmetries may be discrete or continuous. Continuous symmetries are those that may be continuously deformed to the identity. Regarded as CTs, they can be built by composing a

succession of infinitesimal CTs. Consider an infinitesimal symmetry, there must be a function on phase space $f(q,p)$ that generates the corresponding CT, called the generator of the symmetry. E.g. $f(q,p) = p_i a^i$ for a fixed vector $\vec{a}$ generates a translation of coordinates by $\vec{a}$, since

$$\delta q^i = \frac{\partial f}{\partial p^i} = a^i \quad \text{and} \quad \delta p_i = -\frac{\partial f}{\partial q^i} = 0. \tag{232}$$

Now the change in any observable g due to the symmetry transformation generated by f is $\delta g = \{g, f\}$. In particular, since the hamiltonian is invariant under a symmetry, we must have $0 = \delta H = \{H, f\} = 0$. By hamilton's equation this means $\dot{f} = \{f, H\} = 0$. It follows that the generator f of the symmetry is a constant of motion. Thus we have a Hamiltonian version of Noether's theorem. The symmetry generator is the conserved quantity. In the above example, it means $p \cdot a$ is a conserved quantity if the hamiltonian is invariant under translations of coordinates by $\vec{a}$.

5.4.7 Liouville's theorem

• We will apply the idea of infinitesimal generator for a CT to establish an interesting theorem of Liouville on the geometric nature of CT. Previously, we saw that for one degree of freedom, CTs preserve areas in phase space. This is a special case of Liouville's theorem. For n degrees of freedom, it says that CTs preserve $2n$-dimensional 'volumes' in phase space. In other words, suppose a $2n$-dimensional region in phase space $D \subset \mathbb{R}^{2n}$ is mapped by a CT to a new region $D' \subset \mathbb{R}^{2n}$. Then $\text{Vol}(D) = \text{Vol}(D')$. Alternatively, it says that the volume element in phase space is invariant under a CT

$$\prod_{i=1}^{n} dQ^i \prod_{j=1}^{n} dP_j = \prod_{i=1}^{n} dq^i \prod_{j=1}^{n} dp_j. \tag{233}$$

For a general transformation, the determinant of the Jacobian matrix of first partials appears as a pre-factor on the rhs

$$J = \begin{pmatrix} \frac{\partial Q^i}{\partial q^j} & \frac{\partial Q^i}{\partial p_j} \\ \frac{\partial P_i}{\partial q^j} & \frac{\partial P_i}{\partial p_j} \end{pmatrix}_{2n \times 2n}, \quad \text{where each sub-matix is an } n \times n \text{ block with } 1 \le i, j \le n. \tag{234}$$

So Liouville's theorem says that $\det J = 1$ for a canonical transformation. Note that unlike for one degree of freedom, for $n > 1$, $\det J = 1$ is *not* a sufficient condition for a transformation to be canonical.

• Let us establish Liouville's theorem for infinitesimal canonical transformations by using our expressions for Q^i, P_j in terms of an infinitesimal generator[17] ϵf

$$Q^i \approx q^i + \epsilon \frac{\partial f}{\partial p_i} \quad \text{and} \quad P_i \approx p_i - \epsilon \frac{\partial f}{\partial q^i} \tag{235}$$

Let us first look at the simple case of $n = 2$ degrees of freedom, where

$$Q^1 \approx q^1 + \epsilon f_{p_1}, \;\; Q^2 \approx q^2 + \epsilon f_{p_2}, \;\; P_1 \approx p_1 - \epsilon f_{q^1} \;\text{ and }\; P_2 \approx p_2 - \epsilon f_{q^2} \tag{236}$$

[17] ϵ is a small parameter which will help us keep track of infinitesimals, we will ignore quantities of order ϵ^2.

and sub-scripts denote partial derivatives. In this case the Jacobian matrix

$$J \approx I + \epsilon \begin{pmatrix} f_{q^1p_1} & f_{q^2p_1} & f_{p_1p_1} & f_{p_1p_2} \\ f_{q^1p_2} & f_{q^2p_2} & f_{p_1p_2} & f_{p_2p_2} \\ -f_{q^1q^1} & -f_{q^2q^1} & -f_{p_1q^1} & -f_{p_2q^1} \\ -f_{q^1q^2} & -f_{q^2q^2} & -f_{p_1q^2} & -f_{p_2q^2} \end{pmatrix} = I + \epsilon F \tag{237}$$

departs from the identity by an infinitesimal matrix of second partials of f. Now[18]

$$\det J = \det[I + \epsilon F] = 1 + \epsilon \text{ tr } F + \mathcal{O}(\epsilon^2) = 1 + \mathcal{O}(\epsilon^2) \tag{238}$$

since F is traceless. So for two degrees of freedom we have shown that an infinitesimal canonical transformation preserves the (4-dimensional) volume element in phase space.

• The case of n-degrees of freedom is analogous. The $2n \times 2n$ Jacobian matrix is made of $n \times n$ blocks

$$J = \begin{pmatrix} \delta_{ij} + \epsilon \frac{\partial^2 f}{\partial p_i \partial q^j} & \epsilon \frac{\partial^2 f}{\partial p_i \partial p_j} \\ -\epsilon \frac{\partial^2 f}{\partial q^i \partial q^j} & \delta_{ij} - \epsilon \frac{\partial^2 f}{\partial q^i \partial p_j} \end{pmatrix} \quad \Rightarrow \quad \det J \approx 1 + \epsilon \sum_{i=1}^{n} \frac{\partial^2 f}{\partial p_i \partial q^i} - \epsilon \sum_{i=1}^{n} \frac{\partial^2 f}{\partial q^i \partial p_i} = 1 \tag{239}$$

Thus, an infinitesimal canonical transformation preserves the volume element in phase space. Synthesizing a finite canonical transformation by composing a succession of N infinitesimal ones and letting $N \to \infty$ and $\epsilon \to 0$, we argue that finite canonical transformations also preserve the phase volume. One needs to show that the terms of order ϵ^2 and higher, will not contribute to the Jacobian of a finite CT.

• In particular, hamiltonian time evolution preserves phase volume. This is true even if the hamiltonian is explicitly time dependent. All we need is for the equations of motion to be expressible in Hamiltonian form $\dot{q}^i = \frac{\partial H}{\partial p_i}, \dot{p}_i = \frac{\partial H}{\partial q^i}$ and this is true even if the Lagrangian depends explicitly on time (see the section on Hamilton's equations). At each instant of time, H generates an infinitesimal CT that preserves the phase volume. Of course, if H is explicitly time-dependent, the CT will change with time, but phase volume will still be preserved. Note that dissipative systems do not admit a standard Lagrangian or hamiltonian description, there is no function $H(q, p, t)$ for which hamilton's equations reproduce the equations of motion. Typically, for dissipative systems, the volume in phase space is a decreasing function of time (e.g. for the damped harmonic oscillator $m\ddot{x} = -kx - \gamma\dot{x}$, irrespective of what initial conditions one considers, the mass comes to rest at the equilibrium point $(x = 0, m\dot{x} = 0)$, so the phase space area shrinks to zero).

• Application to statistical mechanics: Consider the gas molecules in a room, modeled as a system of N classical point particles. The phase space is $6N$ dimensional with coordinates $\vec{q}^1 \cdots \vec{q}^N, \vec{p}_1 \cdots \vec{p}_N$. Now owing to the difficulty of determining the initial values of these variables, we may at best be able to say that the initial conditions lie within a certain region D of phase space. Each of the phase points in D will evolve in time and trace out a phase trajectory. In this manner D itself will evolve in time to a new region D' which contains the possible phase

[18] Suppose the eigenvalues of $J = I + \epsilon F$ are $\lambda_1, \cdots, \lambda_{2n}$. Then from the characteristic equation $\det(J - \lambda I) = \det(\epsilon F - (\lambda - 1)I) = 0$ we see that the eigenvalues of ϵF are $\lambda_1 - 1, \cdots \lambda_{2n} - 1$. Hence the eigenvalues of F are $f_1 = \frac{\lambda_1 - 1}{\epsilon}, \cdots \frac{\lambda_{2n} - 1}{\epsilon}$. Thus $\det J = \lambda_1 \cdots \lambda_{2n} = (1 + \epsilon f_1) \cdots (1 + \epsilon f_{2n}) = 1 + \epsilon(f_1 + \cdots + f_{2n}) + \mathcal{O}(\epsilon^2) = 1 + \epsilon \text{ tr } F + \mathcal{O}(\epsilon^2)$. Alternatively, assuming the identity $\det J = \exp(\text{ tr } \log(I + \epsilon F))$, one may proceed by expanding in powers of ϵ.

points at a later time. We are often not interested in locations and momenta of individual gas molecules but average properties of the gas (such as pressure or internal energy). These may be obtained by computing an average over the region of phase space D'. Liouvilles's theorem says that this region of phase space evolves in time as an 'incompressible fluid'. In general, the shape of the region will get distorted with time, while maintaining a constant $6N$-dimensional volume.

5.4.8 Generating functions for finite canonical transformations from variational principles

• Transformations between different sets of canonical coordinates and momenta are called canonical transformations. Here we seek to express finite canonical transformations in terms of generating functions. We have already done this for infinitesimal canonical transformations. To do so, we will use Hamilton's variational principle for his equations. Consider the (possibly explicitly time-dependent) map from $(q^i, p_j) \mapsto (Q_i, P_j)$ with the equations of transformation given by the functions

$$Q^i = Q^i(q, p, t) \quad \text{and} \quad P_i = P_i(q, p, t) \tag{240}$$

Such a change is canonical provided there is a new Hamiltonian $K(Q, P, t)$ (previously called $\tilde{H}$) such that the eom in the new variables take the same form as those in the old variables, i.e.,

$$\dot{Q}^i = \frac{\partial K}{\partial P_i} \quad \text{and} \quad \dot{P}_i = -\frac{\partial K}{\partial Q^i} \quad \text{while} \quad \dot{q}^i = \frac{\partial H}{\partial p_i} \quad \text{and} \quad \dot{p}_i = -\frac{\partial H}{\partial q^i}. \tag{241}$$

When the transformation is not explicitly dependent on time, $K(Q, P)$ is got by expressing q, p in terms of Q, P in the old Hamiltonian $H(q, p)$. We will see that essentially the same thing continues to be true, but with a slight modification. Now both these sets of Hamilton equations should be equivalent in the sense that if we express Q and P in terms of q and p in the second set, they should reduce to the old Hamilton equations.

• Each set of Hamilton's equations follows from a variational principle:

$$\delta \int_{t_i}^{t_f} \left[p_i \dot{q}^i - H(q, p) \right] dt = 0 \quad \text{and} \quad \delta \int_{t_i}^{t_f} \left[P_i \dot{Q}^i - K(Q, P) \right] dt = 0. \tag{242}$$

The extrema of these two functionals are the same equations (just in different coordinates). One way for this to happen is for the integrands to be the same. But there is also a more general way for this to happen, the integrands could differ by the total time derivative of a function $F_1(q, Q, t)$. Let us see why. Subtracting, we find that the condition for the functional

$$I[q, p, Q, P] = \int_{t_i}^{t_f} \left(p\dot{q} - H - P\dot{Q} + K \right) dt \tag{243}$$

to be extremal is identically satisfied, since it is the difference between two equivalent sets of equations. So this integral must be a constant functional with respect to variations of q, p, Q, P subject to the boundary conditions $\delta q(t_i) = \delta q(t_f) = \delta Q(t_i) = \delta Q(t_f) = 0$. A way for this to happen is for the integrand to be a total time derivative of a function $\dot{F}_1(q, Q, t)$. For, then

$$I = \int_{t_i}^{t_f} \dot{F}_1 \, dt = F_1(q(t_f), Q(t_f), t_f) - F_1(q(t_i), Q(t_i), t_i). \tag{244}$$

And I is then a constant since q and Q are held fixed at the fixed times t_i and t_f. Note that F_1 cannot be taken as a function of p or P since $\delta p(t_i), \delta p(t_f), \delta P(t_i), \delta P(t_f)$ are unconstrained in Hamilton's variational principle and the total derivative of such a term would violate the constancy of I. In other words, a way by which the equations in both old and new variables take the hamiltonian form is for the relation

$$p_i \dot{q}^i - H = P_i \dot{Q}^i - K + \frac{dF_1}{dt}, \tag{245}$$

to hold for some function $F_1(q, Q, t)$. Multiplying through by dt we get

$$pdq - Hdt = PdQ - Kdt + \frac{dF_1}{dt}dt. \tag{246}$$

That the independent variables in F_1 are q, Q, t is also consistent with the fact that the independent differentials appearing in the rest of the terms above are dt, dq, dQ. So as an equation among the independent differentials dq, dQ, dt we have

$$pdq - Hdt = PdQ - Kdt + \frac{\partial F_1}{\partial q}dq + \frac{\partial F_1}{\partial Q}dQ + \frac{\partial F_1}{\partial t}dt. \tag{247}$$

Comparing coefficients, we read off the relations

$$p = \frac{\partial F_1}{\partial q}, \quad P = -\frac{\partial F_1}{\partial Q} \quad \text{and} \quad K(Q, P, t) = H(q, p) + \frac{\partial F_1(q, Q, t)}{\partial t}. \tag{248}$$

$F_1(q, Q)$ is called the generator of the CT. The first two equations determine the equations of transformation. The first may be solved to find $Q = Q(q, p, t)$ and using it, the second may be solved to express $P = P(q, p, t)$. The last relation fixes the new hamiltonian in terms of the old one and the generator. If F_1 does not depend explicitly on time, then it just says that $K(Q, P) = H(q(Q, P), p(Q, P)) = \tilde{H}(Q, P)$ as before. But in general, the new and old hamiltonians differ by the partial time derivative of the generator.

• Not every function $F_1(q, Q, t)$ is a legitimate generator. E.g., $F_1(q, Q) = q + Q$ would imply $p = 1$ and $P = -1$ which in general cannot be solved to express Q, P in terms of q, p. Similarly, $F_1 = q^2 + Q^2$ also does not generate a CT since it implies $p = 2q, P = -2Q$ which cannot be solved to express Q, P as functions of q, p. On the other hand, a choice that does generate a CT is $F_1(q, Q) = qQ$, in which case, $Q = p$ and $P = -q$ exchanges coordinates and momenta up to a sign. What CT does $F_1 = -qQ$ generate?

• In general, for $F_1(q, Q)$ to generate a CT, we need the 'hessian' of unlike second partials $\frac{\partial^2 F_1}{\partial q \partial Q}$ to be non-vanishing[19]. This will allow us to use $p = \frac{\partial F_1(q,Q)}{\partial q}$ to solve for Q in terms of q, p, at least locally. When the second partial is non-vanishing $\frac{\partial F_1(q,Q)}{\partial q}$ depends non-trivially on Q which can then be solved for and then inserted in $P = -\frac{\partial F_1(q,Q)}{\partial Q}$ to express $P = P(q, p)$.

• The generator of a finite CT $F_1(q, Q, t)$ is distinct from the infinitesimal generator $f(q, p)$ encountered before. Unlike $f(q, p)$, which generates all infinitesimal CTs, $F_1(q, Q, t)$ does not generate all finite CTs. In particular, the identity transformation $Q = q, P = p$ is not expressible via a generating function $F_1(q, Q, t)$. The latter expresses $p = \frac{\partial F_1(q,Q)}{\partial q} = p(q, Q)$ and $P =$

[19] More generally an adequate condition should be that the hessian $\frac{\partial^2 F_1}{\partial q^i \partial Q^j}$ of 'unlike' second partials be invertible.

$-\frac{\partial F_1(q,Q)}{\partial Q} = p(q,Q)$. But for the identity transformation, it is not possible to express P as a function of Q and q. Roughly, F_1 is good at generating CTs that are in the vicinity of the one that exchanges coordinates and momenta upto a sign $Q = p,\ P = -q$. It is not a good way of generating CTs in the vicinity of the identity transformation.

• To find a generator for other canonical transformations, we make use of the second variational principle $\tilde{S}[Q,P]$ for Hamilton's equations. Here the momenta are held fixed at the end points $\delta P(t_i) = \delta P(t_f) = 0$. For the old hamilton equations, we use the first variational principle $S[q,p]$ where $\delta q(t_i) = \delta q(t_f) = 0$:

$$\delta \int_{t_i}^{t_f} [p\dot{q} - H(q,p)]\, dt = 0 \quad \text{and} \quad \delta \int_{t_i}^{t_f} [-Q\dot{P} - K(Q,P)]\, dt = 0. \tag{249}$$

These two variational principles give the same equations even if the integrands differ by the total time derivative of a function $F_2(q,P,t)$ since $\delta q, \delta P$ are held fixed at the end points. So we must have

$$pdq - Hdt = -QdP - Kdt + \frac{\partial F_2}{\partial q}dq + \frac{\partial F_2}{\partial P}dP + \frac{\partial F_2}{\partial t}\, dt \tag{250}$$

Thus $F_2(q,P)$ generates a CT, with the equations of transformation given by

$$p = \frac{\partial F_2}{\partial q}, \quad Q = \frac{\partial F_2}{\partial P} \quad \text{and} \quad K = H + \frac{\partial F_2}{\partial t}. \tag{251}$$

• It is easily seen that if $F_2(q,P) = qP$, then the resulting transformation is the identity $Q = q, p = P$. In the absence of explicit time dependence, $F_2(q,P)$ is sometimes denoted $W(q,P)$. The above arguments show that F_2 generates a CT and must therefore preserve Poisson brackets.

• The difference between the generating functions $F_1(q,Q)$ and $F_2(q,P)$ lies in the independent variables they depend on. As we have seen, $F_1(q,Q)$ cannot be used to get the identity transformation and one checks that $F_2(q,P)$ cannot be used to get the exchange transformation $Q = p, P = -q$. But there are many CTs that may be generated by both a generating function $F_1(q,Q)$ and one of type $F_2(q,P)$ (we will give non-trivial examples in the context of the harmonic oscillator). In these cases, one wonders whether F_1 and F_2 are related by a Legendre transform, as they produce the same CT. From the difference of the above two relations among differentials,

$$pdq - Hdt = PdQ - Kdt + dF_1 \quad \text{and} \quad pdq - Hdt = -QdP - Kdt + dF_2 \tag{252}$$

we get

$$-QdP + dF_2 = PdQ + dF_1 \ \Rightarrow\ dF_2(q,P) = d\left[F_1(q,Q) + QP\right] \quad \text{where} \quad P = -\frac{\partial F_1}{\partial Q}. \tag{253}$$

In other words, up to an additive constant, $F_2 = QP + F_1$ with P given as above, or in short,

$$F_2(q,P,t) = \mathrm{ext}_Q\left[QP + F_1(q,Q,t)\right]. \tag{254}$$

• We may obtain two more types of generators $F_3(p,Q,t)$ and $F_4(p,P,t)$ for finite canonical transformations by suitable choices of variational principles for the old and new Hamilton equations.

$$\tilde{S}[q,p] \ \ \& \ \ S[Q,P] \ \ \Longrightarrow \ \ F_3(p,Q) \quad \text{while} \quad \tilde{S}[q,p] \ \ \& \ \ \tilde{S}[Q,P] \ \ \Longrightarrow \ \ F_4(p,P) \tag{255}$$

One finds

$$-qdp - Hdt = PdQ - Kdt + dF_3(p,Q,t) \quad \Rightarrow \quad q = -\frac{\partial F_3}{\partial p}, \;\; P = -\frac{\partial F_3}{\partial Q} \quad \text{and} \quad K = H + \frac{\partial F_3}{\partial t} \tag{256}$$

and

$$-qdp - Hdt = -QdP - Kdt + dF_4 \quad \Rightarrow \quad q = -\frac{\partial F_4}{\partial p}, \;\; Q = \frac{\partial F_4}{\partial P} \quad \text{and} \quad K = H + \frac{\partial F_3}{\partial t}. \tag{257}$$

As with $F_2(q,P)$ we may obtain $F_3(p,Q)$ and $F_4(p,P)$ via Legendre transforms from the others. E.g.,

$$F_3(p,Q) = \text{ext}_q[F_1(q,Q) - qp] \quad \& \quad F_4(p,P) = \text{ext}_Q[QP + F_3(p,Q)] = \text{ext}_q[F_2(q,P) - pq]. \tag{258}$$

• **One wonders if there are generating functions $F_5(q,p)$ and $F_6(Q,P)$ for finite CTs.** The above variational approach doesn't lead to such generators. In Hamilton's action principle, both q and p cannot be held fixed at the end points, so the total time derivative of F_5 would non-trivially modify hamilton's equations and not lead to a CT in general. Similarly, a generator $F_6(Q,P)$ is also disallowed in general.

• **Example:** We began our study of canonical transformations with coordinate changes $Q^i(q)$ on configuration space ('point' transformations). The identity is included among such transformations. So let us look for a generator of type $W(q,P)$ that effects a change of coordinates on $\mathcal{Q}$, for simplicity when $n = 1$. We must have $Q = \frac{\partial W}{\partial P}$ and $p = \frac{\partial W}{\partial q}$. The first equation then implies

$$W(q,P) = PQ(q) + g(q) \tag{259}$$

for some function $g(q)$ of the old coordinates alone. Then $p = PQ'(q) + g'(q)$ or $P = (p - g'(q))/Q'(q)$. This determines the new momentum. A CT that effects a change of coordinates on $\mathcal{Q}$ is clearly not unique, $g(q)$ being an arbitrary function. Different functions $g(q)$ produce different possible new momenta. In our earlier discussion, the new momenta were determined using a Lagrangian. Specification of a Lagrangian ($L(q,\dot{q})$ with a particular dependence on velocities), which 'induces' a change in momenta $P = \frac{\partial \tilde{L}}{\partial \dot{Q}}$ where $\tilde{L}(Q,\dot{Q}) = L(q(Q), \dot{q}(Q,\dot{Q}))$, is like selecting a specific function g. Of course, the simplest possibility is to take $g = 0$, which we will see below corresponds to a Lagrangian with the standard kinetic terms.

• Let us illustrate with the example of the 'point' transformation from cartesian to plane polar coordinates on configuration space. The old coordinates and momenta are x, y, p_x, p_y and the new coordinates and momenta are $r = \sqrt{x^2+y^2}, \theta = \arctan(y/x), p_r, p_\theta$ with p_r, p_θ yet to be determined. By the above arguments, the simplest generating function of the second type, that should take cartesian to plane polar coordinates is one with $g = 0$:

$$W(x,y,p_r,p_\theta) = Q^i(q)P_i = r(x,y)p_r + \theta(x,y)p_\theta = \sqrt{x^2+y^2}\, p_r + \arctan\left(\frac{y}{x}\right) p_\theta \tag{260}$$

The new coordinates are given by partial derivatives of W and satisfy the defining relations as expected:

$$r = \frac{\partial W}{\partial p_r} = \sqrt{x^2+y^2} \quad \text{and} \quad \theta = \frac{\partial W}{\partial p_\theta} = \arctan\left(\frac{y}{x}\right). \tag{261}$$

The old momenta are given by the following partial derivatives of W

$$p_x = \frac{\partial W}{\partial x} = \frac{x}{r}p_r - \frac{y}{r^2}p_\theta \quad \text{and} \quad p_y = \frac{\partial W}{\partial y} = \frac{y}{r}p_r + \frac{x}{r^2}p_\theta. \tag{262}$$

We may invert these relations and express p_r and p_θ in terms of the old coordinates and momenta

$$p_r = \frac{x}{r}p_x + \frac{y}{r}p_y = p_x\cos\theta + p_y\sin\theta = \mathbf{p}\cdot\hat{r} \quad \text{and} \quad p_\theta = xp_y - yp_x = L_z. \tag{263}$$

We see that p_r and p_θ are the familiar radial and angular momenta. So our generating function reproduces the usual conjugate momenta that we derived using the standard Lagrangian $L = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) - V(r,\theta)$. On the other hand, if we took

$$W(x,y,p_r,p_\theta) = rp_r + \theta p_\theta + g(x,y) \quad \text{for} \quad g \neq 0, \tag{264}$$

then the resulting transformation would still be a CT, but the momenta $p_x = \frac{x}{r}p_r - \frac{y}{r^2}p_\theta + \frac{\partial g}{\partial x}$ and $p_y = \frac{\partial W}{\partial y} = \frac{y}{r}p_r + \frac{x}{r^2}p_\theta + \frac{\partial g}{\partial y}$, would not be the usual ones (arising from the above Lagrangian).

• Another simple example of a CT is got by choosing $W(q,P) = \lambda q^i P_i$. The resulting CT is a scaling,

$$Q^j = \frac{\partial W}{\partial P_j} = \lambda q^j \quad \text{and} \quad p_i = \frac{\partial W}{\partial q^i} = \lambda P_i \quad \Rightarrow \quad P_i = \lambda^{-1}p^i. \tag{265}$$

The p.b. are preserved, $\{Q^i, P_j\} = \{\lambda q^i, \lambda^{-1}p_j\} = \delta^i_j$ etc. If $\lambda = 1+\epsilon$ we get an infinitesimal scaling. We could also do a different rescaling in each of the $q-p$ planes, by choosing $W(q,P) = \sum_i \lambda_i q^i P_i$.

• Choosing $\lambda = -1$, we see that reversing the signs of all coordinates and momenta $Q^i = -q^i, P_j = -p_j$ is a canonical transformation.

5.5 Action-Angle variables and Hamilton-Jacobi equation

• In our discussion of CTs so far, the specific hamiltonian of the system played no role. A transformation is canonical irrespective of what the hamiltonian may be. Among canonical systems of coordinates and momenta on phase space, those which admit more cyclic coordinates *for a given hamiltonian*, are more suited to solving Hamilton's equations for the given system. The momenta conjugate to cyclic coordinates are constants of motion, determined by the initial conditions. The best possibility is if all the coordinates $q^i = \theta^i$ are cyclic. Then the hamiltonian is a function of the conjugate momenta alone $H = H(I_1, \cdots I_n)$ which are constants of motion $\dot{I}_i = -\frac{\partial H}{\partial \theta^i} = 0$. Furthermore, the coordinates are then linear functions of time since we may easily integrate Hamilton's equations.

$$\dot{\theta}^i = \frac{\partial H(I_1,\ldots,I_n)}{\partial I_i} = \omega^i(I_1,\ldots,I_n) \quad \text{which implies} \quad \theta^i(t) = \theta^i(0) + \omega^i t \quad \text{and} \quad I_i(t) = I_i(0) \tag{266}$$

since the 'frequencies' ω^i are *constant* in time. We call such a canonical system angle-action variables. The coordinates θ^i are called angle variables and their conjugate constant momenta I_i are action variables. This terminology will be explained using the harmonic oscillator.

• E.g., the position and momentum of a free particle $H = \frac{p^2}{2m}$ are angle and action variables since $\{q,p\} = 1$, momentum is conserved $p(t) = p(0)$ and position is linear in time $q(t) = q(0) + \frac{p(0)t}{m}$.

• Not every hamiltonian system with n degrees of freedom admits action-angle variables. A pre-requisite is that the system possess n independent conserved quantities that are in involution (Poisson commute pairwise) so that they can serve as action variables. When they exist,

angle-action variables for a given hamiltonian are not uniquely determined. E.g., we may add a constant to the action or angle variables without affecting their Poisson brackets nor the conservation of the action variables. We may also rescale the action variable I_i by constant λ_i and the angle variable θ^i by $1/\lambda_i$ while retaining their status as action-angle variables.

5.5.1 Action-angle variables for the harmonic oscillator

• The harmonic oscillator hamiltonian is $H = \frac{p^2}{2m} + \frac{1}{2}kq^2$ with $\omega = \sqrt{\frac{k}{m}}$. Hamilton's equations $\dot{q} = p/m$ and $\dot{p} = -kq$ imply Newton's equation $\ddot{q} = -\omega^2 q$, whose solution is

$$q(t) = A\sin(\omega(t-t_0)) \quad \text{and} \quad p(t) = Am\omega\cos(\omega(t-t_0)) \equiv B\cos(\omega(t-t_0)). \tag{267}$$

$A > 0$ implies clockwise motion in the q-p phase plane along an ellipse with semi-axes $A = \sqrt{\frac{2E}{m\omega^2}}$ and $B = \sqrt{2mE}$ in the q and p directions. The phase point begins at the the northernmost point of the ellipse at $t = t_0$. The constant A is fixed in terms of the energy $E = \frac{1}{2}m\omega^2 A^2$. So

$$q(t) = \sqrt{\frac{2E}{m\omega^2}}\sin\theta(t) \quad \text{and} \quad p(t) = \sqrt{2mE}\cos\theta(t) \quad \text{where} \quad \theta(t) = \omega(t-t_0). \tag{268}$$

Our aim is to identify canonically conjugate angle and action variables for this system. $\theta(t)$ varies linearly with time, so it is a natural candidate for an angle variable. It is of course the angle subtended by the phase point with respect to the p axis measured clockwise. This explains the name angle. Taking a quotient we express the angle variable in terms of q and p:

$$\theta = \arctan\left(\frac{m\omega q}{p}\right). \tag{269}$$

• An action variable must be a constant of motion. Since there is only one degree of freedom, there can be at most one independent constant of motion, which can be taken as energy E. All other constants of motion must be functions of energy. So we suppose that $I = I(E)$. We try to fix $I(E)$ by requiring that it be canonically conjugate to θ. Since I depends on q, p only via E, we have

$$1 = \{\theta, I\} = \frac{\partial\theta}{\partial q}\frac{\partial I}{\partial p} - \frac{\partial\theta}{\partial p}\frac{\partial I}{\partial q} = \frac{\partial\theta}{\partial q}I'(E)\frac{\partial E}{\partial p} - \frac{\partial\theta}{\partial p}I'(E)\frac{\partial E}{\partial q} = I'(E)\left[\frac{p}{m}\frac{\partial\theta}{\partial q} - kq\frac{\partial\theta}{\partial p}\right]. \tag{270}$$

Taking the differential of the formula $\tan\theta = \frac{m\omega q}{p}$ for θ we get (using $\cos^2\theta = p^2/2Em$)

$$d\theta = \sqrt{km}\left(\frac{dq}{p} - \frac{q\,dp}{p^2}\right)\cos^2\theta = \frac{\omega}{2E}(p\,dq - q\,dp) \Rightarrow \quad \frac{\partial\theta}{\partial q} = \frac{\omega p}{2E} \quad \text{and} \quad \frac{\partial\theta}{\partial p} = -\frac{\omega q}{2E}. \tag{271}$$

Thus the condition that angle and action be canonically conjugate becomes an ODE for $I(E)$

$$1 = I'(E)\frac{\omega}{E}\left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2\right) \quad \Rightarrow \quad I'(E) = \frac{1}{\omega} \quad \Rightarrow \quad I(E) = \frac{E}{\omega} + c \tag{272}$$

I is not uniquely determined, as mentioned earlier. For simplicity we pick $c = 0$ and arrive at a pair of angle-action variables for the harmonic oscillator

$$\theta(q,p) = \arctan\left(\frac{m\omega q}{p}\right) \quad \text{and} \quad I(q,p) = \frac{E(q,p)}{\omega} = \frac{p^2}{2m\omega} + \frac{1}{2}m\omega q^2 \tag{273}$$

By construction we know that $\theta(t) = \omega(t - t_0)$ is linear in time, I is constant in time and they are canonically conjugate $\{\theta, I\} = 1$. Moreover, the hamiltonian when expressed in action-angle variables $H(\theta, I) = \omega I$ is a function of I alone, the angle variable is a cyclic coordinate. The action variable I has dimensions of action, energy $\times$ time. As mentioned before, θ is the angle that the phase point makes with respect to the p axis clockwise. On the other hand, we notice that the action variable $I(E)$ is $1/2\pi$ times the area enclosed by the ellipse traced out by the phase point during one complete oscillation: the ellipse has semi-axes $A = \sqrt{\frac{2E}{k}}$ and $B = \sqrt{2mE}$ and area πAB:

$$I(E) = \frac{1}{2\pi}\text{Area}(E). \tag{274}$$

We could have anticipated this relation between $I(E)$ and the area for the harmonic oscillator. It follows from the fact that a CT on the phase plane preserves areas. The area enclosed by a closed phase trajectory of energy E may be found in two sets of canonical coordinates and equated. On the one hand,

$$\text{Area}(E) = \oint p\, dq \tag{275}$$

where we could choose a clockwise orientation since the phase trajectory went clockwise with $A > 0$. On the other hand, by preservation of areas, we must have

$$\oint p\, dq = \oint I\, d\theta = \int_0^{2\pi} I(E) d\theta = 2\pi I(E) \tag{276}$$

by constancy of I along the trajectory. Again we choose θ to increase clockwise. Thus $I(E) = \text{Area}(E)/2\pi$ as we obtained by explicit calculation.

• Suppose E is an energy for which the trajectory is periodic with period $T(E)$. This is of course always true for the SHO with $E \geq 0$. The action variable is related to the time period in a simple way: $I'(E) = T(E)/2\pi$. This is seen by differentiating in E

$$I'(E) = \frac{1}{2\pi}\oint p'(E) dq = \frac{1}{2\pi}\oint \frac{2m\, dq}{2\sqrt{2m(E-V)}} = \frac{1}{2\pi}\sqrt{\frac{m}{2}}\oint \frac{dx}{\sqrt{E - V(x)}} = \frac{1}{2\pi}T(E). \tag{277}$$

We know the time period of SHO trajectories, $T(E) = 2\pi/\omega$. So we could have used this to identify the angle variable. What ever θ may be, it must satisfy Hamilton's equation in the new variables,

$$\dot\theta = \frac{\partial E}{\partial I} = \frac{dE}{dI} = \frac{1}{I'(E)} = \frac{2\pi}{T(E)} = \frac{2\pi}{2\pi/\omega} = \omega \quad \text{so} \quad \theta(t) = \omega t + \theta(0). \tag{278}$$

• The formula $E = I\omega$ for the harmonic oscillator is a classical precursor to the quantum mechanical formula $E = \hbar(n + \frac{1}{2})\omega$ where $h = 2\pi\hbar$ is Planck's unit of action. Indeed, Ehrenfest proposed that it is the action variables of certain classical systems that may take discrete values in the quantum theory. A quantity that takes discrete values in the quantum theory (such as the number of nodes of a bound state wave function), cannot change under small slow perturbations or continuous time-evolution. He asserted that classical quantities that were 'ripe' for quantization should not only be conserved under hamiltonian time-evolution, but also be unchanged under some slow perturbations of the system. It was found that the action variable (like the above phase integral $\oint p dq$) is an adiabatic invariant of the classical system. If the spring

constant is increased slowly, the energy of oscillations increases, but the action E/ω remains unchanged. These ideas are implemented in the Bohr-Sommerfeld quantization rule $\oint pdq = nh$ for the possible values of a phase space action integral in the quantum theory.

• We have found a canonical transformation to action-angle variables for the harmonic oscillator problem. What is the generator of the finite canonical transformation from q, p to θ, I? The Hamilton-Jacobi equation gives us a method to find it.

5.5.2 Generator of canonical transformation to action-angle variables: Hamilton-Jacobi equation

• Consider a dynamical system[20] with hamiltonian $H(q,p)$ and canonical variables $\{q,p\} = 1$. An example to keep in mind is $H(q,p) = \frac{p^2}{2m} + V(q)$ and more specifically the harmonic oscillator. We are interested in trajectories with energy E. So q, p must satisfy the condition $H(q,p) = E$. Now we seek the generator of a canonical transformation to new co-ordinates and momenta $Q = \theta, P = I$ where all coordinates are cyclic. In other words, the hamiltonian depends only on the new momenta P, $H(q,p) = K(P)$. The new canonical variables would be action-angle variables: as $\dot{Q} = \frac{\partial K}{\partial P}$ are constant, the Q's evolve linearly in time. Moreover, $\dot{P} = -\frac{\partial K}{\partial Q} = 0$, so the new momenta are constants of motion[21]. So we use I, θ in place of P, Q. Let us look for a generating function of the second type[22], depending on old coordinates and new momenta $F_2(q, I, t)$. In terms of F_2,

$$\theta = \frac{\partial F_2}{\partial I} \quad \text{and} \quad p = \frac{\partial F_2}{\partial q} \quad \text{and} \quad K = H + \frac{\partial F_2}{\partial t} \tag{279}$$

Furthermore, let us consider only the case where F_2 is not explicitly dependent on time. This should be adequate for the harmonic oscillator since in that case we found $K = H$ simply by substitution and I, θ depended on time only via their dependence on q, p, and not explicitly. In this case, it is conventional to denote $F_2(q, I) = W(q, I)$. The equations of transformation simplify,

$$\theta = \frac{\partial W(q,I)}{\partial I}, \qquad p = \frac{\partial W(q,I)}{\partial q} \quad \text{and} \quad K(I(q,p)) = H(q,p). \tag{280}$$

We hope that the trajectories of energy E are simpler to describe in terms of I, θ. Whatever this generating function may be, it must satisfy the energy constraint $H(q,p) = E$ which is in general a non-linear first order PDE for $W\left(\vec{q}, \vec{I}\right)$. For the above example with one degree of freedom, it is

$$H\left(q, \frac{\partial W}{\partial q}\right) = E \quad \text{or} \quad \frac{1}{2m}\left(\frac{\partial W}{\partial q}\right)^2 + V(q) = E. \tag{281}$$

This equation is called the time-independent Hamilton-Jacobi (HJ) equation and W is called Hamilton's characteristic function.

[20] Our notation will be for one degree of freedom, though some of this generalises to $n > 1$ degrees of freedom. For a system with one degree of freedom with conserved hamiltonian, one may usually pass to action-angle variables. But this is not always possible for systems with $n > 1$ degrees of freedom.

[21] Of course, there may not be n independent conserved quantities to serve as action variables. Then it is not possible to find action-angle variables and we say the system is not integrable. Note also that the action variables must Poisson commute with each other, so that they form a canonical family with their conjugate angle variables $\{\theta^i, I_j\} = \delta^i_j$, $\{I_i, I_j\} = \{\theta^i, \theta^j\} = 0$.

[22] In the sequel, we will indicate, how to proceed with a generator of type $F_1(q, \theta)$.

• In general, W will generate a CT to new canonical variables. The HJ equation does not by itself pick out the CT to action-angle variables. To impose this additional requirement, we seek solutions $W(q,I)$ of the HJ equation subject to the condition that the action variable I be a constant of motion. This will ensure that θ is a cyclic coordinate, since $\frac{\partial K}{\partial \theta} = -\dot{I} = 0$, so that θ evolves linearly in time.

• The time derivative of W is

$$\frac{dW(q,I)}{dt} = \frac{\partial W}{\partial q}\frac{dq}{dt} = p\dot{q} \quad \text{since} \quad \dot{I} = 0. \tag{282}$$

Thus we must have

$$W(q(t),I) = W(q(t_0),I) + \int_{t_0}^{t} p\dot{q}\, dt = W(q(t_0),I) + \int_{q_0}^{q} p dx \quad \text{where} \quad p(x,E) = \sqrt{2m(E-V(x))}.$$

Any such W is a solution of the HJ equation for some E as we check: differentiating the integral, $\frac{\partial W}{\partial q} = p = \sqrt{2m(E-V(q))}$ so the time-independent HJ equation is satisfied. These solutions of HJ are parametrized by a 'constant of integration' $W(q(t_0),I)$ which can be an arbitrary function of the action variable, since it drops out of $\frac{\partial W}{\partial q}$. However, $W(q(t_0),I)$ does affect the dependence of W on I, and through this, it affects the angle variable $\theta = \frac{\partial W}{\partial I}$.

• In particular, we see that there are many sets of action-angle variables for the same system, obtained by different choices of the constant of integration.

• The second term $\int_{q_0}^{q} p\, dq'$ is sometimes called an abbreviated action integral[23]. It depends in a specific way on both q and I. The dependence on q is via the upper limit of integration, while the dependence on I is through p. The integrand p is determined by solving $H(q,p) = E$ for p. For the above example,

$$p(q,I) = \sqrt{2m\,[E(I) - V(q)]}. \tag{283}$$

For a single degree of freedom, E must be a function of I as there is only one independent conserved quantity. More generally, E is a function of the action variables $E = K(I) = H(q,p)$ since the hamiltonian in the new variables depends only on the action variables.

• We could also have proceeded using a generating function of type 1. If we use $F_1(q,\theta)$ instead of $W(q,I)$, then the HJ equation still reads $H(q, \frac{\partial F_1(q,\theta)}{\partial q}) = E$. Now both q and θ depend on time and $\dot{F}_1 = (F_1)_q\dot{q} + (F_1)_\theta\dot{\theta} = p\dot{q} - I\dot{\theta}$. Here subscripts q,θ denote partial derivatives. The condition that I and θ be action-angle variables is imposed by requiring that both I and $\dot{\theta} \equiv \omega$ be a constant. We could then integrate and find F_1 as before, but with the extra term.

5.5.3 Generating function for CT to action-angle variables for harmonic oscillator

• For the SHO, we already found action-angle variables and we now seek a generating function from:

$$(q,p) \quad \text{to} \quad I = \frac{E}{\omega} \quad \text{and} \quad \theta = \arctan\left[\frac{qm\omega}{p}\right]. \tag{284}$$

Based on the previous section, a candidate generating function for the CT to action-angle variables is provided by hamilton's characteristic function $W(q,I)$, which is a solution of the HJ

[23] Recall that $S = \int_{t_i}^{t_f}(p\dot{q} - Hdt)$ was also called the action.

equation. So let us consider the abbreviated action integral, which is automatically a solution of HJ

$$W(q,I) = \int_0^q p\,dx = \int_0^q \sqrt{2m(I\omega - V(x))}\,dx \quad \text{where} \quad \omega^2 = \frac{k}{m} \quad \text{and} \quad V(x) = \frac{1}{2}kx^2. \tag{285}$$

We fixed the constant of integration by the convenient choice $W(q(0),I) = 0$. Evaluate the integral and find $W(q,I)$ explicitly. Verify that the resulting function generates the desired transformation.

$$\frac{\partial W}{\partial q} \stackrel{?}{=} p = \sqrt{2m(E-V)} \quad \text{and} \quad \frac{\partial W}{\partial I} \stackrel{?}{=} \theta = \arcsin\left(q\sqrt{\frac{k}{2I\omega}}\right). \tag{286}$$

So we have found a generating function of the second kind $W(q,I)$ that allows us to pass to action-angle variables for the harmonic oscillator.

• The generating function takes a simpler form when expressed in terms of the old coordinates and the new coordinates, i.e., as $F_1(q,Q)$, which is obtained via a Legendre transform

$$F_1(q,\theta) = \text{ext}_I\left[W(q,I) - I\theta\right] \tag{287}$$

Exercise: Find $F_1(q,\theta)$. For this CT we are free to use a generator of either kind.

5.5.4 Action-angle variables for systems with one degree of freedom

• Based on our experience with the SHO, we briefly comment on a passage to action-angle variables for a system with one degree of freedom and conserved hamiltonian, say

$$H(q,p) = \frac{p^2}{2m} + V(q) \tag{288}$$

We will suppose that $V(q)$ is such that all the phase space trajectories are bounded and periodic in time as for $V(q) = \frac{1}{2}q^2 + q^4$. This is guaranteed if $V(q) \to \infty$ sufficiently fast, as $|q| \to \infty$. Further assume that for a given energy there is a unique periodic trajectory in phase space[24]. Then we *define* the action variable as the area enclosed by that phase trajectory

$$I(E) = \frac{1}{2\pi}\oint p(E,q)\,dq = \frac{1}{2\pi}\oint \sqrt{2m\left(E - V(q)\right)}\,dq. \tag{289}$$

This also defines E as a function of I, there is only one independent conserved quantity. As before, we look for a generating function of the second kind that allows us to transform to action-angle variables. We do this by solving the HJ equation via an abbreviated action integral with a convenient choice of constant of integration (set to zero below)

$$W(q,I) = \int_0^q p(E(I),x)\,dx = \int_0^q \sqrt{2m\left(E - V(q)\right)}\,dx \tag{290}$$

The angle variable is *defined* by $\theta = \frac{\partial W}{\partial I}$ and moreover, $p = \frac{\partial W}{\partial q}$. By virtue of having a generating function, we are guaranteed that $\{\theta, I\} = 1$, i.e., they are canonically conjugate. Moreover, since the hamiltonian $H = E(I) = K(I)$ is a function of I alone, θ is cyclic, I is conserved, and θ is linear in time. Thus we have a way of identifying action-angle variables for such a system with 1 degree of freedom.

[24] There are potentials such as $V = -q^2 + q^4$ for which there may be more than one phase trajectory for a given energy. Then $I(E)$ is a multi-valued function of energy.

5.5.5 Action-angle variables for simple pendulum

• Let us obtain action-angle variables for the simple pendulum with hamiltonian $H = \frac{p_\theta^2}{2ml^2} - mgl\cos\theta$ and canonical variables with p.b. $\{\theta, p_\theta\} = 1$ and angular frequency $\omega = \sqrt{g/l}$. We abbreviate $p \equiv p_\theta$ and will restrict to the region of phase space inside the separatrix where we have libration, i.e., $E < mgl$. The action variable may be written as twice the integral between the left and right turning points $\pm\theta_{\max} = \pm\arccos(-\epsilon)$

$$I(E) = \frac{1}{2\pi}\oint p\,d\theta = \frac{\sqrt{2ml^2}}{2\pi}2\int_{-\theta_{\max}}^{\theta_{\max}}\sqrt{E + mgl\cos\theta}\;d\theta = \frac{\sqrt{2}m\omega l^2}{\pi}\int_{-\theta_{\max}}^{\theta_{\max}}\sqrt{\epsilon+\cos\theta}\;d\theta \quad (291)$$

where $\epsilon = E/mgl$. This implicitly defines the energy $E(I)$ as a function of action I. The integral can be expressed in terms of complete elliptic integrals of the first two kinds though we do not do so here.

• Hamilton's characteristic function $W(q, I)$ that generates the CT to action-angle variables is an incomplete elliptic integral:

$$W(q,I) = \int^{\theta} p(\theta')d\theta' = \int^{\theta}\sqrt{(2ml^2)(E+mgl\cos\theta)}\;d\theta = \sqrt{2}m\omega l^2\int^{\theta}\sqrt{\epsilon+\cos\theta}\;d\theta. \quad (292)$$

If we evaluate this integral explicitly, then we could find the angle variable by differentiation $\Theta = \frac{\partial W}{\partial I}$ and $p = \frac{\partial W}{\partial\theta}$. However, there is another way of proceeding that exploits our knowledge of a formula for the time period $T(E)$ of a pendulum, as a function of energy.

• To get the angle variable Θ (not to be confused with θ!) we begin with Hamilton's equation $\dot\Theta = \frac{\partial E}{\partial I} = \frac{dE}{dI}$ which is just 2π times the reciprocal of the time period for the periodic librational trajectory

$$\dot\Theta = \frac{dE}{dI} = \left(\frac{dI}{dE}\right)^{-1} = \frac{2\pi}{T(E)} = \frac{\pi\omega}{2K(k)} \quad \text{where} \quad k = \sqrt{\frac{1}{2}\left(1+\frac{E}{mgl}\right)} \quad (293)$$

and $K(k)$ is the complete elliptic integral of the first kind. Since the elliptic modulus k is a constant, the angle varies linearly in time

$$\Theta(t) = \frac{\pi\omega t}{2K(k)} + \Theta(0) \quad (294)$$

We will work with the initial condition $\Theta(0) = 0$ for simplicity. To specify the canonical transformation, let us now express the old variables θ, p_θ in terms of the new ones Θ, I. Recall that the librational trajectory with initial condition $\theta(0) = 0$ is given by $\theta(t) = 2\arcsin[k\,\mathrm{sn}(\omega t, k)]$ substituting for t in terms of $\Theta(t)$ we get (note that the initial conditions for θ and Θ are consistent)

$$\theta(t) = 2\arcsin\left[k\,\mathrm{sn}\left(\frac{2K(k)\Theta(t)}{\pi}, k\right)\right] \quad (295)$$

The old momentum is given by $p_\theta^2 = 2ml^2(E + mgl\cos\theta)$. Show that it can be expressed as

$$p_\theta(t) = 2ml^2\omega k\,\mathrm{cn}\left(\frac{2K(k)\Theta(t)}{\pi}, k\right). \quad (296)$$

The last two equations give the old variables θ, p_θ in terms of the new angle Θ and action I, thus specifying the CT.

5.5.6 Time dependent Hamilton-Jacobi evolution equation

• Time evolution is particularly simple in action-angle variables where the hamiltonian is independent of all coordinates. An even more extreme case of canonical variables is that in which the hamiltonian is independent of all coordinates as well as momenta, i.e., if the hamiltonian is a constant. By a choice of zero of energy, this constant may be taken as zero. Now if the hamiltonian in the new variables $K = 0$, then the new coordinates and momenta are both constant in time, and are therefore determined by their initial values: $Q^i(t) = Q^i(0) = \beta^i$ and $P_i(t) = P_i(0) = \alpha_i$. Time evolution is very simple in such variables! However, it is not always possible to find canonical variables in which $K = 0$. But if it is possible, then the generator of the CT to such variables must satisfy an interesting non-linear first order PDE called the (time-dependent) Hamilton-Jacobi equation. Let us look for a generating function of the second type $F_2(q, P, t)$ for the transformation from $(q, p, H) \to (Q, P, K)$. For reasons to be clarified later, it is conventional in this context to denote F_2 by $S(q, P, t)$ and call it Hamilton's principal function. P_i are the new *constant* momenta and $p_i = \frac{\partial S}{\partial q^i}$. Then S must satisfy[25]

$$K = H(q, p, t) + \frac{\partial S(q, P, t)}{\partial t} = 0 \qquad \text{or} \qquad H\left(q^i, \frac{\partial S}{\partial q^j}, t\right) + \frac{\partial S}{\partial t} = 0. \tag{297}$$

This is the Hamilton-Jacobi equation (HJ), a first order (generally non-linear) PDE for the unknown generating function S in $n+1$ variables $q^1, \cdots, q^n, t$. For a particle in a 1D potential $V(q)$, it is a PDE for one unknown function S of two independent variables q, t:

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 + V(q) = 0. \tag{298}$$

• We will be interested in so-called 'complete integrals/solutions' of HJ, which depend on $n+1$ constants of integration. These are of the form

$$S = S(q^1, \cdots q^n, \alpha_1 \cdots \alpha_n, t). \tag{299}$$

We haven't indicated the dependence on the $(n+1)^{\text{th}}$ constant of integration α_{n+1}. α_{n+1} may be taken as an additive constant in S, since only derivatives of S appear in the HJ eqn. We will choose $\alpha_{n+1} = 0$ since it will be seen not to enter the equations of transformation $p = \frac{\partial S}{\partial q}$, $Q = \frac{\partial S}{\partial P}$ and $K = H + \frac{\partial S}{\partial t}$. The origin of these constants of integration will be clarified when we discuss the method of separation of variables to solve the HJ equation. In favorable cases (such as the free particle), the HJ PDE can be reduced to a set of n *decoupled first order* ODEs, whose solution introduces the required constants of integration.

• The virtue of a 'complete' solution of the HJ equation is that it provides a way of solving for the time evolution of the original mechanical system, i.e., of expressing $q^i(t)$ and $p_j(t)$ in terms of their initial values. First, we are free to take (i.e., *define*) the new constant momenta to equal the constants of integration, i.e., $P_j = \alpha_j$. (We could also take the P_j to be some n independent functions of the α_j.)

[25] If H is explicitly time-dependent, then one wonders whether we may end up with a new hamiltonian $K(t)$ which is a constant on phase space, but a different constant at different times. Such a time-dependent K can be got rid of by adding to S a function $f(t)$ satisfying $K(t) = \frac{\partial f}{\partial t}$. So any residual time dependence in the new hamiltonian can be removed.

• The equations of transformation in terms of the generator S read

$$p_j = \frac{\partial S(q,\alpha,t)}{\partial q^j} \quad \text{and} \quad \beta^i = Q^i = \frac{\partial S(q,\alpha,t)}{\partial \alpha_i}. \tag{300}$$

The second equation may be used to solve for $q^i = q^i(\alpha_j, \beta^k, t)$. This may be put in the first equation to find $p_i = p_i(\alpha_j, \beta^k, t)$. Now the solution of the mechanical problem in the sense mentioned above would be obtained if we express α_j, β^k in terms of the initial values of the old variables $q^i(0)$ and $p_i(0)$. To do this, let us consider these equations at $t = 0$. We get

$$p_j(0) = \frac{\partial S(q,\alpha,t)}{\partial q^j} \quad \text{and} \quad \beta^i = \frac{\partial S(q(t),\alpha,t)}{\partial \alpha_i} \quad \text{evaluated at } t = 0. \tag{301}$$

We may use the first equation to express α_i in terms of $q^i(0)$ and $p_i(0)$. Then the second equation gives us β^i in terms of $q^j(0)$ and $p_k(0)$.

• Using the above results, we get

$$q^i(t) = q^i(q^j(0), p_k(0), t) = q^i(\alpha,\beta,t) \quad \text{and} \quad p_i(t) = p_i(q^j(0), p_j(0), t) = p_i(\alpha,\beta,t) \tag{302}$$

These give the solution to the mechanical problem since they express the old coordinates and momenta in terms of their initial values.

• It is not always possible to find a complete solution of the HJ equation. Sometimes, one may find a solution S depending on less than $n+1$ constants of integration. Even this can be used to provide a partial understanding of the original mechanical problem.

5.5.7 Hamilton-Jacobi equation as semi-classical limit of Schrodinger equation

• We began with Newton's formulation of a mechanical system in terms of a system of non-linear ODEs for cartesian coordinates. We progressed to Lagrange's equations which are still ODEs, but whose form is invariant under changes of coordinates on configuration space. Then came hamilton's ODEs which are form-invariant under canonical transformations on phase space. The Poisson bracket formulation of hamilton's equations $\dot{f} = \{f, H\}$ take the same form for any observable and any system of coordinates on phase space (canonical or not). Now we have reformulated time-evolution of a hamiltonian system in terms of a single non-linear first order PDE for a generating function $S(q, P, t)$. This brings the equations of particle mechanics closer in spirit to the PDEs for waves: classical EM waves in the short wavelength Eikonal approximation and quantum matter waves in the semi-classical approximation. Recall the Schrodinger equation for time evolution of the wave function of a particle in a potential V:

$$i\hbar\frac{\partial \Psi}{\partial t} = H\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi \tag{303}$$

As we know from the free particle stationary state wave function $\Psi(x,t) = e^{i(px-Et)/\hbar}$, which has an essential singularity at $\hbar = 0$, the wave function itself does not have a good classical limit. But the quantity S defined by $\Psi = e^{iS/\hbar}$ is better placed to have a finite $\hbar \to 0$ limit. We have

$$\nabla\Psi = \frac{i}{\hbar}\Psi\nabla S, \quad \nabla^2\Psi = -\frac{1}{\hbar^2}\Psi\nabla S\cdot\nabla S + \frac{i}{\hbar}\Psi\nabla^2 S, \tag{304}$$

so the Schrodinger equation becomes, upon cancelling $e^{iS/\hbar} \neq 0$,

$$-\frac{\partial S}{\partial t} = \frac{1}{2m}|\nabla S|^2 + V - \frac{i\hbar}{2m}\nabla^2 S \tag{305}$$

No approximation has been made, though we assume that ψ is expressible as $e^{iS/\hbar}$ for some S[26]. In the limit $\hbar \to 0$ we ignore the last term and get the Hamilton-Jacobi evolution equation:

$$\frac{\partial S}{\partial t} + \frac{|\nabla S|^2}{2m} + V = 0 \quad \text{or} \quad \frac{\partial S}{\partial t} + H(q, \nabla S) = 0. \tag{306}$$

5.5.8 Separation of variables (SOV) in Hamilton-Jacobi equation

• Ironically, many of us are more familiar with solving the Schrödinger equation than the HJ equation, which predates it. We may use this experience to motivate the method of separation of variables to solve the HJ equation. Recall that if the hamiltonian isn't explicitly dependent on time, then we may multiplicatively separate the time-dependence by writing $\Psi(t, q) = T(t)\psi(q)$. $\psi(q)$ must solve the time-independent Schrodinger eigenvalue problem, and $T(t) = e^{-iEt/\hbar}$ where E is the separation constant and energy eigenvalue. Since $\Psi \sim e^{iS/\hbar}$, multiplicative separation of variables in the quantum wave function is replaced by additive SOV in hamilton's principle function. So, if $H = H(q, p)$ is not explicitly dependent on time, so that the hamiltonian is a constant of motion, then we may seek a solution of the HJ equation $H(q, \frac{\partial S}{\partial q}) + \frac{\partial S}{\partial t} = 0$ in the form

$$S(q, P, t) = W(q, P) - Et \tag{307}$$

Inserting this in HJ, we find that it is satisfied provided W solves the time-independent HJ equation for Hamilton's characteristic function

$$E = H\left(q, \frac{\partial W}{\partial q}\right). \tag{308}$$

• **Free particle in 1D:** The simplest case to consider is $H = p^2/2m$. The HJ equation is

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 = 0. \tag{309}$$

Since H isn't time dependent, we take $S = -Et + W(q, P)$ and get the time-independent HJ equation $\frac{1}{2m}(\frac{\partial W}{\partial q})^2 = E$ which is now an ODE. Upto an additive constant $W(q) = q\sqrt{2mE}$. Thus we have found a complete solution $S = -Et + q\sqrt{2mE}$ of the HJ equation depending on one constant of integration. For convenience, we take this constant of integration as $\alpha = P = \sqrt{2mE}$. So

$$S = -\frac{P^2}{2m}t + qP + \text{constant}. \tag{310}$$

We notice that $W(q, P) = qP$ generates the identity CT, while S deviates from the identity by an amount that grows linearly with time, as we might expect. The additive constant in S may be set to zero. The first equation of transformation says $p = \frac{\partial S}{\partial q} = P$. So the new

[26] S would have to diverge at points where Ψ vanishes.

momentum is conserved and equals the old momentum, and so, $P = p(0)$. The second equation of transformation gives us the new coordinate

$$Q = \frac{\partial S}{\partial P} = q - \frac{Pt}{m} = q(t) - \frac{p(0)t}{m}. \tag{311}$$

Since the new coordinate is guaranteed to be a constant of motion, we evaluate it at $t = 0$ and find $Q = q(0)$. Thus the new coordinate is equal to the initial location. This allows us to solve the initial value problem $q(t) = Q + \frac{p(0)t}{m}$. Finally, the new hamiltonian vanishes by construction: $K = H + \frac{\partial S}{\partial t} = E - E = 0$.

• **The free particle in 3D:** may be treated similarly. The HJ equation

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\left(\frac{\partial S}{\partial q^1}\right)^2 + \left(\frac{\partial S}{\partial q^2}\right)^2 + \left(\frac{\partial S}{\partial q^3}\right)^2\right) = 0. \tag{312}$$

reduces to the time independent HJ equation $E = \frac{1}{2m}\left(\left(\frac{\partial W}{\partial q^1}\right)^2 + \left(\frac{\partial W}{\partial q^2}\right)^2 + \left(\frac{\partial W}{\partial q^3}\right)^2\right)$ upon putting $S = -Et + W(q)$. We further separate variables by taking $W = W_1(q^1) + W_2(q^2) + W_3(q^3)$ to get

$$W_1'(q^1)^2 + W_2'(q^2)^2 + W_3'(q^3)^2 = 2mE \tag{313}$$

Since rhs is a constant and lhs is a sum of terms depending on different variables, each must be a constant that we denote α_j^2. The new momenta P_j are taken to equal the α_j,

$$W_1'(q^1)^2 = P_1^2, \quad W_2'(q^2)^2 = P_2^2, \text{ and } W_3'(q^3)^2 = P_3^2 \quad \text{where} \quad \frac{1}{2m}(P_1^2 + P_2^2 + P_3^2) = E. \tag{314}$$

We have a complete solution of the HJ equation depending on 3 constants of integration P_1, P_2, P_3:

$$S = -\frac{1}{2m}(P_1^2 + P_2^2 + P_3^2)t + q^1 P_1 + q^2 P_2 + q^3 P_3. \tag{315}$$

A 4^{th} constant of integration is an additive constant that we omit. Partial derivatives of hamilton's principal function with respect to the old coordinates give

$$p_j = \frac{\partial S}{\partial q^j} \quad \Rightarrow \quad p_j = P_j \tag{316}$$

So the constant new momenta are just the old momenta, which must be constants of motion $P_i = p_i = p_i(0)$. Partial derivatives of S with respect to the new momenta give the new coordinates

$$Q^i = \frac{\partial S}{\partial P_i} \Rightarrow Q^i = -\frac{tP_i}{m} + q^i \tag{317}$$

Since Q^i must be constant, we evaluate them at $t = 0$ and find $Q^i = q^i(0)$ are just the initial values of the old coordinates. Thus the solution of the initial value problem is

$$q^i(t) = q^i(0) + \frac{p_i(0)t}{m}. \tag{318}$$

• For the free particle we were able to *separate* all the variables (t, q^1, q^2, q^3) in the HJ equation and write Hamilton's principal function as a sum of terms involving just one variable each.

The HJ equation for a free particle is said to be separable. If the time-dependent HJ equation is separable, we may reduce it to a collection of ODEs, each of which is solved separately. Separability of the HJ equation is another viewpoint on what it means for a system to be 'solvable'.

• This additive SOV $S = -Et + W(q)$ in the classical HJ equation is replaced in QM by multiplicative SOV $\Psi(q,t) = e^{-iEt/\hbar}\psi(q)$ in the Schrodinger equation for a system with conserved energy. Moreover, the stationary state wave function is related to hamilton's characteristic function via $\psi(q) \propto e^{iW(q)/\hbar}$ in the semiclassical limit $\hbar \to 0$. The further additive SOV for hamilton's characteristic function $W(q) = W_1(q^1) + W_2(q^2)$ is replaced in QM by the multiplicative SOV of the stationary state wave function $\psi(q^1, q^2) = \psi_1(q^1)\psi_2(q^2)$.

5.5.9 Hamilton's principal function is action regarded as a function of end point of a trajectory

• We introduced hamilton's principal function $F_2(q,P,t) = S(q,P,t)$ as the generating function of a CT to coordinates and momenta, both of which are time-independent. It satisfies the time dependent HJ equation $\frac{\partial S}{\partial t} + H\left(q, \frac{\partial S}{\partial q}, t\right) = 0$. Hamilton's principal function is related to the action, which is the reason we use the same letter S for both. To see this, we compute the time derivative of an F_2 that satisfies the HJ equation

$$\dot{F}_2 = \frac{\partial F_2}{\partial q^i}\dot{q}^i + \frac{\partial F_2}{\partial t} = p_i\dot{q}^i + \frac{\partial F_2}{\partial t} = p_i\dot{q}^i - H = L \quad \Rightarrow \quad F_2(q(t),t) - F_2(q(t_0),t_0) = \int_{t_0}^{t} [p\dot{q} - H]dt' \tag{319}$$

t_0 was taken to be zero in the previous section. So S is like the action that appears in Hamilton's variational principle. But now, it is regarded as a *function* of the (variable) final location and final time of a *trajectory*, rather than as a *functional* of a whole *path* holding the end points fixed[27]. Furthermore, the variables conjugate to the (final) time and coordinates, namely the (final) hamiltonian and momenta, are expressed as partial derivatives

$$H = -\frac{\partial F_2}{\partial t} \quad \text{and} \quad p_i = \frac{\partial F_2}{\partial q^i}. \tag{320}$$

Note that to specify a trajectory that begins at fixed $q(t_0)$ at t_0, we need to say what the initial momenta are. So $F_2(q(t),t)$ also depends on the initial momenta $p(t_0)$, though we did not indicate this explicitly above. It is through these initial momenta and initial coordinates that hamilton's principal function $F_2 = S(q,P,t)$ acquires a dependence on P_i. Indeed, for the free particle, we saw that we could take $P_i = p_i(t_0)$. In general, the relation is obtained by evaluating $p_i = \frac{\partial S(q,P,t)}{\partial q^i}$ at $t = t_0$.

• Just as Hamilton's principal function is related to the action, Hamilton's characteristic function $W(q,P)$ is related to the abbreviated action. To see this, we compute

$$\frac{dW}{dt} = \frac{\partial W}{\partial q^i}\dot{q}^i + \frac{\partial W}{\partial P_i}\dot{P}_i = p_i\dot{q}^i. \tag{321}$$

Thus $W(q(t),P) = W(q(t_0),P) + \int_{t_0}^{t} p_i\dot{q}^i\, dt'$ where the integration is along the trajectory which starts at $q(t_0)$ at t_0 with initial momentum $p(t_0)$. Here the constant P is determined in terms of

[27] Recall that a trajectory is a path (in this context, a path on phase space) that satisfies the equations of motion.

$q(t_0), p(t_0)$ using $p(t_0) = \frac{\partial W(q,P)}{\partial q}_{|_{t=t_0}}$. So hamilton's characteristic function is the abbreviated action evaluated on a trajectory with fixed initial point and viewed as a function of a variable end point.

5.5.10 Geometric interpretation of HJ: trajectories are orthogonal to HJ wave fronts

• Let us discuss a geometric interpretation of Hamilton's principal function $S(q, P, t)$. For fixed constant new momenta P, we think of $S(q, P, t)$ as a time-dependent scalar function of q on the n-dimensional configuration manifold $\mathcal{Q}$. Then at each instant of time, $S(q, P, t)$ defines a family of hyper-surfaces in $\mathcal{Q}$, namely, the constant S hyper-surfaces of dimension $n-1$. A hyper-surface is a manifold of dimension one less than that of the ambient space. We will call these constant S hyper-surfaces 'wave fronts'. These are to be regarded as the instantaneous wave fronts of a propagating wave/disturbance that is governed by the HJ wave equation $\frac{\partial S}{\partial t} + H(q, \frac{\partial S}{\partial q}) = 0$. At a given time, each wave front is labeled by the value of S on it. As time progresses, the wave front with a given value of $S = S_0$ moves. In addition, we also have a family of curves in $\mathcal{Q}$, namely the trajectories for various possible initial locations $q^i(0)$ and fixed initial momenta $p_i(0) = \frac{\partial S}{\partial q^i}$, which are determined by the constants P_j and $q^i(0)$. Now, let us display a geometric relation between the wave fronts and trajectories by first examining the solution of the free particle HJ equation.

• **For a free particle moving in 2D,** Hamilton's principal function is $S = -Et + xP_1 + yP_2$ where $\vec{q} = (x, y)$, P_1 and P_2 are constants and $2mE = P_1^2 + P_2^2$. At any fixed time t_0, the constant $S = S_0$ hypersurfaces are a family of lines $xP_1 + yP_2 = S_0 + Et_0$. These are the wave fronts at $t = t_0$, they are the lines perpendicular to the vector (P_1, P_2). Though individual wave fronts move, the set of wave fronts at any other time is the same set of lines as at t_0. This is essentially because E is time independent.

• On the other hand, trajectories are $(x(t), y(t)) = (x_0 + \frac{P_1 t}{m}, y_0 + \frac{P_2 t}{m})$. Subtracting, trajectories are the family of lines $P_2 x - P_1 y = P_2 x_0 - P_1 y_0$, which is the same as $(P_2, -P_1) \cdot (x, y) = P_2 x_0 - P_1 y_0$. In other words, trajectories are the lines (not necessarily through the origin), orthogonal to the vector $(P_2, -P_1)$.

• Since the normal (P_1, P_2) to the wave fronts is perpendicular to the normal $(P_2, -P_1)$ to the trajectories, it follows that the trajectories are everywhere orthogonal to the wave fronts.

• **For a free particle in 3D**, the complete solution of the HJ equation is

$$S = -Et + xP_1 + yP_2 + zP_3 \quad \text{where} \quad 2mE = P_1^2 + P_2^2 + P_3^2. \tag{322}$$

In this case, the constant S hypersurfaces are planes orthogonal to the vector $\mathbf{P} = (P_1, P_2, P_3)$, i.e., $(x, y, z) \cdot (P_1, P_2, P_3) = S + Et = \text{const}$. The wave fronts evolve but the set of all wave fronts is independent of time. Trajectories are still straight lines $\mathbf{r} = \mathbf{r}_0 + \frac{\mathbf{P}t}{m}$. So trajectories are parallel to the vector $\mathbf{P}$ which is everywhere normal to the wave fronts. Thus the free particle trajectories are everywhere orthogonal to the wave fronts.

• **Particle subject to a potential moving on a Riemannian manfold:** More generally, let us consider a classical system whose configuration space is a Riemannian manifold $\mathcal{Q}$ with metric g_{ij} and whose kinetic energy is quadratic in velocities $L = \frac{1}{2} g_{ij} \dot{q}^i \dot{q}^j - V(q)$. For instance for $V = 0$, this could describe a free particle moving on Q in the absence of any external potential. We know that the conjugate momenta are $p_i = g_{ij} \dot{q}^j$ and the Hamiltonian is $H =$

$\frac{1}{2}g^{ij}p_ip_j + V(q)$. For $V = 0$ Lagrange's equations are the geodesic equations $\ddot{q}^l + \Gamma^l_{ij}\dot{q}^i\dot{q}^j = 0$. The HJ equation for Hamilton's principal function $S(q, P, t)$ is

$$\frac{\partial S}{\partial t} + \frac{1}{2}g^{ij}\frac{\partial S}{\partial q^i}\frac{\partial S}{\partial q^j} + V(q) = 0 \quad \text{where} \quad p_j = \frac{\partial S}{\partial q^j}. \tag{323}$$

For a free particle moving in 2D or 3D Euclidean space, we found that the trajectories are orthogonal to the wave fronts (level hyper-surfaces of S) at each point. We will show the same for the above Lagrangian system even with a potential.

• A normal vector to a hyper-surface of constant S is given by the gradient of S. It has components $n^i = (\text{grad } S)^i = g^{ij}\partial_j S$. Since S is a generating function of second type, $n^i = g^{ij}p_j = \dot{q}^j$. But this just says that the velocity vector at a point along a trajectory is equal to the normal to the wavefront through that point. Thus the trajectories are everywhere normal to the HJ wave fronts!

• **This is a classical version of 'wave-particle' duality.** The same physical system can be described either via point-particle trajectories that solve a system of ODEs, or via evolving wave fronts obtained from solving a PDE. Sometimes, the trajectories are called characteristic curves and Hamilton's ODEs are called the equations for the characteristics associated to the HJ PDE.

• One may use this connection between trajectories and wave fronts to give an alternate derivation of the geodesic equation on $\mathcal{Q}$ from the HJ equation by considering the special case $V = 0$. If $x^i(t)$ is a curve whose tangent vector $\dot{x}$ equals the normal to the HJ wave front at every point, then

$$\dot{x}^i = g^{ij}\partial_j S \tag{324}$$

We may eliminate S and obtain a differential equation for $x^i(t)$. We differentiate once in time and use $\dot{S} = \partial_t S + \partial_k S\dot{x}^k$, the HJ equation $\partial_t S = -H = -\frac{1}{2}g_{ij}\dot{x}^i\dot{x}^j$ and the fact that $\partial_j S = p_j = g_{jk}\dot{x}^k$:

$$\begin{aligned}\ddot{x}^i &= g^{ij}{}_{,k}\dot{x}^k\partial_j S + g^{ij}\partial_j\partial_t S + g^{ij}\partial_j\partial_k S\,\dot{x}^k = g^{ij}{}_{,k}\dot{x}^k p_j - g^{ij}\partial_j H + g^{ij}\partial_j p_k\dot{x}^k \\ &= g^{ij}{}_{,k}\dot{x}^k g_{jl}\dot{x}^l - g^{ij}\frac{1}{2}g_{kl,j}\dot{x}^l\dot{x}^k + g^{ij}g_{kl,j}\dot{x}^k\dot{x}^l = \left[g^{ij}{}_{,k}g_{jl} + \frac{1}{2}g^{ij}g_{kl,j}\right]\dot{x}^l\dot{x}^k. \end{aligned} \tag{325}$$

We also used $\partial_j\dot{x}^k = \frac{d}{dt}\delta^k_j = 0$. Differentiating the identity $g^{ij}g_{jl} = \delta^i_{\ l}$ in x^k one has $g^{ij}{}_{,k}g_{jl} + g^{ij}g_{jl,k} = 0$. Exploiting the symmetry of $\dot{x}^l\dot{x}^k$ under $k \leftrightarrow l$, we find that the curve $x(t)$ satisfies the geodesic equation

$$\ddot{x}^i + \frac{1}{2}g^{ij}\left(g_{jl,k} + g_{jk,l} - g_{kl,j}\right)\dot{x}^k\dot{x}^l = 0. \tag{326}$$

Remark: If $V \neq 0$, trajectories aren't geodesics with respect to the metric g_{ij}, but they remain orthogonal to the wave fronts.

6 Oscillations

6.1 Double pendulum

• The double pendulum is a system with a minimal number of degrees of freedom that displays both regular and chaotic dynamics in various energy regimes. It is an interesting and non-trivial

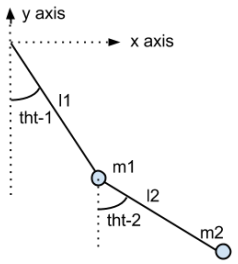


Figure 4: Double pendulum with two bobs of masses m_1, m_2 suspended from a fixed support with massless rods of length l_1, l_2. The respective counterclockwise deflection angles are θ_1, θ_2.

model system to study. As a general rule of thumb, if a system admits more conserved quantities, then the dynamics is more constrained and may display more regularity (the best possibility is integrability). A system with 2 degrees of freedom has a 4d phase space. In the absence of any conserved quantity, the trajectory could explore the whole of phase space. If energy is conserved, the trajectory must lie on a 3d constant energy sub-manifold of phase space, determined by initial conditions. If there is another conserved quantity Q functionally independent of energy, then trajectories must lie on the intersection of a constant E and constant Q sub-manifold, which is in general a 2D surface in phase space. We see that the presence of more conserved quantities restricts the dynamics.

• We consider a double pendulum with 'lower' bob of mass m_2 suspended by a massless rod of length l_2 from an 'upper' bob of mass m_1 which is in turn suspended from a fixed pivot by a massless rod of length l_1 (see figure 4). The system has 2 degrees of freedom, it is free to move in a vertical plane subject to gravity. The rods make angles θ_1, θ_2 counterclockwise relative to the downward vertical. The cartesian coordinates of the two bobs are

$$\begin{aligned} \mathbf{r}_1 &= (x_1, y_1) \quad \text{where} \quad x_1 = l_1 \sin\theta_1 \quad \text{and} \quad y_1 = -l_1 \cos\theta_1, \quad \text{and} \\ \mathbf{r}_2 &= (x_2, y_2) \quad \text{where} \quad x_2 = l_1 \sin\theta_1 + l_2 \sin\theta_2 \quad \text{and} \quad y_2 = -l_1 \cos\theta_1 - l_2 \cos\theta_2. \end{aligned} \tag{327}$$

• Assuming the potential energy vanishes at the height of the pivot, the potential and kinetic energies are

$$\begin{aligned} V &= -m_1 g l_1 \cos\theta_1 - m_2 g (l_1 \cos\theta_1 + l_2 \cos\theta_2) \quad \text{and} \\ T &= \frac{m_1}{2}\left(\dot{x}_1^2 + \dot{y}_1^2\right) + \frac{m_2}{2}\left(\dot{x}_2^2 + \dot{y}_2^2\right) = \frac{m_1}{2} l_1^2 \dot{\theta}_1^2 + \frac{m_2}{2}\left[l_1^2\dot{\theta}_1^2 + l_2^2\dot{\theta}_2^2 + 2 l_1 l_2 c_{12} \dot{\theta}_1 \dot{\theta}_2\right]. \end{aligned} \tag{328}$$

Here we abbreviate $s_{12} = \sin(\theta_1 - \theta_2)$ and $c_{12} = \cos(\theta_1 - \theta_2)$. To simplify things, we take bobs of equal masses m and rods of equal length l. In this case, $|V| \leq 3mgl$ while $0 \leq T < \infty$.

• The configuration space of the double pendulum is a torus $\mathbb{T}^2 = S^1 \times S^1$ with coordinates $\theta_1 \in S^1, \theta_2 \in S^1$. The Lagrangian is

$$L = T - V = \frac{1}{2} m l^2 \left[2\dot{\theta}_1^2 + \dot{\theta}_2^2 + 2 c_{12} \dot{\theta}_1 \dot{\theta}_2\right] + mgl\left[2\cos\theta_1 + \cos\theta_2\right]. \tag{329}$$

The momenta conjugate to θ_1, θ_2 are

$$p_1 = \frac{\partial L}{\partial \dot{\theta}_1} = m l^2 \left[2\dot{\theta}_1 + c_{12}\dot{\theta}_2\right] \quad \text{and} \quad p_2 = \frac{\partial L}{\partial \dot{\theta}_2} = m l^2 \left[\dot{\theta}_2 + c_{12}\dot{\theta}_1\right]. \tag{330}$$

The conjugate momenta do not coincide with the angular momenta of the two bobs, though their sum coincides with the total angular momentum of the pendulum. The angular momenta are

$$\mathbf{L}_1 = m\mathbf{r}_1 \times \dot{\mathbf{r}}_1 = ml^2\dot{\theta}_1\,\hat{z} \quad \text{and} \quad \mathbf{L}_2 = m\mathbf{r}_2 \times \dot{\mathbf{r}}_2 = ml^2\left[\dot{\theta}_1 + \dot{\theta}_2 + c_{12}\left(\dot{\theta}_1 + \dot{\theta}_2\right)\right]\hat{z} \tag{331}$$

$\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2 = (p_1 + p_2)\hat{z}$. We will use the conjugate momenta p_1, p_2 rather than the angular momenta.

• The 'generalized forces' are

$$\frac{\partial L}{\partial \theta_1} = -ml\left[2g\sin\theta_1 + ls_{12}\,\dot{\theta}_1\dot{\theta}_2\right] \quad \text{and} \quad \frac{\partial L}{\partial \theta_2} = ml\left[ls_{12}\,\dot{\theta}_1\dot{\theta}_2 - g\sin\theta_2\right]. \tag{332}$$

Lagrange's equations of motion are a pair of second order non-linear ODEs

$$2\ddot{\theta}_1 + c_{12}\,\ddot{\theta}_2 + s_{12}\,\dot{\theta}_2^2 + 2\omega^2\sin\theta_1 = 0 \qquad \text{and} \qquad \ddot{\theta}_2 + c_{12}\,\ddot{\theta}_1 - s_{12}\,\dot{\theta}_1^2 + \omega^2\sin\theta_2 = 0. \tag{333}$$

They involve only one material parameter $\omega^2 = g/l$. Upon expressing the generalized velocities in terms of momenta,

$$\dot{\theta}_1 = \frac{p_1 - c_{12}p_2}{ml^2(1+s_{12}^2)} \quad \text{and} \quad \dot{\theta}_2 = \frac{2p_2 - c_{12}p_1}{ml^2(1+s_{12}^2)} \tag{334}$$

we find the conserved hamiltonian $H = p_1\dot{\theta}_1 + p_2\dot{\theta}_2 - L = T + V$

$$H = \frac{1}{2ml^2(1+s_{12}^2)}\left[p_1^2 + 2p_2^2 - 2c_{12}p_1p_2\right] - mgl[2\cos\theta_1 + \cos\theta_2]. \tag{335}$$

The conserved energy may also be expressed in terms of coordinates and velocities:

$$E = \frac{1}{2}ml^2\left[2\dot{\theta}_1^2 + \dot{\theta}_2^2 + 2c_{12}\dot{\theta}_1\dot{\theta}_2\right] - mgl[2\cos\theta_1 + \cos\theta_2]. \tag{336}$$

The phase space of the double pendulum is four dimensional, with coordinates $\theta_1 \in S^1, \theta_2 \in S^1, p_1, p_2 \in \mathbb{R}$. The phase space is the cartesian product of a torus and a plane $\mathbb{T}^2 \times \mathbb{R}^2$

• Besides energy, the double pendulum does not possess any obvious conserved quantity. However, when the energy is very large, most of it is kinetic since the gravitational potential energy is bounded between $\pm 3mgl$. For example, the two bobs could just go round very fast in uniform circular motion. So in the limit of high energies ($E \gg 3mgl$) we should be able to ignore the gravitational force, and the torque it imparts. As a consequence, total angular momentum $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$ should be conserved at asymptotically high energies. We already know that

$$\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2 = ml^2\left[2\dot{\theta}_1 + \dot{\theta}_2 + 2c_{12}(\dot{\theta}_1 + \dot{\theta}_2)\right]\hat{z} = (p_1 + p_2)\hat{z} \tag{337}$$

This expression for the conserved total angular momentum may also be obtained using Noether's theorem. The Lagrangian ignoring gravity

$$L = T = \frac{1}{2}ml^2\left[2\dot{\theta}_1^2 + \dot{\theta}_2^2 + 2\cos(\theta_1 - \theta_2)\dot{\theta}_1\dot{\theta}_2\right] \tag{338}$$

is invariant under (infinitesimal) rotations $\theta_1 \to \theta_1 + \delta\phi, \theta_2 \to \theta_2 + \delta\phi$. Noether's theorem guarantees conservation of

$$p_1\,\delta\theta_1 + p_2\,\delta\theta_2 = \delta\phi\, ml^2[2\dot\theta_1 + c_{12}\dot\theta_2] + \delta\phi\, ml^2[\dot\theta_2 + c_{12}\dot\theta_1] \tag{339}$$

Since $\delta\phi$ is arbitrary, we may omit it and get an expression for the conserved angular momentum

$$\mathbf{L} = (p_1 + p_2)\hat z = ml^2\left[(2 + c_{12})\dot\theta_1 + (1 + c_{12})\dot\theta_2\right]\hat z \tag{340}$$

Numerical solutions of the equations of motion of the double pendulum show that $\mathbf{L}$ fluctuates around a mean value. As the energy increases, the fluctuations in $\mathbf{L}$ get smaller, and in the limit of infinite energy, angular momentum is exactly conserved just as for the simple pendulum (see fig.2).

6.1.1 Small oscillations of a double pendulum: normal modes

• In general, it has not been possible to solve the equations of motion of a double pendulum in closed form due to their non-linearities (not even with elliptic functions! The motion is chaotic!). However, if the deflection angles are always small, we may linearize the equations of motion and solve them. The motion reduces to the integrable dynamics of a pair of coupled harmonic oscillators. Let us see why.

• If both $|\theta_1|, |\theta_2| \ll 1$ we may approximate the trigonometric functions cos and sin by their quadratic Taylor polynomials in the kinetic and potential energies, so that the resulting equations of motion become linear. The Lagrangian becomes

$$L = \frac{1}{2}ml^2\left[2\dot\theta_1^2 + \dot\theta_2^2 + 2\dot\theta_1\dot\theta_2\right] + mgl\left[3 - \theta_1^2 - \frac{1}{2}\theta_2^2\right] = T - V. \tag{341}$$

We omit the constant $3mgl$ from the Lagrangian: it doesn't affect the eom. The conjugate momenta are

$$p_1 = ml^2\left(2\dot\theta_1 + \dot\theta_2\right) \quad \text{and} \quad p_2 = ml^2\left(\dot\theta_1 + \dot\theta_2\right). \tag{342}$$

and

$$\dot\theta_1 = \frac{p_1 - p_2}{ml^2} \quad \text{and} \quad \dot\theta_2 = \frac{2p_2 - p_1}{ml^2}. \tag{343}$$

The equations of motion depend only on one physical parameter $\omega^2 = g/l$:

$$2\ddot\theta_1 + \ddot\theta_2 + 2\omega^2\theta_1 = 0 \quad \text{and} \quad \ddot\theta_1 + \ddot\theta_2 + \omega^2\theta_2 = 0. \tag{344}$$

The corresponding conserved energy is $H = T + V$,

$$H = \frac{ml^2}{2}\left[2\dot\theta_1^2 + \dot\theta_2^2 + 2\dot\theta_1\dot\theta_2\right] + mgl\left[\theta_1^2 + \frac{\theta_2^2}{2}\right] \;=\; \frac{1}{2ml^2}\left[p_1^2 + 2p_2^2 - 2p_1p_2\right] + mgl\left[\theta_1^2 + \frac{\theta_2^2}{2}\right]. \tag{345}$$

The equations of motion are now a pair of coupled second order linear ODEs with constant coefficients. It is possible to change variables to normal modes to get a pair of de-coupled linear ODEs. Let us first write the eom in matrix form

$$\frac{d^2}{dt^2}\begin{pmatrix}2 & 1\\ 2 & 2\end{pmatrix}\begin{pmatrix}\theta_1\\ \theta_2\end{pmatrix} = -2\omega^2\begin{pmatrix}\theta_1\\ \theta_2\end{pmatrix} \tag{346}$$

If we let B be the constant coefficient matrix,

$$B = \begin{pmatrix} 2 & 1 \\ 2 & 2 \end{pmatrix} \quad \text{and} \quad \theta = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \quad \text{then} \quad \frac{d^2}{dt^2} B\theta = -2\omega^2 \theta \tag{347}$$

Though B is not a symmetric matrix, it has distinct eigenvalues $\lambda_\pm = 2 \pm \sqrt{2}$, and therefore can be diagonalized. The corresponding eigenvectors are not orthogonal, but may be taken as

$$a_+ = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \end{pmatrix} \quad \text{and} \quad a_- = \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \end{pmatrix}. \tag{348}$$

B may be diagonalized by a (non-orthogonal) similarity transformation S whose matrix representation has columns that are the eigenvectors of B

$$S^{-1}BS = D \quad \text{where} \quad S = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ \sqrt{2} & -\sqrt{2} \end{pmatrix}, \; S^{-1} = \begin{pmatrix} 1 & \frac{1}{\sqrt{2}} \\ 1 & -\frac{1}{\sqrt{2}} \end{pmatrix} \text{ and } D = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}. \tag{349}$$

The equations of motion become

$$\frac{d^2}{dt^2} SDS^{-1}\theta = -2\omega^2\theta \;\; \Rightarrow \;\; \frac{d^2}{dt^2}(S^{-1}\theta) = -2\omega^2 D^{-1}(S^{-1}\theta) \tag{350}$$

If we denote

$$S^{-1}\theta = \xi = \begin{pmatrix} \xi_+ \\ \xi_- \end{pmatrix} = \begin{pmatrix} \theta_1 + \frac{\theta_2}{\sqrt{2}} \\ \theta_1 - \frac{\theta_2}{\sqrt{2}} \end{pmatrix} \quad \text{and} \quad 2\omega^2 D^{-1} = \begin{pmatrix} \frac{2\omega^2}{\lambda_+} & \\ 0 & \frac{2\omega^2}{\lambda_-} \end{pmatrix} = \begin{pmatrix} \omega_+^2 & 0 \\ 0 & \omega_-^2 \end{pmatrix}, \tag{351}$$

then the components $\xi_\pm$ evolve via *decoupled* 2nd order ODEs

$$\ddot{\xi}_+(t) = -\omega_+^2 \xi_+(t) \quad \text{and} \quad \ddot{\xi}_-(t) = -\omega_-^2 \xi_-(t) \quad \text{where} \quad \omega_\pm^2 = \frac{2\omega^2}{2 \pm \sqrt{2}}. \tag{352}$$

$\xi_\pm(t)$ are called normal modes of the system, they are periodic functions of time with periods

$$T_\pm = \frac{2\pi}{\omega_\pm} = \frac{2\pi}{\omega} \sqrt{1 \pm \frac{1}{\sqrt{2}}}. \tag{353}$$

$\xi_\pm(t)$ may be expressed in terms of trigonometric functions of time

$$\xi_+(t) = c_1 \cos(\omega_+ t) + c_2 \sin(\omega_+ t) \quad \text{and} \quad \xi_-(t) = c_3 \cos(\omega_- t) + c_4 \sin(\omega_- t). \tag{354}$$

The four coefficients c_i are to be fixed using the initial conditions. The original deflection angles are determined via $\theta = S\xi$

$$\theta_1 = \frac{1}{2}(\xi_+ + \xi_-) \quad \text{and} \quad \theta_2 = \frac{1}{\sqrt{2}}(\xi_+ - \xi_-). \tag{355}$$

Note that the general motion of the double pendulum in the small angle approximation is not periodic. The above solution is a linear combination of periodic functions whose periods are not in rational ratio

$$\frac{T_+}{T_-} = \frac{\omega_-}{\omega_+} = \sqrt{\frac{\lambda_+}{\lambda_-}} = 1 + \sqrt{2} \;\notin\; \mathbb{Q} \tag{356}$$

In general, the motion is quasi-periodic. The double pendulum does not return to its initial state, but approaches it arbitrarily closely if we are willing to wait long enough. However, if initial conditions are chosen so that only one of the two normal modes ξ_+ or ξ_- is present (e.g. if $c_3 = c_4 = 0$), then the motion is periodic.

• We may use the normal modes to find a new conserved quantity for small oscillations of a double pendulum. As for the simple pendulum or harmonic oscillator, from the equations of motion,

$$\ddot{\xi}_+ = -\omega_+^2 \xi_+ \quad \text{and} \quad \ddot{\xi}_- = -\omega_-^2 \xi_- \tag{357}$$

we infer that the energy of each normal mode is a constant of motion

$$H_+ = \frac{1}{2} m l^2 \left[\dot{\xi}_+^2 + \omega_+^2 \xi_+^2 \right] \quad \text{and} \quad H_- = \frac{1}{2} m l^2 \left[\dot{\xi}_-^2 + \omega_-^2 \xi_-^2 \right]. \tag{358}$$

The pre-factor ml^2 is chosen so that $H_\pm$ have dimensions of energy. The total energy

$$H = \frac{1}{2} m l^2 [2\dot{\theta}_1^2 + \dot{\theta}_2^2 + 2\dot{\theta}_1 \dot{\theta}_2] + mgl[\theta_1^2 + \frac{1}{2}\theta_2^2] \tag{359}$$

is of course also conserved. Are $H, H_\pm$ functionally independent? This is unlikely since we would expect the total energy to be a sum of energies contributed by the various normal modes, which do not interact with each other. In fact, we will show that H is a weighted sum of the energies of the normal modes $H = 2\lambda_+ H_+ + 2\lambda_- H_-$. To see this we write the total energy as a quadratic form and express θ_i in terms of normal modes ξ_i:

$$\begin{aligned} H &= \frac{1}{2} m l^2 \begin{pmatrix} \dot{\theta}_1 \\ \dot{\theta}_2 \end{pmatrix}^t \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \dot{\theta}_1 \\ \dot{\theta}_2 \end{pmatrix} + mgl \begin{pmatrix} \dot{\theta}_1 \\ \dot{\theta}_2 \end{pmatrix}^t \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \dot{\theta}_1 \\ \dot{\theta}_2 \end{pmatrix} = \frac{1}{2} m l^2 \dot{\theta}^t \tau \dot{\theta} + mgl \theta^t v \theta \\ \text{where} \qquad \tau &= \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \quad \text{and} \quad v = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{2} \end{pmatrix}. \end{aligned} \tag{360}$$

The kinetic and potential matrices τ and v are not uniquely defined. But if they are chosen symmetric, then they are unique. We may add any anti-symmetric matrices to τ and v without affecting the formula for energy. Writing $\theta = S\xi$ and using $S^t \tau S = 2D = 2\text{diag}(\lambda_+, \lambda_-)$ and $S^t v S = 2I$ we get

$$\begin{aligned} H &= \frac{1}{2} m l^2 \, \dot{\xi}^t \left(S^t \tau S \right) \dot{\xi} + mgl \, \xi^t \left(S^t v S \right) \xi \\ &= (2\lambda_+) \frac{1}{2} m l^2 \dot{\xi}_+^2 + (2\mu_-) \frac{1}{2} m l^2 \dot{\xi}_-^2 + (2\lambda_+) \frac{mgl}{\lambda_+} \xi_+^2 + (2\lambda_-) \frac{mgl}{\lambda_-} \xi_-^2 \\ &= 2\lambda_+ H_+ + 2\lambda_- H_-. \end{aligned} \tag{361}$$

In the last step we used $\omega_\pm^2 = 2\omega^2/\lambda_\pm$ to write

$$\frac{mgl}{\lambda_\pm} = \frac{ml^2 \omega^2}{\lambda_\pm} = \frac{1}{2} m l^2 \, \omega_\pm^2 \tag{362}$$

So of H, H_1 and H_2, only two are independent conserved quantities. Thus we have identified a second conserved quantity for small oscillations of a double pendulum. In the limit of low energies, we find that the motion of a double pendulum is integrable, we have explicitly found the general solution. Before we attempt to study the dynamics of a double pendulum at higher energies, let us discuss some general features of small oscillations (engineers use the term vibrations) around static and periodic solutions.

6.2 Normal modes of oscillation around a static solution: general framework

• Small oscillations of a double pendulum illustrate some features of the general method of passage to normal modes of vibration for a system with $n \geq 2$ degrees of freedom. Many interesting mechanical systems have a Lagrangian of the form $L = \frac{1}{2} g_{ij}(q)\dot{q}^i\dot{q}^j - U(q)$ where $g_{ij}(q)$ is a positive definite matrix on configuration space and $U(q)$ is a potential energy. Lagrange's equations take the form

$$\frac{d}{dt}\left(g_{ij}(q)\dot{q}^j\right) + \frac{\partial U}{\partial q^i} = 0. \tag{363}$$

For the double pendulum, $g_{ij} = ml^2 \begin{pmatrix} 2 & \cos(\theta_1 - \theta_2) \\ \cos(\theta_1 - \theta_2) & 1 \end{pmatrix}$ and $U(\theta) = -mgl(2\cos\theta_1 + \cos\theta_2)$.

• If q_0 is an extremum of U, then $\frac{\partial U}{\partial q^i}(q_0) = 0$ and a static solution of the eom is given by

$$q^i(t) \equiv q_0^i \quad (\text{so that} \quad \dot{q}^i(t) \equiv 0). \tag{364}$$

For the double pendulum, $\theta_1 = \theta_2 = 0$ is a static solution. If a static solution occurs at a minimum of the potential, we expect it to be stable under small perturbations, and may look for small oscillations around the static solution. Let $x^i = q^i - q_0^i$ be the departure from equilibrium, we expect it to remain small for all times. Then the Lagrangian may be expanded to quadratic order (so that the equations of motion will be linear) in x by Taylor expanding $g_{ij}(q)$ and $U(q)$ around $q = q_0$:

$$L = g_{ij}(q_0)\dot{x}^i\dot{x}^j - U(q_0) - \frac{1}{2}\frac{\partial^2 U(q_0)}{\partial q^i \partial q^j} x^i x^j + \mathcal{O}(x^3). \tag{365}$$

Without loss of generality we may take $U(q_0) = 0$, a constant addition to the potential does not affect the equations of motion. Let us abbreviate

$$g_{ij}(q_0) = m_{ij} \quad \text{a mass matrix and} \quad \frac{\partial^2 U(q_0)}{\partial q^i \partial q^j} = k_{ij} \quad \text{a spring constant matrix.} \tag{366}$$

Then the Lagrangian to quadratic approximation around equilibrium is

$$L = \frac{1}{2} m_{ij}\dot{x}^i\dot{x}^j - \frac{1}{2} k_{ij} x^i x^j. \tag{367}$$

For small oscillations of a double pendulum about the minimum energy static solution, we found

$$L = \frac{1}{2}ml^2(2\dot{\theta}_1^2 + \dot{\theta}_2^2 + 2\dot{\theta}_1\dot{\theta}_2) - \frac{1}{2}mgl(2\theta_1^2 + \theta_2^2) \quad \Rightarrow \quad M = ml^2 \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \quad \text{and} \quad K = mgl \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}. \tag{368}$$

Check that both M and K are real symmetric positive matrices.

• The corresponding equations of motion are a system of n homogeneous linear 2nd order ODEs with constant coefficients

$$m_{ij}\ddot{x}^j + k_{ij}x^j = 0 \quad \text{or} \quad M\ddot{x} = -Kx \tag{369}$$

defined by a pair of real symmetric positive matrices $M = m_{ij}$ and $K = k_{ij}$ which act on the vector space $V \cong \mathbb{R}^n$ in which x lives. For the double pendulum, the equations for small oscillations are

$$ml^2 \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \ddot{\theta}_1 \\ \ddot{\theta}_2 \end{pmatrix} = -mgl \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix}. \tag{370}$$

• Linearity of the equations means the space of solutions $x(t)$ is a linear space, we can add and rescale solutions to get other solutions. One checks that this system of ODEs admits a conserved energy $E = \frac{1}{2}\dot{x}^t M\dot{x} + \frac{1}{2}x^t Kx$. The momentum conjugate to x^i is $p_i = m_{ij}\dot{x}^j$. If we denote the matrix elements of the inverse of M by m^{ij}, then the Hamiltonian is

$$H = \frac{1}{2}m^{ij}p_i p_j + \frac{1}{2}k_{ij}x^i x^j. \tag{371}$$

• To find the vector function of time $x^i(t)$, we try to separate the time and vectorial dependences by making the ansatz $x^i(t) = a^i f(t)$ where $a^i \in \mathbb{R}^n$ is a constant vector and f an ordinary real function of time. One hopes there are sufficiently many separable solutions to span the space of all solutions. Then

$$(Ma)\ddot{f} = -(Ka)f \quad \text{or} \quad (Ma)(\ddot{f}/f) = -Ka \tag{372}$$

The rhs is time-independent while the lhs depends on time via the scalar $\ddot{f}/f$. The only way for this equation to hold at all times is for $\ddot{f}/f$ to be a negative[28] constant, say $-\omega^2$. Thus $\ddot{f} = -\omega^2 f$ and so $f = A\cos\omega t + B\sin\omega t$. Sometimes one simply says $f \sim e^{i\omega t}$ with the understanding that the real and imaginary parts are the linearly independent real solutions. a must then satisfy a linear equation which is reminiscent of an eigenvalue problem

$$(-\omega^2 M + K)a = 0. \tag{373}$$

For non-trivial solutions a to exist, the matrix of coefficients must have zero determinant, leading to the characteristic equation for ω^2

$$\det(-\omega^2 M + K) = 0. \tag{374}$$

This equation in general has n roots ω_α^2 (including possibly repeated roots), which must all be real and positive if K, M are positive matrices, as noted above. Physically, the roots must be positive to ensure that $x(t) = \Re a e^{i\omega t}, \Im a e^{i\omega t}$ do not grow or decay exponentially with time, which would violate conservation of energy H, as well as stability of the static solution q_0. Alternatively, we could multiply the linear equation by M^{-1} , to get a standard eigenvalue equation[29]

$$\left(M^{-1}K\right)\, a = \omega^2 a. \tag{375}$$

Note that the product of two positive matrices need not be positive, it need not even be symmetric[30]. But despite this, our earlier argument tells us that if M, K are positive, then the n eigenvalues $\omega_\alpha^2 = \frac{\langle a|M|a\rangle}{\langle a|K|a\rangle}$ are real and positive.

• For small oscillations of a double pendulum,

$$M^{-1}K = \frac{1}{ml^2}\begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix} mgl \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} = \frac{g}{l}\begin{pmatrix} 2 & -1 \\ -2 & 2 \end{pmatrix}. \tag{376}$$

[28] That the constant must be negative is seen by multiplying by the transpose of a from the left and using the fact that both M and K are positive matrices so that their diagonal matrix elements $\langle a|K|a\rangle, \langle a|M|a\rangle$ in the 'state' a must be positive.

[29] Assuming M is positive definite, M^{-1} is positive definite as well, as is seen by going to the basis in which M is diagonal. M^{-1} is also diagonal in this basis, with positive eigenvalues equal to the reciprocals of those of M.

[30] However, the product of two positive matrices that commute is again positive, check this!

Notice that $M^{-1}K$ is not a symmetric matrix, and that M and K do not commute in this example. Yet, $M^{-1}K$ has positive eigenvalues $\frac{g}{l}(2 \pm \sqrt{2})$.

• The corresponding n eigenvectors are denoted $a_{(\alpha)}$. Since $M^{-1}K$ may not be symmetric, the $a_{(\alpha)}$ may not be orthogonal (as we found for the double pendulum. The $a_{(\alpha)}$ can be chosen orthogonal if M and K commute so that $M^{-1}K$ is symmetric). Thus we have n normal modes of small oscillations with eigenfrequencies ω_α for $\alpha = 1, 2, \ldots$

$$\xi_{(\alpha)}(t) = a_{(\alpha)} \left[c_1^{(\alpha)} \cos(\omega_\alpha t) + c_2^{(\alpha)} \sin(\omega_\alpha t) \right] \qquad (\text{no sum on } \alpha). \tag{377}$$

Physically, the vector $a_{(\alpha)}$ for each α is a direction in the tangent space to the configuration space at the equilibrium point q_0. The corresponding normal mode is an oscillation in that direction. $c_{1,2}^{(\alpha)}$ are constants of integration. In terms of the normal modes, the equations of motion decouple for each eigenfrequency,

$$\ddot{\xi}_{(\alpha)}(t) = -\omega_\alpha^2 \, \xi_{(\alpha)}(t) \qquad (\text{no sum on } \alpha). \tag{378}$$

The general solution of the equations $M\ddot{x} + Kx = 0$ for small vibrations is a linear combination of normal modes

$$x(t) = \sum_\alpha \xi_{(\alpha)}(t) = \sum_{\alpha=1}^{n} a_{(\alpha)} \left[c_1^{(\alpha)} \cos(\omega_\alpha t) + c_2^{(\alpha)} \sin(\omega_\alpha t) \right]. \tag{379}$$

• A negative eigenvalue ω^2 (i.e., imaginary ω) would imply that the static solution is, in general, exponentially unstable in the linear approximation. Small perturbations would grow exponentially (or decay) with time $\xi \sim a(c_1 e^{|\omega| t} + c_2 e^{-|\omega| t})$, and the energy $H = \frac{1}{2} m_{ij} \dot{x}^i \dot{x}^j + \frac{1}{2} k_{ij} x^i x^j$ would not be conserved. This happens if we were perturbing around a static solution q_0 that is not a local minimum, but a local maximum or saddle point of the potential. Of course, this cannot happen if both M and K are positive matrices. Illustrate with a diagram.

• A 'zero mode' corresponding to a zero eigenvalue $\omega^2 = 0$ could grow linearly with time $\xi \sim a(c_1 + c_2 t)$ since $\ddot{f} = 0$. In this case, the static solution is said to be marginally unstable within the linear approximation. This happens, for instance, if the static solution q_0 is at a degenerate minimum of the potential, such as at one of the minima of the Mexican hat potential $U(x, y) = (x^2 + y^2 - 1)^2$. The corresponding zero mode points in the direction in which the potential is flat, i.e., along the valley of the Mexican hat potential. Illustrate with a diagram.

• **Remark:** Another way to reduce the equation $(-M\omega^2 + K)a = 0$ to a standard eigenvalue problem is given here, emphasizing concepts from tensor algebra. We are given a vector space V along with a pair of covariant symmetric positive tensors $M = m_{ij}$ and $K = k_{ij}$. We may regard M as defining a positive definite inner product on V. Let e_i denote the standard basis vectors for V with components $(e_i)^j = \delta_i^j$. Explicitly, $e_1 = (1000\cdots)^t, e_2 = (0100\cdots)^t$ etc. The inner products of basis vectors are $(e_i, e_j) = m_{ij}$. For a general pair of vectors $u = u^i e_i, v = v^j e_j$, their inner product is $(u, v) = m_{ij} u^i v^j$ with $(u, u) > 0$ for all $u \neq 0$, since the kinetic energy is positive. Then there is a basis for V consisting of vectors f_i which are orthonormal with respect to this inner product $(f_i, f_j) = \delta_{ij}$. The f_i basis vectors are some linear combinations of the e_j, $f_i = T_i{}^\alpha e_\alpha$, so

$$\delta_{ij} = (f_i, f_j) = (T_i{}^\alpha e_\alpha, T_j{}^\beta e_\beta) = T_i{}^\alpha T_j{}^\beta (e_\alpha, e_\beta) = T_i{}^\alpha T_j{}^\beta m_{\alpha\beta} \tag{380}$$

In other words, in the standard basis e_α, M is the matrix with entries $m_{\alpha\beta}$, while in the f_i basis, M is the identity matrix. Note that being a covariant tensor of rank two, M transforms via 'TT' (rather than '$T^{-1}T$'), which is *not* a similarity transformation[31], and in particular *does not* preserve the eigenvalues of $m_{\alpha\beta}$. In the new basis, M is the identity, all of whose eigenvalues are equal to one. K also transforms as a covariant symmetric tensor to

$$\tilde{k}_{ij} = T_i^{\ \alpha} T_j^{\ \beta} k_{\alpha\beta}. \tag{381}$$

Finally, the vector $a = a^i e_i$ also has new components in the f basis. Indeed

$$f_i = T_i^{\ j} e_j \quad \Rightarrow \quad e_j = (T^{-1})_j^{\ i} f_i \quad \Rightarrow \quad a = \tilde{a}^i f_i \quad \text{where} \quad \tilde{a}^i = (T^{-1})_j^{\ i} a^j \tag{382}$$

So the linear equation for a is transformed from

$$(-m_{ij}\omega^2 + k_{ij})a^j = 0 \quad \text{to} \quad (-\delta_{ij}\omega^2 + \tilde{k}_{ij})\tilde{a}^j = 0 \quad \text{or} \quad \tilde{k}_{ij}\tilde{a}^j = -\omega^2 \tilde{a}^j. \tag{383}$$

which is now a standard eigenvalue problem for a matrix $\tilde{k}_{ij}$.

6.3 Small perturbations around a periodic solution

• In the last 2 sections we studied small oscillations around a static solution. This is what results when the static solution is stable to small perturbations. More generally, we could consider a time dependent solution (may be even an approximate solution) and ask about its stability and perturbations around it. Consider a system with Lagrangian $L = \frac{1}{2} m_{ij} \dot{q}^i \dot{q}^j - V(q)$ where for simplicity we take m_{ij} constant. For simplicity, let us suppose $q_0(t)$ is a periodic solution with period T:

$$m_{ij}\ddot{q}_0^j + \frac{\partial V(q_0)}{\partial q^i} = 0 \quad \text{with} \quad q_0(t+T) = q_0(t) \quad \forall\, t. \tag{384}$$

This is reasonably common in potential wells or planetary orbits etc. We seek a nearby solution of the form $q^i(t) = q_0^i(t) + x^i(t)$ where x^i is a small perturbation, $|x(t)| \ll |q_0(t)|$. Expanding in x we get

$$m_{ij}(\ddot{q}_0^j + \ddot{x}^j) + \frac{\partial V(q_0(t))}{\partial q^i} + \frac{\partial^2 V(q_0(t))}{\partial q^i \partial q^j} x^j + \mathcal{O}(x^2) = 0. \tag{385}$$

We get a system of 2nd order homogeneous linear ODEs with periodic coefficients for the perturbation $x(t)$:

$$m_{ij}\ddot{x}^j + k_{ij}(t)x^j = 0 \quad \text{where} \quad k_{ij}(t) = \frac{\partial^2 V(q_0(t))}{\partial q^i \partial q^j} \quad \text{and} \quad k_{ij}(t+T) = k_{ij}(t). \tag{386}$$

The time-dependent spring 'constants' $k_{ij}(t)$ inherit the periodicity of the unperturbed solution $q_0(t)$, since the hessian of the potential is evaluated at $q_0(t)$. The simplest case is that of one degree of freedom

$$m\,\ddot{x}(t) + k(t)\,x(t) = 0. \tag{387}$$

An interesting case is $k(t) = a + b\cos t$, which leads to Mathieu's equation.

• Such ODEs were studied by Hill in the context of solar perturbations to the moon's periodic motion around the earth and also by Floquet. For the earth-moon-sun system, $q_0(t)$ is an

[31] On the other hand, a mixed tensor with one upper and one lower index h_j^i transforms via $T^{-1}T$.

approximate periodic solution (when the sun's effect is ignored), namely the Earth and moon going round their common center of mass in a nearly circular orbit with a period of about $T = 1$ month. $q_0(t) + x(t)$ is the perturbed lunar orbit when effects of the sun's gravity are included to first order.

• An equation of this sort (for $n = 1$) arises also in quantum mechanics when considering the time-independent Schrödinger eigenvalue problem for a particle moving in one dimension subject to a periodic potential $V(x)$, such as that presented by an ionic crystal to an electron. Here one considers a 1 dimensional crystal with spacing between adjacent ions equal to a. The crystal as a whole is of length L, but we assume that L is so large that the effects of the edges of the crystal can be ignored. This is often implemented via periodic boundary conditions on the wave function (as would be the case if the ions are arranged on a circle). To go from the classical mechanics problem to the QM one, x is replaced by the wave function ψ and time t is replaced by the spatial coordinate x and the spring 'constant' $k(t)$ by the potential $E - V(x)$. Newton's equation is replaced by the Schrödinger eigenvalue problem, a class of solutions of which are called Bloch wave functions:

$$-\frac{\hbar^2}{2m}\psi''(x) + (V(x) - E)\psi(x) = 0. \tag{388}$$

• A qualitative feature of an ODE with periodic coefficients is that the solutions need not have the same periodicity, nor even be periodic at all. In fact, we are familiar with this phenomenon from the simplest such equation for a harmonic oscillator. $m\ddot{x} + kx = 0$ describes oscillations around a static equilibrium point at $x = 0$. Here the coefficients are constant, and therefore periodic with period 0. Nevertheless, solutions are not constant functions, they are periodic with period $T = 2\pi/\omega$ where $\omega = \sqrt{k/m}$. Loosely, this may be regarded as an example of '*spontaneous symmetry breaking*'. A 'symmetry' of the equation of motion, (i.e. periodicity of coefficients with period 0) is not realized in some/all solutions.

6.3.1 Formulation as a system of first order equations

• In the simplest case of one degree of freedom, the equation for small oscillations around a periodic solution takes the form $m\ddot{x}+k(t)x(t) = 0$ with $k(t+T) = k(t)$ for all t. It is convenient to rewrite this as a pair of first order equations on phase space

$$\frac{d}{dt}\begin{pmatrix} x(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} 0 & m^{-1} \\ -k(t) & 0 \end{pmatrix}\begin{pmatrix} x(t) \\ p(t) \end{pmatrix} \quad \text{and denote} \quad A(t) = \begin{pmatrix} 0 & m^{-1} \\ -k(t) & 0 \end{pmatrix}. \tag{389}$$

$A(t)$ is periodic with period T. These equations follow from the (explicitly time-dependent) hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}k(t)x^2$. Let $\psi(t) = (x(t), p(t))^t$ denote the instantaneous 'state vector' of the system. Then the equation takes the form $\dot{\psi}(t) = A(t)\psi(t)$. Notice the formal similarity of $\dot{\psi} = A\psi$ with the time-dependent Schrödinger equation $i\hbar\dot{\psi} = H(t)\psi$. Unlike the hermitian $H(t)$ in quantum mechanics, here $A(t)$ is not hermitian, but traceless. This has interesting consequences, as we shall see.

• For n degrees of freedom, the equation $m_{ij}\ddot{x}^j + k_{ij}x^j = 0$ may similarly be formulated as a first order system. We first define the momenta $p_i = m_{ij}\dot{x}^j$. Then

$$\dot{x}^i = (m^{-1})^{il}p_l \quad \text{and} \quad \dot{p}_j = -k_{jk}x^k \quad \Rightarrow \quad \frac{d}{dt}\begin{pmatrix} x^i \\ p_j \end{pmatrix} = \begin{pmatrix} 0 & (m^{-1})^{il} \\ -k_{jk}(t) & 0 \end{pmatrix}\begin{pmatrix} x^k \\ p_l \end{pmatrix}. \tag{390}$$

We see that the $2n \times 2n$ matrix $A(t) = \begin{pmatrix} 0 & m^{-1} \\ -k & 0 \end{pmatrix}$ is again traceless. These equations for small oscillations again follow from an explicitly time-dependent hamiltonian

$$H(x,p,t) = \frac{1}{2}(m^{-1})^{il} p_i p_l + \frac{1}{2} k_{jk}(t)\, x^j x^k. \tag{391}$$

As before, we define the phase space 'state vector' $\psi(t) = (x^i, p_j)^t$, in terms of which $\dot{\psi}(t) = A(t)\psi(t)$. Here too, $A(t+T) = A(t)$ inherits the periodicity of the solution q_0.

6.3.2 Time evolution matrix

Given an initial state $\psi(0)$, the equation $\dot{\psi}(t) = A(t)\psi(t)$ determines the state $\psi(t)$ at any subsequent time. For instance if t is small, then

$$\psi(t) = (1 + A(0)\, t)\psi(0) + \mathcal{O}(t^2). \tag{392}$$

To get the state after a longer time we could compose time evolution over several short times.

$$\psi(t) = \lim_{n\to\infty} (1 + A((n-1)t/n))(1 + A((n-2)t/n)) \dots (1 + A(t/n))(1 + A(0))\psi(0) \tag{393}$$

We will give an alternate formula shortly, but for now we notice that since the equation is linear, $\psi(t)$ must depend linearly on the initial state, i.e.,

$$\psi(t) = \begin{pmatrix} x(t) \\ p(t) \end{pmatrix} = U(t,0) \begin{pmatrix} x(0) \\ p(0) \end{pmatrix} = U(t,0)\psi(0), \tag{394}$$

where $U(t,0)$ is a 2×2 time evolution matrix.

• For n degrees of freedom we again have $\dot{\psi} = A(t)\psi(t)$ where the $2n \times 2n$ matrix $A(t) = \begin{pmatrix} 0 & m^{-1} \\ -k & 0 \end{pmatrix}$ is block off diagonal and traceless and we may write $\psi(t) = U(t,0)\psi(0)$. $U(t,0)$ satisfies the same 1st order ODE as $\psi(t)$

$$AU(t,0)\psi(0) = \dot{\psi} = \dot{U}(t,0)\psi(0) \quad \forall \quad \psi(0) \quad \Rightarrow \quad \dot{U}(t,0) = A(t)U(t,0). \tag{395}$$

with the initial condition $U(0,0) = I$. Of course, there is nothing special about $t = 0$ and one defines

$$\psi(t) = U(t,t')\psi(t') \quad \text{for any} \quad t \geq t'. \tag{396}$$

It is convenient to combine the ODE and initial condition into an integral equation

$$U(t,0) = I + \int_0^t A(t')U(t',0)\, dt' \tag{397}$$

Notice that this is similar to the equation for the time evolution operator in quantum mechanics $i\hbar\dot{U}(t,0) = H(t)U(t,0)$ where $H(t)$ is the hamiltonian. As in QM, from its definition ($\psi(t) = U(t,t')\psi(t')$), U satisfies a composition law or reproducing property (alternatively, one checks that both the LHS and RHS satisfy the same differential equation $\frac{d}{dt}U = A(t)U$, and initial condition.)

$$U(t,t'') = U(t,t')U(t',t'') \quad \text{for any} \quad t \geq t' \geq t''. \tag{398}$$

• However, there are some differences as well. Unlike the hermitian hamiltonian $H(t)$ in QM, the matrix $A(t)$ is not hermitian in general. However, it is traceless. Using this, one may show that unlike in QM where $U(t)$ is *unitary*, here $U(t)$ is *unimodular* (i.e. of determinant one) under time evolution. Physically, we know that hamiltonian evolution, (even by a time-dependent hamiltonian) defines a canonical transformation. The time evolution matrix defines linear CTs on phase space. By Liouville's theorem, these CTs must preserve the volume element on phase space, which means U must have unit determinant. (For one degree of freedom, it is shown in the problem set that a linear canonical transformation is an element of the group $\mathrm{SL}_2(\mathbb{R})$).

• Proving $\det U = 1$ is easy when A is time-independent. Then $U(t,0) = e^{tA}$ and $\log\det U = \mathrm{tr}\,\log e^{tA} = \mathrm{tr}\,(tA) = 0$. When A is time-dependent, we have for short times,

$$U(t,0) = I + \int_0^t A(t')dt' + \mathcal{O}(t^2). \tag{399}$$

Using $\det(I+\epsilon A) \approx 1 + \epsilon\,\mathrm{tr}\,A$ for small ϵ we get

$$\det U(t,0) \approx 1 + \int_0^t \mathrm{tr}\,A(t')dt' = 1 + \mathcal{O}(t^2). \tag{400}$$

We see that infinitesimal time-evolution preserves the unimodularity of U. For longer times, we write $U(t,t_0)$ as a product of several short-time evolutions and let the time-step go to zero:

$$U(t,t_0) = U(t,t_{n-1})U(t_{n-1},t_{n-2})\cdots U(t_2,t_1)U(t_1,t_0) \tag{401}$$

where, say $t_{i+1} - t_i = \Delta t = (t-t_0)/n$ is constant. Then defining $t_n \equiv t$, which is held fixed,

$$\det U(t,t_0) = \prod_{i=1}^n \det U(t_{i+1},t_i) = \prod_{i=1}^n (1+\mathcal{O}(\Delta t)^2) \to 1 \quad \text{as} \quad n\to\infty. \tag{402}$$

The unimodularity of $U(t,t')$ can also be established using the identity $\log\det U = \mathrm{tr}\,\log U$. One first shows that $\frac{d}{dt}\log\det U(t,0) = \mathrm{tr}\,\dot U U^{-1} = \mathrm{tr}\,A = 0$ and then uses the initial condition $\det U(0,0) = 1$ to conclude that $\det U(t,0) = 1$.

• By iterating the above integral equation, we get a series for the time-evolution operator

$$\begin{aligned} U(t,0) &= I + \int_0^t dt'\,A(t') + \int_0^t dt' A(t') \int_0^{t'} dt''\,A(t'') + \cdots \\ &= 1 + \sum_{n=1}^\infty \iiint_{t\ge t_1\ge t_2\ge\cdots t_n\ge 0} dt_1\cdots dt_n\,A(t_1)A(t_2)\cdots A(t_n) \\ &= \sum_{n=0}^\infty \frac{1}{n!}\int_0^t dt_1\cdots\int_0^t dt_n \mathcal{P}(A(t_1)\cdots A(t_n)) \equiv \mathcal{P}\exp\int_0^t A(t')dt' \end{aligned} \tag{403}$$

In the last line we extended the integrals from simplices $t \ge t_1 \ge \cdots \ge t_n \ge 0$ to the full hypercube $[0,t]^n$ by dividing by $n!$, but made sure the matrices $A(t_i)$ in the product are ordered with 'younger ones to the right'. This expression is called the time- or path-ordered exponential, denoted symbolically by $\mathcal{P}\exp$. Note that in general, it is not the exponential of $\int A(s)\,ds$, though it reduces to this if A is time independent or if the matrices $A(s)$ commute at

distinct times. If $A(t)$ is uniformly bounded, i.e., if the largest eigenvalue of A is bounded above by some constant Λ for all times in the interval $[0,t]$, then the norm of this sum of operators is dominated by a constant multiple of the exponential series $\sum(\Lambda t)^n/n! = e^{\Lambda t}$, and is therefore absolutely convergent. In general

$$U(t,t') = \sum_{n=0}^{\infty} \frac{1}{n!} \int_t^{t'} dt_1 \cdots \int_t^{t'} dt_n \mathcal{P}\left(A(t_1)\cdots A(t_n)\right) \equiv \mathcal{P}\exp\int_t^{t'} A(s)\, ds. \tag{404}$$

• A virtue of $U(t,t')$ is that its columns are solutions of the original equation $\dot{\psi} = A(t)\psi(t)$, as is easily seen from $\dot{U}(t,t') = A(t)U(t)$. Since $\det U \neq 0$, the columns of U are a complete set of $2n$ linearly independent solutions to the equation for small oscillations. So U is called the fundamental matrix solution. Every solution of $\dot{\psi} = A(t)\psi$ is a linear combination of the columns of U.

6.3.3 Monodromy matrix

• So far, we have not used the T-periodicity of $A(t)$. We are especially interested in the behavior of U after one period, i.e., $U(t+T,t)$. The reproducing formula says in particular that

$$U(t+T,0) = U(t+T,t)U(t,0). \tag{405}$$

The operator $U(t+T,t)$ advances a solution by one period of the unperturbed q_0

$$\psi(t+T) = U(t+T,t)\psi(t). \tag{406}$$

What is more, by periodicity of A, it follows that $U(t+T,t)$ is independent of t, since the above time-ordered exponential series for $U(t+T,t)$ only involves integrals of A over a complete period. So we may unambiguously denote $U(t+T,t)$ by $M(T)$, which is also called the monodromy matrix

$$M(T) = U(t+T,t) = \mathcal{P}\exp\int_0^T A(s)\, ds. \tag{407}$$

Being a special case of the time evolution operator, $\det M = 1$. So $\psi(t+T) = M\psi(t)$. In other words, the solution need not be periodic, but is periodic up to multiplication by a unimodular matrix. This is one of the main results of Floquet's theory. It finds application in Bloch's analysis of the energy eigenfunctions of an electron in a 1D periodic potential, which underpins the band theory of electrons in a crystal.

6.3.4 Stability of periodic solution

• Long-term stability of the original periodic solution $q_0(t)$ is related to the spectrum of M. After one period T of the unperturbed motion, the initial perturbation $\psi(0)$ becomes $\psi(T) = M\psi(0)$. After n time periods, $\psi(nT) = M^n\psi(0)$. For long-term stability, we would want $\psi(nT)$ to remain bounded as $n \to \infty$ for any choice of $\psi(0)$. This puts restrictions on the monodromy matrix M. M is a real matrix with unit determinant, it defines a finite linear canonical transformation. To determine M explicitly for given $A(t)$ is usually quite hard (the time-ordered exponential gives a series for M), but a lot can be said about the qualitative nature of the motion, if the spectrum of M is known.

• Let us consider the simplest example of one degree of freedom, where M is a 2×2 matrix with product of eigenvalues $\lambda_1 \lambda_2 = 1$. There are various cases to consider, and the analysis is simplest in a basis in which M is either diagonal or takes a canonical form.

• If the eigenvalues are **real and unequal**, then M is diagonalizable via a similarity transformation $S^{-1}MS = D$ where $D = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda^{-1} \end{pmatrix}$. The eigenvalues must both have the same sign. One of the eigenvalues is necessarily larger than 1 in magnitude, say $1/\lambda$. An initial state $\psi(0)$ that has a component in the direction of the corresponding eigenvector will grow exponentially with time since $D^n = \begin{pmatrix} \lambda^n & 0 \\ 0 & \lambda^{-n} \end{pmatrix} \to \begin{pmatrix} 0 & 0 \\ 0 & \pm\infty \end{pmatrix}$ as $n \to \infty$. So if the monodromy matrix has real and distinct eigenvalues, the periodic solution $q_0(t)$ is in general unstable over long times.

• If the eigenvalues are **real and equal** $\lambda_1 = \lambda_2 = 1$, or $\lambda_1 = \lambda_2 = -1$ then M in general cannot be diagonalized, though it is similar to a Jordan matrix $S^{-1}MS = J = \begin{pmatrix} 1 & c \\ 0 & 1 \end{pmatrix}$ or $J = \begin{pmatrix} -1 & c \\ 0 & -1 \end{pmatrix}$ and $J^n = \begin{pmatrix} 1 & nc \\ 0 & 1 \end{pmatrix}$ or $J^n = (-1)^n \begin{pmatrix} 1 & -nc \\ 0 & 1 \end{pmatrix}$. Working in the Jordan basis, we see that a perturbation that initially has a component in the second direction, grows linearly with time ($t = nT$) if $c \neq 0$. So if $M \neq \pm I$ has coincident real eigenvalues, then the periodic solution is linearly unstable in general. It is stable if $M = \pm I$.

• If M has a **non-real** eigenvalue, then both eigenvalues must be non-real and complex conjugates of each other ($\lambda \neq \bar{\lambda}$), since the characteristic equation has real coefficients. Moreover $|\lambda|^2 = \lambda\bar{\lambda} = \det M = 1$, so the eigenvalues have unit absolute values. Let $\lambda = e^{i\theta} = a + ib$ with $a = \Re\lambda, b = \Im\lambda$ and $a^2 + b^2 = 1$. Since it has distinct eigenvalues, M may be diagonalized by a non-real similarity transformation $S^{-1}MS = D = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}$ and $D^n = \begin{pmatrix} e^{in\theta} & 0 \\ 0 & e^{-in\theta} \end{pmatrix}$. It is clear that the matrix elements do not grow in magnitude, so we expect stability. However, x, p are real, and M cannot be diagonalized by a real similarity transformation. However, it may be brought by a similarity transformation to the real Jordan form $J = \begin{pmatrix} a & b \\ -b & a \end{pmatrix}$ with $a^2 + b^2 = 1$. So we may write $a = \cos\theta, b = \sin\theta$. Then $J = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$ is just a rotation in the phase plane and $J^n = \begin{pmatrix} \cos n\theta & \sin n\theta \\ -\sin n\theta & \cos n\theta \end{pmatrix}$ is also a rotation. It is clear that perturbations do not grow in size if the eigenvalues of M are non-real. If $\theta = 2\pi(p/q)$ is a rational multiple of 2π (with the g.c.d. $(p, q) = 1$), then the perturbation $\psi(t)$ is periodic with period qT.

• Thus the eigenvalues of the monodromy matrix determine the stability of the unperturbed periodic trajectory $q_0(t)$. If the eigenvalues are non-real or $M = \pm I$, we have stability, perturbations remain bounded. Otherwise, if the eigenvalues are real and equal, then generic perturbations grow linearly. If the eigenvalues are real and unequal then generic perturbations grow exponentially.

6.4 Chaotic oscillations of a double pendulum

6.4.1 Poincare sections for double pendulum

• The phase space of the double pendulum is 4-dimensional, with coordinates $\theta_1 \in S^1, \theta_2 \in S^1, p_1, p_2 \in \mathbb{R}$. The phase space is the cartesian product of a torus and a plane $\mathbb{T}^2 \times \mathbb{R}^2$. It is difficult to visualize trajectories in this space. Of course, we know energy is conserved, so the trajectory must lie on a constant energy 3D sub-manifold of phase space determined by initial conditions.

• The constant energy $H = E$ sub-manifold of phase space is a compact (bounded and closed) 3D manifold. $\theta_{1,2} \in S^1$ are always bounded, and on a constant energy sub-manifold, $|p_1|$ and $|p_2|$ are also bounded. To see this, we first notice that the potential energy is bounded both above and below $-3mgl \leq V \leq 3mgl$. Thus for fixed E, the kinetic energy is also bounded both above and below: $0 \leq \max(0, E - 3mgl) \leq T \leq E + 3mgl$. Now one uses the fact that T is bounded above to argue that $|p_1|$ and $|p_2|$ are also bounded above

$$|T| = T = \frac{1}{2ml^2(1+s_{12}^2)} \left[p_1^2 + 2p_2^2 - 2c_{12}p_1p_2\right] \geq \frac{1}{4ml^2} \left[p_1^2 + 2p_2^2 - 2|p_1||p_2|\right] \tag{408}$$

Here we replaced $(1 + s_{12}^2)$ by the larger quantity 2 and subtracted the larger quantity $2|p_1||p_2|$ instead of $2p_1p_2c_{12}$. This may be expressed as a sum of two squares

$$E + 3mgl \geq T \geq \frac{1}{4ml^2} \left[(|p_1| - |p_2|)^2 + p_2^2\right]. \tag{409}$$

Therefore $|p_2|$ is bounded above and so is $|p_1| - |p_2|$. It follows that both $|p_1|$ and $|p_2|$ are bounded above. Thus any constant energy submanifold occupies a bounded region of phase space and the trajectory explores it.

• However, it is still difficult to plot or visualize trajectories in a 3D manifold. A Poincare section is a 2D slice through a constant energy sub-manifold. For example, we could choose a Poincare section corresponding to $\theta_1 = 0$, i.e., focus on those instants when the first bob hangs vertically downward. This section intersects the constant energy manifold on a 2D surface that may be parametrized by θ_2, p_2 (very roughly, the 'phase space' of the second bob). The fourth coordinate p_1 at any point on this section is fixed by the condition $H(\theta_1 = 0, \theta_2, p_1, p_2) = E$. Now each point (θ_2, p_2) where the trajectory intersects the Poincare section, is marked with a dot. Thus, for fixed initial conditions (and energy) one gets a picture of the set of points on the Poincare section where the trajectory intersected it.

• A Poincare section can convey a lot of qualitative information on the nature of the dynamics. For instance, if there is a second conserved quantity Q, independent of the energy H, then the trajectory must lie on the 2D surface on which the constant H and constant Q manifolds intersect. This 2D surface generically intersects the Poincare slice along a 1D curve. So if there is a 2^{nd} conserved quantity, we expect the points on a Poincare section to lie along a 1D curve (or union of curves). If Q is 'nearly conserved', then we would expect the points in a Poincare section to be concentrated in a neighborhood of 1D curves. If there is no additional conserved quantity, then points on the Poincare slice are expected to fill out 2D regions rather than be concentrated along curves. In all cases, since the constant energy hyper surface is compact, the points in a Poincare section must lie in a bounded region.

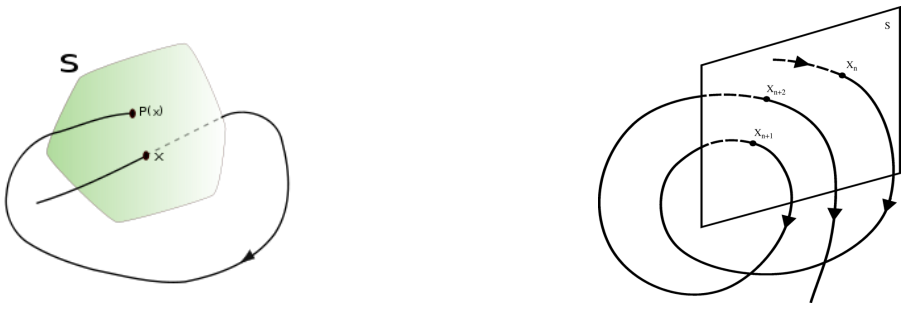
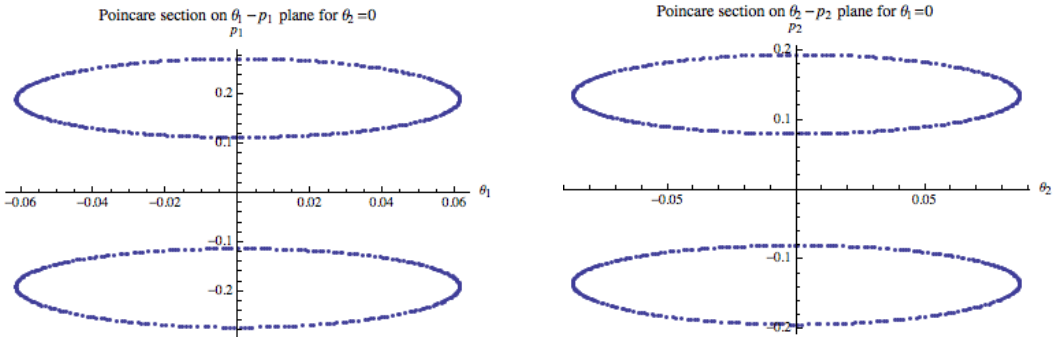


Figure 5: Poincare section: points where a trajectory intersects the 2D Poincare slice are marked. These two figures are from http://en.wikipedia.org/wiki/Poincare_map and http://www.unice.fr/DeptPhys/sem6/2011-2012/PagesWeb/PT/Pendule/En/more3.html



(a) 588 points for $t < 1000$ on θ_1-p_1 plane when $\theta_2 = 0$

(b) 588 points for $t < 1000$ on θ_2-p_2 plane when $\theta_1 = 0$

Figure 6: Poincare sections for double pendulum in small angle approximation: $m = 1, l = 1, g = 1, \theta_1(0) = \pi/15, \theta_2(0) = -\pi/15, \dot{\theta}_1(0) = \dot{\theta}_2(0) = 0$, $E = 0.0658$. On the left, the lower oval corresponds to $\dot{\theta}_2 > 0$ and the upper oval to $\dot{\theta}_2 < 0$. The points lie on a curve indicating the presence of a second conserved quantity and absence of chaos.

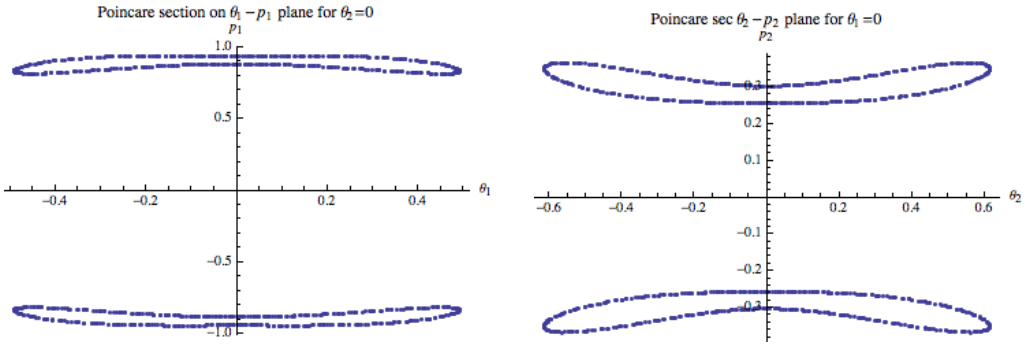
• **Small oscillations of a double pendulum:** Numerically obtained points on Poincare sections are shown in fig. 6.4.1. The points on the Poincare section lie along 1d curves. This indicates there is a **second conserved quantity** other than total energy. Indeed, we already found two conserved quantities for small oscillations, the energies of the two normal modes:

$$E_+ = \frac{1}{2}ml^2\left[\dot{\xi}_+^2 + \omega_+^2\xi_+^2\right] \quad \text{and} \quad E_- = \frac{1}{2}ml^2\left[\dot{\xi}_-^2 + \omega_-^2\xi_-^2\right]. \tag{410}$$

The conserved total energy $E = 2\lambda_+E_+ + 2\lambda_-E_-$ is a weighted sum of these two conserved quantities ($\lambda_\pm = 2 \pm \sqrt{2}$). Though the motion is not periodic (only quasi-periodic), small oscillations of our double pendulum are fairly regular, there is no sign of chaos.

• As energy is increased and oscillations become larger, $E_\pm$ are no longer exactly conserved, though total energy is always conserved. For relatively low energies, Poincare sections are still concentrated near deformed 1D curves indicating that $E_\pm$ are approximately conserved.

• **Onset of chaos:** As the energy is increased to intermediate values, the motion becomes



(a) 921 points on θ_1-p_1 plane when $\theta_2 = 0$ (b) 921 points on θ_2-p_2 plane when $\theta_1 = 0$

Figure 7: Double pendulum $m = 1, l = 1, g = .5, \theta_1(0) = \pi/3, \theta_2(0) = -\pi/3, \dot{\theta}_1(0) = \dot{\theta}_2(0) = 0$, $E = -0.75$

increasingly irregular and chaotic. Energy is the lone conserved quantity, points on Poincare sections fill up 2D regions. This is shown in the figures of Poincare sections for various initial conditions and energies. This onset of chaos can be studied in detail both analytically and numerically and forms an interesting branch of physics. One first studies the immediate neighborhood of integrable dynamics (small departure from small oscillations) using perturbation theory. This leads to the concept of invariant tori (which is a replacement for conserved quantities even when the latter cease to exist). The invariant tori are invariant manifolds for the dynamics (trajectories stay on them) which separate regions of possibly chaotic motion ('islands of regularity separating regions of chaos'). As we move farther away from integrability, the invariant tori dissolve. For the double pendulum, the last invariant torus to dissolve is a 'golden' torus (related to the golden ratio). Eventually the trajectories can fill up the whole of the constant energy hyper-surface and the motion can become ergodic (trajectories spending equal times in equal volume regions of the constant energy submanifold). This passage from integrability to chaos is the subject of the Kolmogorov-Arnold-Moser (KAM) theory.

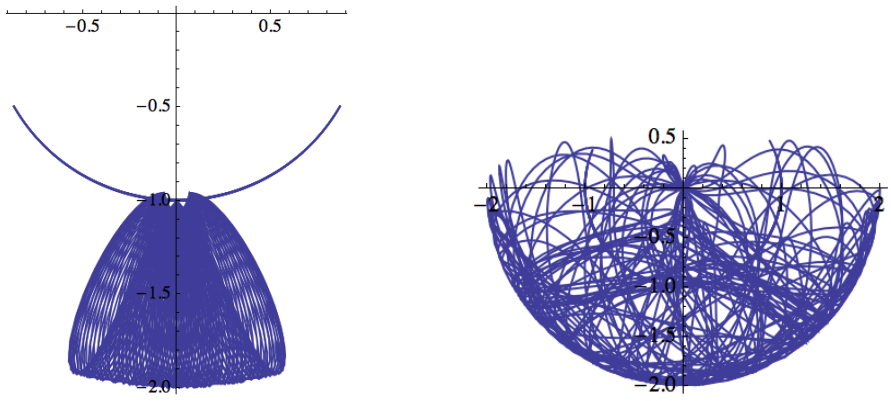
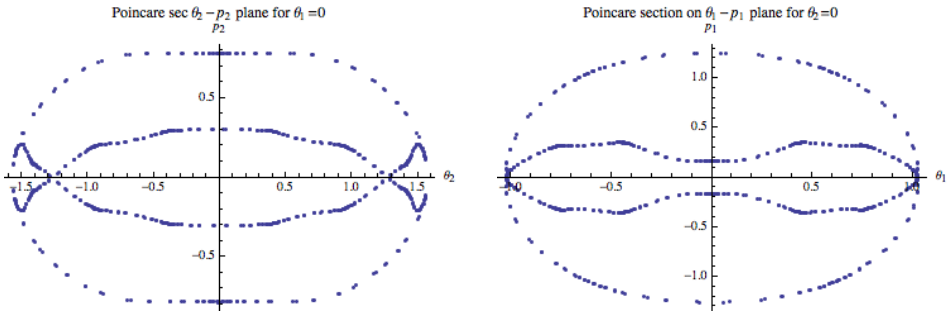


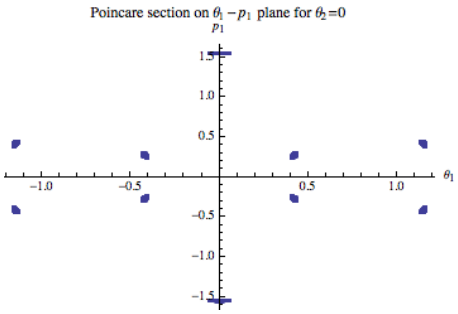
Figure 8: Curves traced out by two bobs of a double pendulum over a significant length of time. The bobs both move on the plane of the paper. The pendulum is suspended from the point $(0, 0)$. Left: Relatively low energy oscillation showing some regularity. Right: Intermediate energy oscillation showing onset of chaos. The 'upper' bob is constrained to lie on the 'upper' circle of radius $l = 1$ centered at the pivot (located at the origin), though its trajectory along this circle can be quite irregular. The curve traced out by the 'lower' bob is much more complicated.



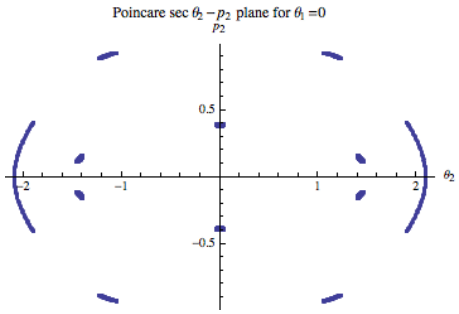
(a) 609 points on θ_1-p_1 plane when $\theta_2 = 0$

(b) 610 points on θ_2-p_2 plane when $\theta_1 = 0$

Figure 9: Double pendulum $m = 1, l = 1, g = .5, \theta_1(0) = 0, \theta_2(0) = \pi/2, \dot{\theta}_1(0) = \dot{\theta}_2(0) = 0,\ E = -1$.

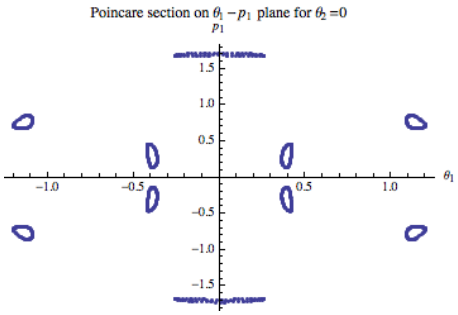


(a) 698 points on θ_1-p_1 plane when $\theta_2 = 0$

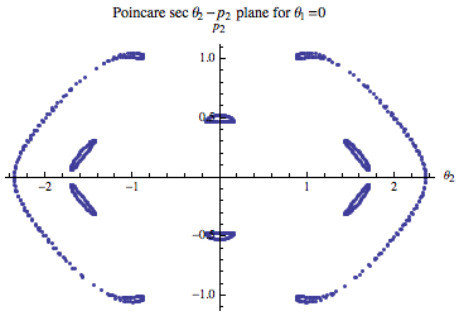


(b) 972 points on θ_2-p_2 plane when $\theta_1 = 0$

Figure 10: Double pendulum $m = 1, l = 1, g = .5, \theta_1(0) = 0, \theta_2(0) = 2\pi/3, \dot{\theta}_1(0) = \dot{\theta}_2(0) = 0$, $E = -0.75$.

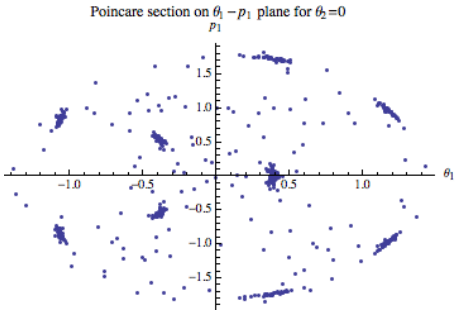


(a) 681 points on θ_1-p_1 plane when $\theta_2 = 0$

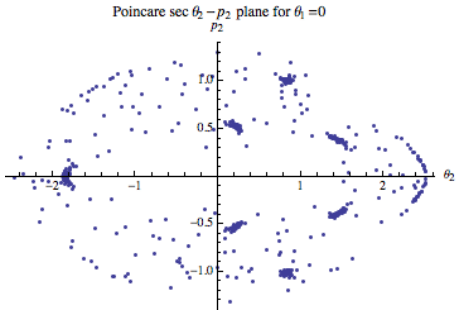


(b) 810 points on θ_2-p_2 plane when $\theta_1 = 0$

Figure 11: Double pendulum $m = 1, l = 1, g = .5, \theta_1(0) = 0, \theta_2(0) = 3\pi/4, \dot{\theta}_1(0) = \dot{\theta}_2(0) = 0$, $E = -0.6464$.

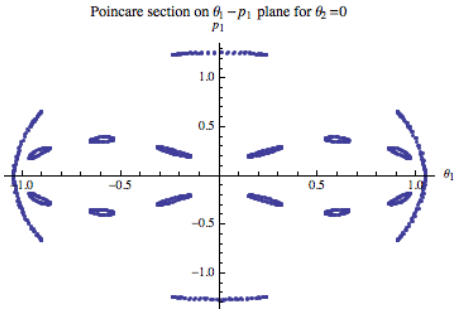


(a) 486 points on θ_1-p_1 plane when $\theta_2 = 0$

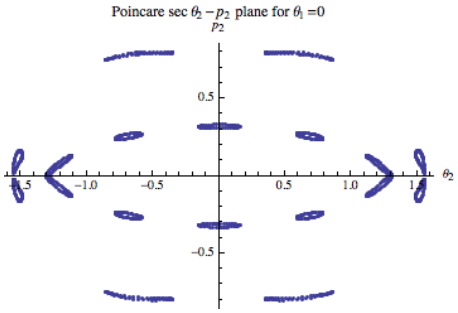


(b) 497 points on θ_2-p_2 plane when $\theta_1 = 0$

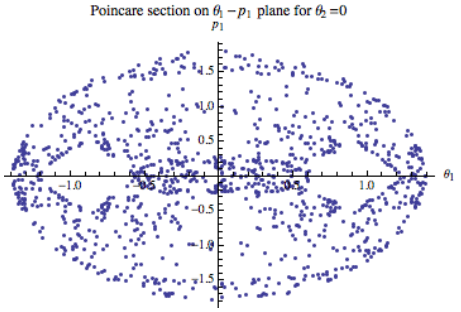
Figure 12: Double pendulum $m = 1, l = 1, g = .5, \theta_1(0) = 0, \theta_2(0) = 4\pi/5, \dot{\theta}_1(0) = \dot{\theta}_2(0) = 0$, $E = -0.595$.



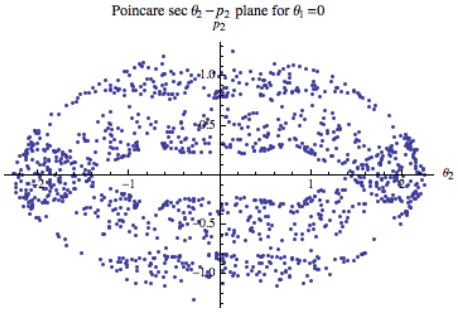
(a) 1072 pts on θ_1-p_1 plane, $\theta_2 = 0$



(b) 1072 pts on θ_2-p_2 plane, $\theta_1 = 0$

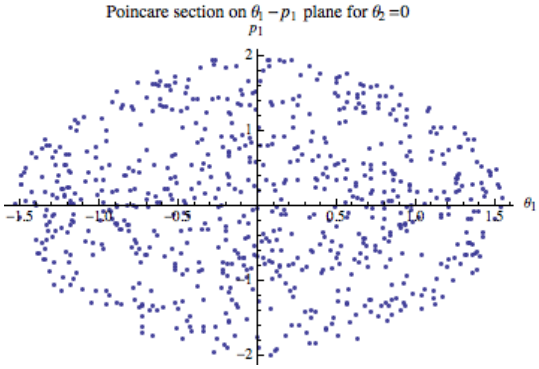


(c) 1125 pts on θ_1-p_1 plane, $\theta_2 = 0$

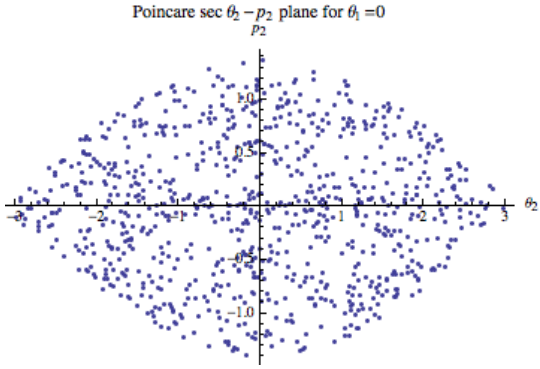


(d) 1196 pts on θ_2-p_2 plane, $\theta_1 = 0$

Figure 13: Double pendulum $m = 1, l = 1, g = .5$, $\theta_2(0) = 0, \dot{\theta}_1(0) = \dot{\theta}_2(0) = 0$. (a) and (b): $\theta_1(0) = \pi/3$, $E = -1$. (c) and (d): $\theta_1(0) = 4\pi/9$, $E = -0.6736$.



(a) 729 points on θ_1-p_1 plane when $\theta_2 = 0$



(b) 854 points on θ_2-p_2 plane when $\theta_1 = 0$

Figure 14: Double pendulum $m = 1, l = 1, g = .5, \theta_1(0) = \pi/2, \theta_2(0) = 0, \dot{\theta}_1(0) = \dot{\theta}_2(0) = 0$, $E = -0.5$.

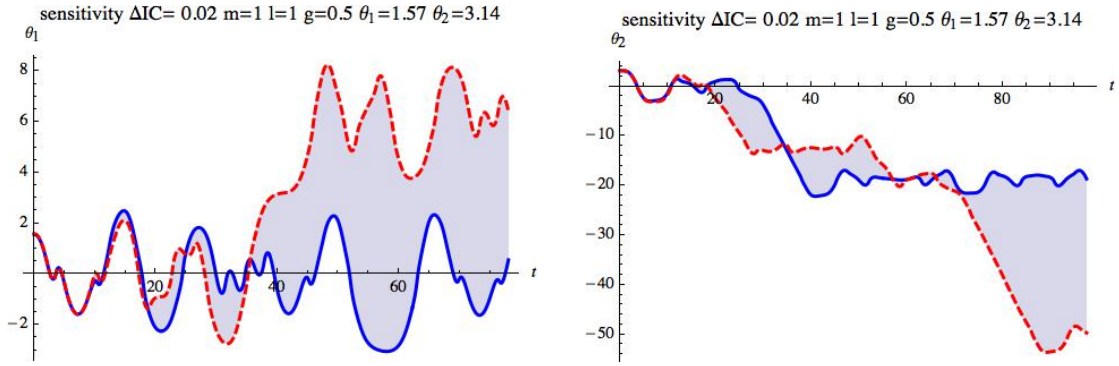
• At very high energies, the Poincare sections again become simpler and are concentrated along 1D curves. A new conserved quantity emerges. Most of the energy is kinetic since the gravitational potential energy is bounded between $\pm 3mgl$, and is negligible. We may ignore the gravitational force, so there is no external torque. Total angular momentum is conserved as $E \to \infty$:

$$\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2 = ml^2 \left[2\dot{\theta}_1 + \dot{\theta}_2 + 2c_{12}(\dot{\theta}_1 + \dot{\theta}_2) \right] \hat{z}. \tag{411}$$

As $E \to \infty$, the two bobs go round in nearly uniform circular motion: dynamics is again regular at high energies!

6.4.2 Sensitivity to initial conditions

• A hallmark of chaos is sensitivity to initial conditions. This means that two trajectories with slightly differing initial conditions could get quite far apart and display qualitatively different behavior. This feature makes chaotic systems behave quite unpredictably. The double pendulum displays sensitive dependence on initial conditions for energies that are neither too high nor too low. We illustrate this in the following figures which show various dynamical variables like angles/positions/momenta of the bobs as a function of time (obtained numerically) for two nearby initial conditions. The parameters used are $m = l = 1, g = .5$. The initial conditions for the blue trajectory are $\theta_1(0) = \pi/2, \theta_2(0) = \pi, \dot{\theta}_1(0) = \dot{\theta}_2(0) = 0$ while those for the red trajectory is $\theta_1(0) = \pi/2 + \delta$ where $\delta = 0.02$. This corresponds to about a 1% change in initial conditions. We can see from the plots that the trajectories do not remain nearby as time progresses. The shaded region encloses the difference between the dynamical variables and it is sometimes seen to be as large as it can be.

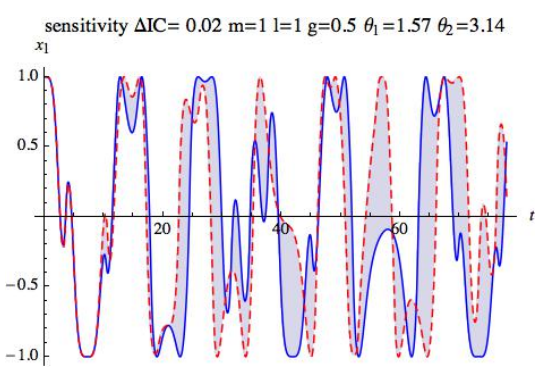


(a) $\theta_1(t)$ for two nearby IC

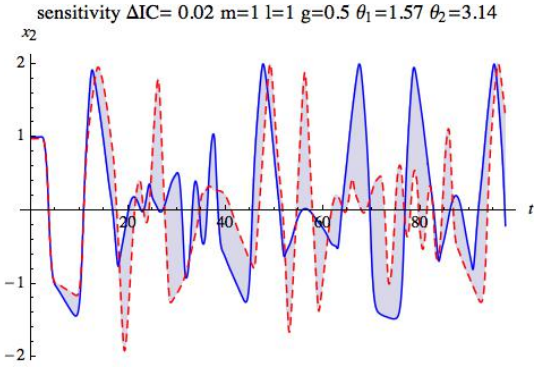
(b) $\theta_2(t)$ for two nearby IC

Figure 15: Double pendulum: sensitivity to IC, deflection angles of bobs. Initial angles for red trajectory are $\Delta IC = .02$ more than for blue trajectory. Initial $\dot{\theta}_1, \dot{\theta}_2 = 0$. Natural time scale $T = 2\pi\sqrt{l/g} = 8.9$.

• Trajectories do not remain nearby with time. Shaded region encloses the difference between angles. It is sometimes maximal (an odd multiple of π).

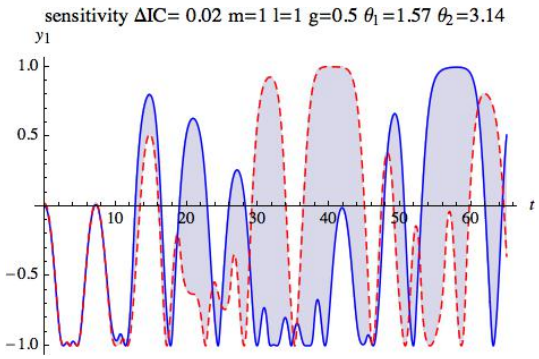


(a) $x_1(t)$ for two nearby IC

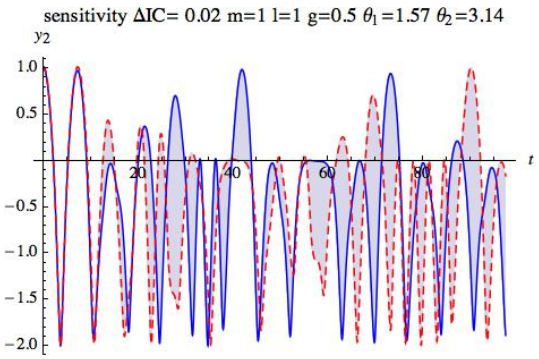


(b) $x_2(t)$ for two nearby IC

Figure 16: Double pendulum: sensitivity to IC, horizontal displacements of bobs. Initial angles for red trajectory are $\Delta IC = .02$ more than for blue trajectory. Initial $\dot{\theta}_1, \dot{\theta}_2 = 0$. Natural time scale $T = 2\pi\sqrt{l/g} = 8.9$.

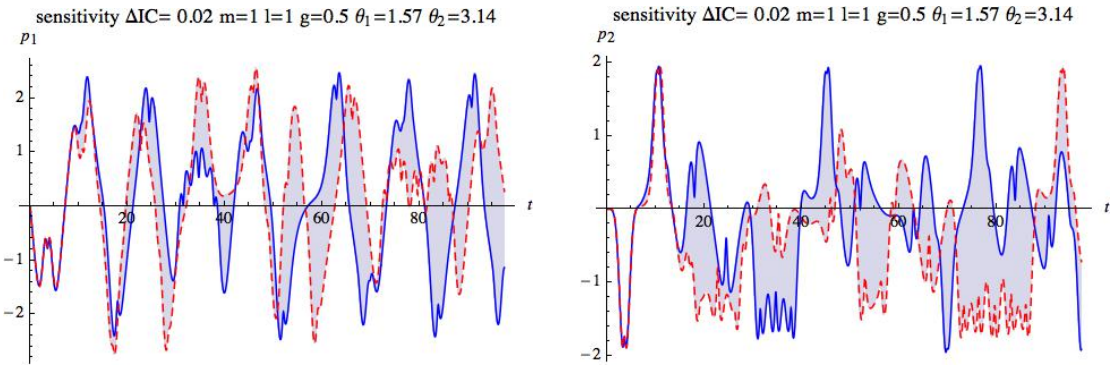


(a) $y_1(t)$ for two nearby IC



(b) $y_2(t)$ for two nearby IC

Figure 17: Double pendulum: sensitivity to IC, heights of bobs. Initial angles for red trajectory are $\Delta IC = .02$ more than for blue trajectory. Initial $\dot{\theta}_1, \dot{\theta}_2 = 0$. Natural time scale $T = 2\pi\sqrt{l/g} = 8.9$.



(a) $p_1(t)$ for two nearby IC

(b) $p_2(t)$ for two nearby IC

Figure 18: Double pendulum: sensitivity to IC, momenta of bobs. Initial angles for red trajectory are $\Delta IC = .02$ more than for blue trajectory. Initial $\dot{\theta}_1, \dot{\theta}_2 = 0$. Natural time scale $T = 2\pi\sqrt{l/g} = 8.9$.