

Classical Mechanics

Hamiltonian Mechanics

- ➡ **Generalized Momenta**
- ➡ **Hamilton's Equations**
- ➡ **Phase Space**
- ➡ **Liouville's Theorem**
- ➡ **The Virial Theorem**

Generalized Momenta

Consider the motion of a single particle moving in one dimension
the kinetic energy is

$$T = \frac{1}{2} m \dot{x}^2$$

m \rightarrow the mass of the particle

x \rightarrow its displacement

the particle's linear momentum is

$$p = m \dot{x}$$

This can also be written as

$$p = \frac{\partial T}{\partial \dot{x}} = \frac{\partial \mathcal{L}}{\partial \dot{x}}$$

because $\mathcal{L} = T - U$ and the potential energy U is independent of \dot{x}

Generalized Momenta (cont'd)

Consider a dynamical system described by \mathcal{F} generalized coordinates q_i
(for $i = 1, \dots, \mathcal{F}$)

By analogy with our previous discussion

⇓

we can define generalized momenta of the form

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$$

p_i is sometimes called the momentum conjugate to the coordinate q_i

Lagrange's equation

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i} \right) - \frac{\partial \mathcal{L}}{\partial q_i} = 0$$

can be re-written as

$$\frac{dp_i}{dt} = \frac{\partial \mathcal{L}}{\partial q_i}$$

Note that a generalized momentum
does not necessarily have the dimensions of linear momentum

Generalized Momenta (cont'd)

Suppose that the Lagrangian \mathcal{L} does not depend explicitly on some coordinate q_k

↓

$$\frac{dp_k}{dt} = \frac{\partial \mathcal{L}}{\partial q_k} = 0$$

↓

$$p_k = \text{const.}$$

The coordinate q_k is said to be ignorable in this case

CONCLUSION

the generalized momentum associated with an ignorable coordinate
is a constant of the motion

EXAMPLE

The Lagrangian for a particle moving in a central potential
is independent of the angular coordinate θ

↓

θ ↗ is an ignorable coordinate

$$p_\theta = \frac{\partial \mathcal{L}}{\partial \dot{\theta}} = m r^2 \dot{\theta} \text{ is a constant of the motion}$$

Of course ↗ p_θ is the angular momentum about the origin
which is conserved because a central force exerts no torque about the origin

Hamilton's Equations

Consider a dynamical system with \mathcal{F} degrees of freedom described by the generalized coordinates $q_i \Leftrightarrow i = 1, \dots, \mathcal{F}$
Suppose that neither T nor U depend explicitly on the time t

In conventional dynamical systems

- ✓ the potential energy is generally independent of the \dot{q}_i
- ✓ the kinetic energy takes the form of a homogeneous quadratic function of the \dot{q}_i

$$T = \sum_{i,j=1,\mathcal{F}} m_{ij} \dot{q}_i \dot{q}_j$$

$\Rightarrow m_{ij}$ depends on the q_i but not on the \dot{q}_i

\Downarrow

$$\sum_{i=1,\mathcal{F}} \dot{q}_i \frac{\partial T}{\partial \dot{q}_i} = 2T$$

The generalized momentum conjugate to the i th generalized coordinate is

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i} = \frac{\partial T}{\partial \dot{q}_i}$$

- ✓ $\mathcal{L} = T - U$ is the Lagrangian of the system
- ✓ U is independent of the \dot{q}_i

Hamilton's Equations (cont'd)

Consider the function

$$H = \sum_{i=1, \mathcal{F}} \dot{q}_i p_i - \mathcal{L} = \sum_{i=1, \mathcal{F}} \dot{q}_i p_i - T + U$$

If all of the conditions discussed above are satisfied

↓

$$H = T + U$$

In other words \Rightarrow the function H is equal to the total energy of the system

Consider the variation of the function H

$$\delta H = \sum_{i=1, \mathcal{F}} \left(\delta \dot{q}_i p_i + \dot{q}_i \delta p_i - \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \delta \dot{q}_i - \frac{\partial \mathcal{L}}{\partial q_k} \delta q_k \right)$$

The first and third terms in the bracket cancel because $\Rightarrow p_i = \partial \mathcal{L} / \partial \dot{q}_i$

Now \Rightarrow Lagrange's equation can be written as $\dot{p}_i = \partial \mathcal{L} / \partial q_i$

↓

$$\delta H = \sum_{i=1, \mathcal{F}} (\dot{q}_i \delta p_i - \dot{p}_i \delta q_i) \quad (\clubsuit)$$

Hamilton's Equations (cont'd)

Suppose now \Rightarrow that we can express the total energy of the system H solely as a function of the q_i and the p_i \Rightarrow with no explicit dependence on the \dot{q}_i

In other words \Rightarrow suppose that we can write $H = H(q_i, p_i)$

When the energy is written in this fashion



it is generally termed the Hamiltonian of the system

The variation of the Hamiltonian function takes the form

$$\delta H = \sum_{i=1, \mathcal{F}} \left(\frac{\partial H}{\partial p_i} \delta p_i + \frac{\partial H}{\partial q_i} \delta q_i \right) \quad (\spadesuit)$$

A comparison of Eqs. (\clubsuit) and (\spadesuit) yields

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \quad \text{and} \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}$$

for $i = 1, \dots, \mathcal{F}$

These $2\mathcal{F}$ first-order differential equations are known as Hamilton's equations
Hamilton's equations are often a useful alternative to Lagrange's equations
which take the form of \mathcal{F} second-order differential equations

1D Harmonic Oscillator

Consider a one-dimensional harmonic oscillator
 The kinetic and potential energies of the system are written

$$T = (1/2) m \dot{x}^2 \quad \text{and} \quad U = (1/2) k x^2$$

x is the displacement

m is the mass

$k > 0$

The generalized momentum conjugate to x is

$$p = \frac{\partial T}{\partial \dot{x}} = m \dot{x} \Rightarrow T = \frac{1}{2} \frac{p^2}{m}$$

The Hamiltonian of the system takes the form

$$H = T + U = \frac{1}{2} \frac{p^2}{m} + \frac{1}{2} k x^2$$

Hamilton's equations yield

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m} \quad (\text{which is just a restatement of the kinetic energy})$$

$$\dot{p} = -\frac{\partial H}{\partial x} = -k x \quad (\text{Newton's second law of motion for the system})$$

Motion in a Central Potential

Consider a particle of mass m moving in the central potential $U(r)$

The kinetic energy is

$$T = \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\theta}^2)$$

$\Rightarrow (r, \theta) \Leftrightarrow$ are plane polar coordinates

The generalized momenta conjugate to r and θ are

$$p_r = \frac{\partial T}{\partial \dot{r}} = m \dot{r}$$

$$p_\theta = \frac{\partial T}{\partial \dot{\theta}} = m r^2 \dot{\theta}$$

\Downarrow

$$T = \frac{1}{2m} \left(p_r^2 + \frac{p_\theta^2}{r^2} \right)$$

The Hamiltonian of the system takes the form

$$H = \frac{1}{2m} \left(p_r^2 + \frac{p_\theta^2}{r^2} \right) + U(r)$$

Motion in a Central Potential (cont'd)

Hamilton's equations yield

$$\dot{r} = \frac{\partial H}{\partial p_r} = \frac{p_r}{m} \quad \text{and} \quad \dot{\theta} = \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{m r^2}$$

(which are just restatements of the generalized momenta)

$$\dot{p}_r = -\frac{\partial H}{\partial r} = \frac{p_\theta^2}{m r^3} - \frac{\partial U}{\partial r} \quad (F)$$

$$\dot{p}_\theta = -\frac{\partial H}{\partial \theta} = 0$$

The last equation implies that

$$\frac{p_\theta}{m} = r^2 \dot{\theta} = h \quad (\kappa)$$

$\Rightarrow h$ is a constant

This can be combined with Eq. (F) to give

$$\frac{\dot{p}_r}{m} = \ddot{r} = \frac{h^2}{r^3} - \frac{\partial V}{\partial r} \quad (\varkappa)$$

$$\Rightarrow V = U/m$$

Of course \Leftarrow Eqs. (κ) and (\varkappa) are the conventional equations of motion for a particle moving in a central potential

Motion in a Central Potential

Consider a particle of mass m moving in 2D in the central potential $U(r)$
 this is clearly a two degree of freedom dynamical system

The particle's instantaneous position is most conveniently specified



plane polar coordinates r and θ

these are our two generalized coordinates

The square of the particle's velocity can be written as

$$v^2 = \dot{r}^2 + (r \dot{\theta})^2$$

the Lagrangian of the system takes the form

$$\mathcal{L} = \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\theta}^2) - U(r)$$

$$\frac{\partial \mathcal{L}}{\partial \dot{r}} = m \dot{r} \qquad \frac{\partial \mathcal{L}}{\partial r} = m r \dot{\theta}^2 - dU/dr$$

$$\frac{\partial \mathcal{L}}{\partial \dot{\theta}} = m r^2 \dot{\theta} \qquad \frac{\partial \mathcal{L}}{\partial \theta} = 0$$

Motion in a Central Potential (cont'd)

Equations of motion \rightarrow Lagrange equations

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{r}} \right) - \frac{\partial \mathcal{L}}{\partial r} = 0 \quad \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\theta}} \right) - \frac{\partial \mathcal{L}}{\partial \theta} = 0$$

$$\frac{d}{dt} (m \dot{r}) - m r \dot{\theta}^2 + \frac{dU}{dr} = 0$$

$$\frac{d}{dt} (m r^2 \dot{\theta}) = 0$$

$$\ddot{r} - r \dot{\theta}^2 = -\frac{dV}{dr}$$

$$r^2 \dot{\theta} = h$$

$\rightarrow V = U/m$

$\rightarrow h = \text{constant}$

Phase Space

Recall that



The generalized coordinates q_j define an s dimensional configuration space with every point representing a state of the system

Likewise



The generalized momenta p_j define an s -dimensional momentum space representing a certain condition of motion of the system

Hamilton phase space ⇨ $2s$ dimensional space consisting of q_j and p_j which allows us to represent both the positions and the momenta of all particles

If the position and momenta of all the particles in a system are known (at a given time)



these quantities can be used as initial conditions ⇨ $(q_j(0), p_j(0))$



- ✍ the subsequent motion of the system is completely determined
- ✍ the representative point describing the system moves along a unique path phase

Phase Diagrams

State of motion of 1-dimensional oscillator is completely specified by 2 quantities

$$x(t) \text{ and } \dot{x}(t)$$

(two quantities needed because differential equation of motion is second order)

$x(t)$ and $\dot{x}(t)$ define coordinates of points in a 2-dimensional space



The Phase Space

In two dimensions the phase space is a phase plane
for general oscillator with n degrees of freedom \rightarrow $2n$ -dimensional phase space

- \rightarrow As the time varies the point $P(x, \dot{x})$ describing the state of the oscillating particle will move along a certain phase path in the phase plane
- \rightarrow For different initial conditions the motion will be described by different paths
- \rightarrow The totality of all phase paths constitutes the phase diagram of the oscillator

Phase Diagrams (cont'd)

simple harmonic oscillator

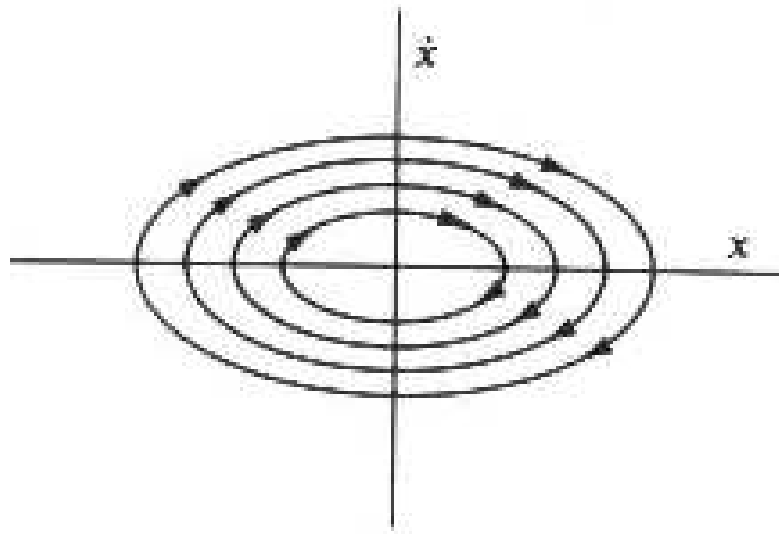
$$x(t) = A \sin(\omega_0 t - \delta)$$

$$\dot{x}(t) = A\omega_0 \cos(\omega_0 t - \delta)$$

Eliminating t

$$\frac{x^2}{A^2} + \frac{\dot{x}^2}{A^2\omega_0^2} = 1$$

This equation represents a family of ellipses



Phase Diagrams (cont'd)

Total Energy $E = kA^2/2$

Angular Frequency $\omega_0^2 = k/m$



$$\frac{x^2}{2E/k} + \frac{\dot{x}^2}{2E/m} = 1$$

Each phase path corresponds to a definite total energy of the oscillator

No two phase paths of the oscillator can cross!!!

If they could cross \rightarrow this would imply that for a given set of initial conditions the motion could proceed along different paths



This is impossible since the solution of the differential equation is unique

Statistical Mechanics

For complex systems with a large collection of particles → gas molecules



we are unable to identify the particular phase space point representing the system



we must devise some alternative approach to study the dynamics of such systems

One possibility is to fill the phase space with a collection of points
each representing a *possible* condition of the system



→ any of which could be the actual system

We imagine a large number of systems

→ each consistent with the known constraints

We are unable to discuss the details of the particles' motion in the actual system



we substitute a discussion of an ensemble of equivalent systems

Each representative point corresponds to a single system of the ensemble
the motion of a particular point represents the independent motion of that system

No two of the phase path may ever intersect!!!

Liouville's Theorem

THEOREM

– Joseph Liouville (1809-1882) –

The density of representative points in phase space corresponding to the motion of a system of particles remains constant during the motion



Define a density in phase ρ

- ✍ must be sufficiently large to contain a large number of representative points
- The volume elements of the phase space defining the density
- ✍ must be also sufficiently small so that the density varies continuously

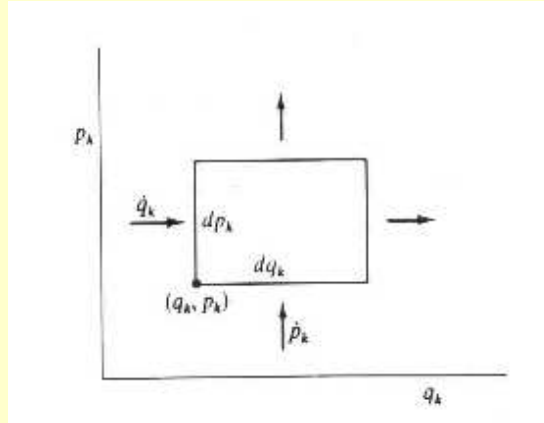
The number N of systems whose representative points lie within a volume dv is

$$N = \rho dv$$

- ✍ $dv = dq_1 dq_2 \dots dq_s dp_1 dp_2 \dots dp_s$
- ✍ s \rightarrow number of degrees of freedom in the ensemble

Liouville's Theorem (cont'd)

Consider an element of area in the $q_k - p_k$ plane in phase space



the number of representative points
moving across the left-hand edge into the area per unit time is

$$\rho \frac{dq_k}{dt} dp_k = \rho \dot{q}_k dp_k$$

and the number moving across the lower edge into the area per unit time is

$$\rho \frac{dp_k}{dt} dq_k = \rho \dot{p}_k dq_k$$

the total number of representative points
moving into the area $dq_k dp_k$ per unit time is

$$\rho(\dot{q}_k dp_k + \dot{p}_k dq_k)$$

Liouville's Theorem (cont'd)

By Taylor series expansion
the number of representative points moving out of the area per unit time is

$$\left[\rho \dot{q}_k + \frac{\partial}{\partial q_k} (\rho \dot{q}_k) dq_k \right] dp_k + \left[\rho \dot{p}_k + \frac{\partial}{\partial p_k} (\rho \dot{p}_k) dp_k \right] dq_k$$

the total increase in density in $dq_k dp_k$ per unit time is

$$\frac{\partial \rho}{\partial t} dq_k dp_k = - \left[\frac{\partial}{\partial q_k} (\rho \dot{q}_k) + \frac{\partial}{\partial p_k} (\rho \dot{p}_k) \right] dq_k dp_k$$

After dividing by $dq_k dp_k$ and summing this expression over all possible values of k

$$\frac{\partial \rho}{\partial t} + \sum_{k=1}^s \left(\frac{\partial \rho}{\partial q_k} \dot{q}_k + \rho \frac{\partial \dot{q}_k}{\partial q_k} + \frac{\partial \rho}{\partial p_k} \dot{p}_k + \rho \frac{\partial \dot{p}_k}{\partial p_k} \right) = 0$$

If the second partial derivatives of H are continuous \Rightarrow Hamilton's equations yield

$$\frac{\partial \dot{q}_k}{\partial q_k} + \frac{\partial \dot{p}_k}{\partial p_k} = 0$$

\Downarrow

$$\frac{\partial \rho}{\partial t} + \sum_{k=1}^s \left(\frac{\partial \rho}{\partial q_k} \frac{dq_k}{dt} + \frac{\partial \rho}{\partial p_k} \frac{dp_k}{dt} \right) = 0 \Rightarrow \frac{d\rho}{dt} = 0$$

The Virial Theorem

Consider a collection of particles whose position vectors \vec{r}_α and momenta \vec{p}_α are bounded
 ☞ i.e., remain finite at all times

Define a quantity

$$S \equiv \sum_{\alpha} \vec{p}_\alpha \cdot \vec{r}_\alpha$$

⇓

the time derivative of S is

$$\frac{dS}{dt} = \sum_{\alpha} (\vec{p}_\alpha \cdot \dot{\vec{r}}_\alpha + \dot{\vec{p}}_\alpha \cdot \vec{r}_\alpha)$$

⇓

The average value of dS/dt over a time interval τ is

$$\begin{aligned} \left\langle \frac{dS}{dt} \right\rangle &= \frac{1}{\tau} \int_0^\tau \frac{dS}{dt} dt \\ &= \frac{S(\tau) - S(0)}{\tau} \end{aligned}$$

The Virial Theorem (cont'd)

$$\left\langle \frac{dS}{dt} \right\rangle = \frac{S(\tau) - S(0)}{\tau}$$

If the system motion is periodic $\Rightarrow S(\tau) = S(0)$ and $\langle \dot{S} \rangle \rightarrow 0$ vanishes
 If the system does not exhibit any periodicity



we can make $\langle \dot{S} \rangle$ as small as desired by allowing $\tau \rightarrow \infty$



in this limit

$$\left\langle \sum_{\alpha} \vec{p}_{\alpha} \cdot \dot{\vec{r}}_{\alpha} \right\rangle = - \left\langle \sum_{\alpha} \dot{\vec{p}}_{\alpha} \cdot \vec{r}_{\alpha} \right\rangle \Rightarrow \left\langle 2 \sum_{\alpha} T_{\alpha} \right\rangle = - \left\langle \sum_{\alpha} \vec{F}_{\alpha} \cdot \vec{r}_{\alpha} \right\rangle$$

The sum over T_{α} is the total kinetic energy of the system

$$\langle T \rangle = -\frac{1}{2} \left\langle \sum_{\alpha} \vec{F}_{\alpha} \cdot \vec{r}_{\alpha} \right\rangle \quad (\mathfrak{V})$$

The rhs of Eq. (\mathfrak{V}) was called by Clausius (1822-1888) the virial of the system
The average kinetic energy of a system of particles is equal to its virial

The Virial Theorem (cont'd)

If the forces \vec{F}_α can be derived from potentials U_α

↓

$$\langle T \rangle = \frac{1}{2} \left\langle \sum_{\alpha} \vec{r}_{\alpha} \cdot \vec{\nabla} U_{\alpha} \right\rangle$$

If two particles interact according to a central power law force

$$F \propto r^n \Rightarrow U = kr^{n+1}$$

↓

$$\vec{r} \cdot \vec{\nabla} U = r \frac{dU}{dr} = k(n+1)r^{n+1} = (n+1)U$$

and the Virial Theorem becomes

$$\langle T \rangle = \frac{n+1}{2} \langle U \rangle$$

If the particles have gravitational interaction $\Rightarrow n = -2$

↓

$$\langle T \rangle = -\frac{1}{2} \langle U \rangle$$

Homework

☹ A particle moves in a circular orbit in a force field given by $F(r) = -k/r^2$
 Show that ☞ if k suddenly decreases to half its original value



the particle's orbit is parabolic

CLUES

☞ the potential energy decreases to half its former value

When $k \rightarrow k/2$

☞ the kinetic energy remains the same

Since the orbital is circular ☞ $T = \langle T \rangle$ and $U = \langle U \rangle$

For $F \propto 1/r^2$ ☞ the Virial Theorem states

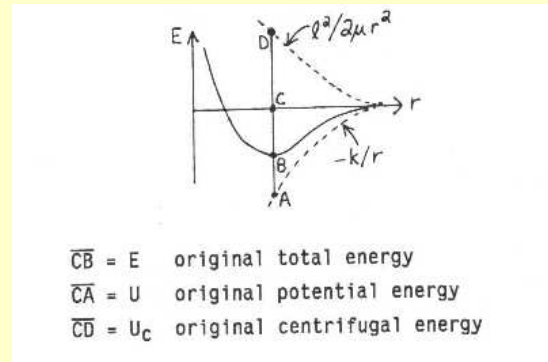
$$\langle T \rangle = -\frac{1}{2} \langle U \rangle$$



$$E = T + U = -\frac{1}{2}U + U = \frac{1}{2}U$$

Homework (cont'd)

Consider the energy diagram



The point B is obtained from $\overline{CB} = \overline{CA} - \overline{CD}$
 According to the Virial Theorem $\Rightarrow E = U/2 \rightarrow \overline{CB} = \overline{CA}/2$

↓

$$\overline{CD} = \overline{CB} = \overline{BA}$$

↓

If U suddenly is halved \Rightarrow the total energy is raised by an amount equal to \overline{CB}

↓

the total energy is raised from B to $C \Rightarrow E_{\text{final}} = 0$ and the orbit is parabolic