PY 408 - Intermediate Mechanics

Lecture notes - September 9, 2011.

Legendre transformation. The Hamiltonian

We already defined the generalized momenta as

$$p_j = \frac{\partial L}{\partial \dot{q}_j} \tag{1}$$

Together with coordinates q_j, the momenta p_j form what are known as "canonical variables".

As we have seen in the example of the double pendulum, it may be useful to formulate the equations of motion in terms of the coordinates q_j and the momenta p_j, i.e. in terms of the canonical variables q_j, p_j, rather that in terms of the q_j and $\dot{q}_j$. Of course, in general it will be possible to solve Eqs. 1, which give $p_j = p_j(q_{j'}, \dot{q}_{j'}, t)$, for $\dot{q}_{j'}$ to express

$$\dot{q}_j = \dot{q}_j(q_{j'}, p_{j'}, t) \tag{2}$$

Substituting into Lagrange's equations, we would then get a system of equations formulated in terms of the variables q_j, p_j and their time derivatives. However the equations giving the variables $\dot{q}_j$ as functions of the coordinates and momenta would normally be rather complex, quite unlike the simple relation Eq. 1 that allows us to get p_j just by taking a derivative of the Lagrangian. In order to be able to obtain the variables $\dot{q}_j$ through a relation similar to Eq. 1 one performs what is known as Legendre transformation[1]. For the purpose, one introduces a new function H, called the Hamiltonian of the system, as follows:

$$H = \sum_j p_j \dot{q}_j - L(q, \dot{q}, t) \tag{3}$$

---

[1] The Legendre transformation plays also a very important role in thermodynamics, where internal energy, free energy, Gibbs free energy and enthalpy are obtained from each other by Legendre transformations.

Let us consider the differential change of H when the variables $p_j, q_j, \dot{q}_j$ undergo differential changes $dp_j, dq_j, d\dot{q}_j$. Please note that it is immaterial which variables we are considering as independent. If for example we take the momenta p_j and coordinates q_j as independent variables, a change of p_j by dp_j and of q_j by dq_j will induce a well defined change $d\dot{q}_j$ of $\dot{q}_j$, which is the varaiation we were referring to just above.

The differential variation of H induced by variations of $p_j, q_j, \dot{q}_j$ is given by

$$dH = d\Big(\sum_j p_j \dot{q}_j\Big) - dL(q, \dot{q}, t) =$$

$$\sum_j (dp_j \dot{q}_j + p_j\, d\dot{q}_j) - \sum_j \left(\frac{\partial L}{\partial q_j}\, dq_j + \frac{\partial L}{\partial \dot{q}_j}\, d\dot{q}_j\right) \tag{4}$$

or

$$dH = \sum_j \left(p_j - \frac{\partial L}{\partial \dot{q}_j}\right) d\dot{q}_j + \sum_j \left(\dot{q}_j\, dp_j - \frac{\partial L}{\partial q_j}\, dq_j\right) \tag{5}$$

But, by virtue of Eq. 1, the first sum in the r.h.s. vanishes and we are left with

$$dH = \sum_j \left(\dot{q}_j\, dp_j - \frac{\partial L}{\partial q_j}\, dq_j\right) \tag{6}$$

On the other hand the Lagrange equations of motion give us

$$\frac{\partial L}{\partial q_j} = \dot{p}_j \tag{7}$$

so that, at the end of the story, we find

$$dH = \sum_j (\dot{q}_j\, dp_j - \dot{p}_j\, dq_j) \tag{8}$$

This remarkable equation tell us that all dependence of H on the differentials $d\dot{q}_j$ simplifies, so that H can be thought of as a function of p_j and q_j. Moreover, comparing Eq. 8 with the expansion

$$dH = \sum_j \left(\frac{\partial H}{\partial p_j}\, dp_j + \frac{\partial H}{\partial q_j}\, dq_j\right) \tag{9}$$

we find

$$\begin{aligned} \dot{q}_j &= \frac{\partial H}{\partial p_j} \\ \dot{p}_j &= -\frac{\partial H}{\partial q_j} \end{aligned} \tag{10}$$

These are Hamilton's equations of motion.

Hamilton's equations of motion are a set of first order differential equations for the generalized coordinates and momenta, which can be obtained from the Hamiltonian function

$$H = H(p_j, q_j, t) \tag{11}$$

As we have seen already, the Hamiltonian H can be found from the Lagrangian L by expressing the variables $\dot{q}_j$ as functions of the generalized coordinate and momenta and then subtracting L from $\sum_j p_j \dot{q}_j$. We note that if, as is often the case in mechanics, the kinetic energy K is a quadratic function of the momenta

$$K = \sum_{j_1, j_2} k_{j_1,j_2}(q_{j'}, t)\, \dot{q}_{j_1} \dot{q}_{j_2} \tag{12}$$

(with symmetric k_{j_1,j_2}) and the potential energy does not depend on $\dot{q}_j$ then

$$p_j = \frac{\partial L}{\partial \dot{q}_j} = \frac{\partial K}{\partial \dot{q}_j} = 2 \sum_{j_2} k_{j,j_2}(q_{j'}, t)\, \dot{q}_{j_2} \tag{13}$$

so that

$$\sum_j p_j \dot{q}_j = 2 \sum_{j, j_2} k_{j,j_2}(q_{j'}, t)\, \dot{q}_j \dot{q}_{j_2} = 2K \tag{14}$$

In this case

$$H = 2K - L = 2K - (K - V) = K + V \tag{15}$$

and we recognize in H the total energy of the system.

Variational derivation of Hamilton's equation.

As Lagrange's equations, Hamilton's equations may also be derived by demanding that the action $S = \int L\, dt$ be stationary with respect to an infinitesimal variation of the trajectory which leaves its end points fixed. However we must now consider the variations δp and δq of momenta and coordinates along the trajectory as independent and must express the action in terms of H. We have

$$S = \int L(q_j, \dot{q}_j, t)\, dt = \int \Big[\sum_j p_j \dot{q}_j - H(p_j, q_j, t) \Big]\, dt \tag{16}$$

From this we get

$$\begin{aligned} \delta S = \int \delta \Big[\sum_j p_j \dot{q}_j - H(p_j, q_j, t) \Big]\, dt = \\ \int \sum_j \left(\delta p_j \dot{q}_j + p_j \delta \dot{q}_j - \frac{\partial H}{\partial p_j}\, \delta p_j - \frac{\partial H}{\partial q_j}\, \delta q_j \right) dt \end{aligned} \tag{17}$$

Using

$$\delta \dot{q}_j = \frac{d}{dt}\, \delta q_j \tag{18}$$

integrating by parts, and using the fact that $\delta q = 0$ at the initial and final times, the second term in the integrand of Eq. 18 can be rewritten as follows

$$\begin{aligned} \int \Big(\sum_j p_j \delta \dot{q}_j \Big)\, dt = \int \Big(\sum_j p_j \frac{d}{dt}\, \delta q_j \Big)\, dt = \\ - \int \Big(\sum_j \frac{d}{dt}\, p_j \delta q_j \Big)\, dt \equiv - \int \Big(\sum_j \dot{p}_j \delta q_j \Big)\, dt \end{aligned} \tag{19}$$

In conclusion we obtain

$$\begin{aligned} \delta S = \int \sum_j \left(\delta p_j \dot{q}_j - \dot{p}_j \delta q_j - \frac{\partial H}{\partial p_j}\, \delta p_j - \frac{\partial H}{\partial q_j}\, \delta q_j \right) dt = \\ \int \sum_j \left[\left(\dot{q}_j - \frac{\partial H}{\partial p_j} \right) \delta p_j - \left(\dot{p}_j + \frac{\partial H}{\partial q_j} \right) \delta q_j \right] dt \end{aligned} \tag{20}$$

Now, since the variations $\delta p_j, \delta q_j$ are arbitrary, the requirement $\delta S = 0$ can only be satisfied if the terms that multiply these variations vanish at all times. Thus we find the conditions

$$\begin{aligned} \dot{q}_j - \frac{\partial H}{\partial p_j} = 0 \\ \dot{p}_j + \frac{\partial H}{\partial q_j} = 0 \end{aligned} \tag{21}$$

which are indeed Hamilton's equations 10.

Hamilton's equations for the double pendulum.

Let us derive Hamilton's equations of motion for the double pendulum considered in Lecture 3. The kinetic and potential energies of the system are (see Lecture 3, Eqs. 12 and 13)

$$\begin{gathered} K = \frac{m}{2}(\dot{x}_1^2 + \dot{z}_1^2 + \dot{x}_2^2 + \dot{z}_2^2) = \\ \frac{ml^2}{2}\left(2\dot{\theta}_1^2 + 2\dot{\theta}_1\dot{\theta}_2\cos(\theta_1 - \theta_2) + \dot{\theta}_2^2\right) \end{gathered} \tag{22}$$

$$V = mg(z_1 + z_2) = -mgl(2\cos\theta_1 + \cos\theta_2) \tag{23}$$

K is quadratic in the generalized velocities $\dot{\theta}_1, \dot{\theta}_2$ and V does not depend on $\dot{\theta}_1, \dot{\theta}_2$. Therefore the Hamiltonian is given by

$$H = K + V \tag{24}$$

K must however be expressed as a function of the momenta, which we denote by p_1, p_2 and are given by

$$p_j = \frac{\partial K}{\partial \dot{\theta}_j} \tag{25}$$

In order to find explicit formulae for p_1, p_2, express $\dot{\theta}_1, \dot{\theta}_2$ as functions of the momenta and substitute their values in K it is convenient to proceed as follows. Let us introduce two vectors $\mathbf{p} \equiv (p_1, p_2)$ and $\dot{\boldsymbol{\theta}} \equiv (\dot{\theta}_1, \dot{\theta}_2)$ and the matrix

$$\mathbf{M} = \begin{pmatrix} 2ml^2 & ml^2\cos(\theta_1 - \theta_2) \\ ml^2\cos(\theta_1 - \theta_2) & ml^2 \end{pmatrix} \tag{26}$$

It is easy to see that the kinetic energy is given by

$$K = \frac{1}{2}\dot{\boldsymbol{\theta}} \cdot \mathbf{M}\dot{\boldsymbol{\theta}} \tag{27}$$

According to Eq. 25 the vector $\mathbf{p}$ is then given by

$$\mathbf{p} = \frac{1}{2}\boldsymbol{\nabla}_{\dot{\boldsymbol{\theta}}}(\dot{\boldsymbol{\theta}} \cdot \mathbf{M}\dot{\boldsymbol{\theta}}) = \mathbf{M}\dot{\boldsymbol{\theta}} \tag{28}$$

We must still solve for $\dot{\boldsymbol{\theta}}$. This is most easily done by multiplying first both sides of Eq. 28 by $\mathbf{M}^{-1}$ which produces

$$\dot{\boldsymbol{\theta}} = \mathbf{M}^{-1}\mathbf{p} \tag{29}$$

and

$$K = \frac{1}{2}\,\mathbf{p}\cdot\mathbf{M}^{-1}\mathbf{p} \tag{30}$$

The explicit form of $\mathbf{M}^{-1}$ is

$$\mathbf{M}^{-1} = \frac{1}{ml^2[2-\cos^2(\theta_1-\theta_2)]}\begin{pmatrix} 1 & -\cos(\theta_1-\theta_2) \\ -\cos(\theta_1-\theta_2) & 2 \end{pmatrix} \tag{31}$$

and thus K, as functions of coordinates and momenta, is

$$K = \frac{p_1^2 - 2p_1p_2cos(\theta_1-\theta_2) + 2p_2^2}{2ml^2[2-\cos^2(\theta_1-\theta_2)]} \tag{32}$$

In conclusion the Hamiltonian $H = K + V$ of the system is given by

$$H = \frac{p_1^2 - 2p_1p_2\cos(\theta_1-\theta_2) + 2p_2^2}{2ml^2[2-\cos^2(\theta_1-\theta_2)]} - mgl(2\cos\theta_1 + \cos\theta_2) \tag{33}$$

From H we get Hamilton's equations

$$\begin{aligned} \dot{\theta}_1 &= \frac{\partial H}{\partial p_1} = \frac{p_1 - p_2\cos(\theta_1-\theta_2)}{ml^2[2-\cos^2(\theta_1-\theta_2)]} \\ \dot{\theta}_2 &= \frac{\partial H}{\partial p_2} = \frac{-p_1\cos(\theta_1-\theta_2) + 2p_2}{2ml^2[2-\cos^2(\theta_1-\theta_2)]} \end{aligned} \tag{34}$$

and

$$\begin{aligned} \dot{p}_1 &= -\frac{\partial H}{\partial \theta_1} = -2mgl\sin\theta_1 - \frac{\partial K}{\partial \theta_1} \\ \dot{p}_2 &= -\frac{\partial H}{\partial \theta_2} = -mgl\sin\theta_2 - \frac{\partial K}{\partial \theta_2} \end{aligned} \tag{35}$$

The last term in Eqs. 35 looks nasty, but we may simplify the algebra by going back to matrix notation. From Eq. 30 we get

$$\begin{aligned} \frac{\partial K}{\partial \theta_1} &= \frac{\partial}{\partial \theta_1}\left(\frac{1}{2}\,\mathbf{p}\cdot\mathbf{M}^{-1}\mathbf{p}\right) = \frac{1}{2}\,\mathbf{p}\cdot\frac{\partial \mathbf{M}^{-1}}{\partial \theta_1}\,\mathbf{p} \\ \frac{\partial K}{\partial \theta_2} &= \frac{\partial}{\partial \theta_2}\left(\frac{1}{2}\,\mathbf{p}\cdot\mathbf{M}^{-1}\mathbf{p}\right) = \frac{1}{2}\,\mathbf{p}\cdot\frac{\partial \mathbf{M}^{-1}}{\partial \theta_2}\,\mathbf{p} \end{aligned} \tag{36}$$

since the only dependence on the variables θ_1, θ_2 is in $\mathbf{M^{-1}}$.

We now use the identity

$$\frac{\partial \mathbf{M}^{-1}}{\partial \theta_j} = -\mathbf{M}^{-1} \frac{\partial \mathbf{M}}{\partial \theta_j} \mathbf{M}^{-1} \tag{37}$$

and

$$\frac{\partial \mathbf{M}}{\partial \theta_1} = -\frac{\partial \mathbf{M}}{\partial \theta_2} = \begin{pmatrix} 0 & -ml^2 \sin(\theta_1 - \theta_2) \\ -ml^2 \sin(\theta_1 - \theta_2) & 0 \end{pmatrix} = \\ -ml^2 \sin(\theta_1 - \theta_2) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{38}$$

to obtain

$$\frac{\partial K}{\partial \theta_1} = -\frac{\partial K}{\partial \theta_2} = \frac{ml^2 \sin(\theta_1 - \theta_2)}{2} \mathbf{p} \cdot \mathbf{M}^{-1} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathbf{M}^{-1} \mathbf{p} \tag{39}$$

The matrix algebra can easily be done and we find

$$\dot{p}_1 = -2mgl \sin\theta_1 \\ -\sin(\theta_1 - \theta_2) \frac{(p_1^2 + 2p_2^2)\cos(\theta_1 - \theta_2) - p_1 p_2 [2 + \cos^2(\theta_1 - \theta_2)]}{ml^2[2 - \cos^2(\theta_1 - \theta_2)^2]^2} \\ \dot{p}_2 = -mgl \sin\theta_2 \\ +\sin(\theta_1 - \theta_2) \frac{(p_1^2 + 2p_2^2)\cos(\theta_1 - \theta_2) - p_1 p_2 [2 + \cos^2(\theta_1 - \theta_2)]}{ml^2[2 - \cos^2(\theta_1 - \theta_2)^2]^2} \tag{40}$$

Of course, we may also go back to Eq. 29 which tells us that $\mathbf{M}^{-1}\mathbf{p} = \dot{\boldsymbol{\theta}}$ to express the derivatives in Eq. 39 as

$$\frac{\partial K}{\partial \theta_1} = -\frac{\partial K}{\partial \theta_2} = \frac{ml^2 \sin(\theta_1 - \theta_2)}{2} \dot{\boldsymbol{\theta}} \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \dot{\boldsymbol{\theta}} = \\ ml^2 \sin(\theta_1 - \theta_2)\, \dot{\theta}_1 \dot{\theta}_2 \tag{41}$$

If we substitute this expression into Eq. 35 we get the simpler set of equations

$$\begin{aligned} \dot{p}_1 &= -2mgl \sin\theta_1 - ml^2 \dot{\theta}_1 \dot{\theta}_2 \sin(\theta_1 - \theta_2) \\ \dot{p}_2 &= -mgl \sin\theta_2 + ml^2 \dot{\theta}_1 \dot{\theta}_2 \sin(\theta_1 - \theta_2) \end{aligned} \tag{42}$$

which coincide with the equations we derived from the Lagrangian (see Lecture 3, Eqs. 16) and show the equivalence of the two formulations. [From the computational point of view, the best strategy is to keep in the program both sets of variables p_j and $\dot{\theta}_j$, and use Eqs. 34 and 42 to implement their evolution.]

Time dependence of the observables. Poisson brackets.

Let us consider an observable A, i.e. a function of the coordinates and momenta, possibly with an explicit dependence on time: $A = A(q_j, p_j, t)$. The value of the observable is thus fully determined when the values of the coordinates and momenta are known. The value of t will also have to be specified, if A has an explicit dependence on time. The time derivative of A is given by:

$$\begin{aligned} \frac{dA}{dt} &= \sum_j \left(\frac{\partial A}{\partial q_j} \frac{dq_j}{dt} + \frac{\partial A}{\partial p_j} \frac{dp_j}{dt} \right) + \frac{\partial A}{\partial t} \\ &\equiv \sum_j \left(\frac{\partial A}{\partial q_j} \dot{q}_j + \frac{\partial A}{\partial p_j} \dot{p}_j \right) + \frac{\partial A}{\partial t} \end{aligned} \tag{43}$$

Using Hamilton's equations the r.h.s. of Eq. 43 can be recast in the form

$$\frac{dA}{dt} = \sum_j \left(\frac{\partial H}{\partial p_j} \frac{\partial A}{\partial q_j} - \frac{\partial H}{\partial q_j} \frac{\partial A}{\partial p_j} \right) + \frac{\partial A}{\partial t} \tag{44}$$

The sum of products of partial derivatives which appears in this equation plays a very important role in classical mechanics and is known as "Poisson bracket."[2] Given two observables A and B their Poisson bracket, denoted by $[A, B]_{\mathrm{PB}}$ or simply $[A, B]$, is defined as

$$[A, B] \equiv \sum_j \left(\frac{\partial A}{\partial p_j} \frac{\partial B}{\partial q_j} - \frac{\partial A}{\partial q_j} \frac{\partial B}{\partial p_j} \right) \tag{45}$$

---

[2] In quantum mechanics classical observables like $A(p_j, q_j)$ are replaced by operators, e.g. $\hat{A}$, defined in a suitable vector space. The role of the Poisson bracket $[A, B]_{PB}$ is played by the commutator $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$ and the relation between the commutator of two observables and the Poisson bracket of their classical counterparts is $[\hat{A}, \hat{B}] = -\imath\hbar \widehat{[A, B]}_{PB}$. (The sign in front of the imaginary unit is a matter of convention and a suitable ordering of operators may have to chosen in the definition of $\widehat{[A, B]}_{PB}$.)

Thus the total time derivative of A is given by the Poisson bracket of the Hamiltonian H with A plus the partial derivative of A with respect to t:

$$\frac{dA}{dt} = [H, A] + \frac{\partial A}{\partial t} \tag{46}$$

Poisson brackets satisfy some important identities[3]:

- The Poisson bracket is antisymmetric in its arguments

  $$[B, A] = -[A, B] \tag{47}$$

  As a consequence

  $$[A, A] = 0 \tag{48}$$

- The Poisson brackets of the canonical variables have a very simple form.

  $$[p_i, p_j] = 0; \quad [p_i, q_j] = \delta_{i,j}; \quad [q_i, q_j] = 0 \tag{49}$$

- The double Poisson brackets of three observables satisfy the equation

  $$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0 \tag{50}$$

(This last identity can be proved with straightforward, albeit rather cumbersome algebra. By taking the derivatives with careful patience, one finds that all second partial derivatives cancel and one is left with products of first derivatives, which cancel as well.)

Note that, as a consequence of Eq, 47, we have

$$\frac{dH}{dt} = [H, H] + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t} \tag{51}$$

In particular, if the Hamiltonian does not depend explicitly on time, it is conserved.

Canonical transformations.

Given a system described by generalized coordinates q_j and generalized momenta p_j, we can change the coordinates to some other set of coordinates

$$q_j \rightarrow Q_j = Q_j(q_k) \tag{52}$$

---

[3] The quantum mechanical counterparts of these identities are: $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$; $[\hat{p}_i, \hat{p}_j] = [\hat{q}_i, \hat{q}_j] = 0$, $[\hat{p}_i, \hat{q}_j] = -\imath\hbar\delta_{i,j}$, $[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0$

This change of variables induces a corresponding change of momenta

$$p_j \to P_j = P_j(q_k, p_k) \tag{53}$$

The change in Eq. 52 will induce a change of the form of the Lagrangian. Given the original Lagrangian $L(q_j, \dot{q}_j, t)$ one must first solve for the old coordinates q_j as functions of the new ones

$$q_j = q_j(Q_k) \tag{54}$$

Substituting into L we will obtain a new Lagrangian

$$L(q_j(Q_k), \dot{q}(Q_k, \dot{Q}_k), t) = L'(Q_k, \dot{Q}_k, t) \tag{55}$$

with a different functional dependence on the new coordinates and their time derivatives than the original L.

This is best illustrated with an example. Let us consider the motion of a point-like object of mass m in the x, y plane under the action of a central force with potential $V(r) = -\alpha/r$. Let us first choose as coordinates q_1, q_2 the Cartesian coordinates of the object

$$\begin{aligned} q_1 &= x \\ q_2 &= y \end{aligned} \tag{56}$$

This gives

$$K = \frac{m(\dot{q}_1^2 + \dot{q}_2^2)}{2} \tag{57}$$

and

$$V = -\frac{\alpha}{\sqrt{q_1^2 + q_2^2}} \tag{58}$$

and the Lagrangian

$$L(q_j, \dot{q}_j) = \frac{m(\dot{q}_1^2 + \dot{q}_2^2)}{2} + \frac{\alpha}{\sqrt{q_1^2 + q_2^2}} \tag{59}$$

Let us now change to polar coordinates with

$$\begin{aligned} Q_1 &= r = \sqrt{q_1^2 + q_2^2} \\ Q_2 &= \phi = \arctan(q_2/q_1) \end{aligned} \tag{60}$$

The inverse relations are

$$\begin{aligned} q_1 &= Q_1 \cos Q_2 \\ q_2 &= Q_1 \sin Q_2 \end{aligned} \tag{61}$$

Substituting into the Lagrangian we get

$$L'(Q_j, \dot{Q}_j) = \frac{m(\dot{Q}_1^2 + Q_1^2 \dot{Q}_2^2)}{2} + \frac{\alpha}{Q_1} \tag{62}$$

which clearly has a different functional dependence on its arguments than L. From the Lagrangians L and L' we get the corresponding momenta

$$\begin{aligned} p_1 &= m\,\dot{q}_1 \\ p_2 &= m\,\dot{q}_2 \end{aligned} \tag{63}$$

and

$$\begin{aligned} P_1 &= m\,\dot{Q}_1 \\ P_2 &= m\,Q_1^2 \dot{Q}_2 \end{aligned} \tag{64}$$

From Eq. 60 we get

$$\begin{aligned} \dot{Q}_1 &= \frac{q_1 \dot{q}_1 + q_2 \dot{q}_2}{\sqrt{q_1^2 + q_2^2}} = \frac{q_1 p_1 + q_2 p_2}{m\sqrt{q_1^2 + q_2^2}} \\ \dot{Q}_2 &= \frac{q_1 \dot{q}_2 - q_2 \dot{q}_1}{q_1^2 + q_2^2} = \frac{q_1 p_2 - q_2 p_1}{m(q_1^2 + q_2^2)} \end{aligned} \tag{65}$$

and therefore

$$\begin{aligned} P_1 &= \frac{q_1 p_1 + q_2 p_2}{\sqrt{q_1^2 + q_2^2}} \\ P_2 &= q_1 p_2 - q_2 p_1 \end{aligned} \tag{66}$$

Equations 60 and 66 express the new canonical variables P_j, Q_j as functions of the old canonical variables p_j, q_j and give an example of a "canonical transformation."

From the Lagrangian $L'(P_j, Q_j)$ we can obtain the Hamiltonian

$$H'(P_j, Q_j) = \frac{P_1^2}{2m} + \frac{P_2^2}{2mQ_1^2} + \frac{\alpha}{Q_1} \tag{67}$$

If we substitute for P_j, Q_j their expressions in terms of p_j, q_j we obtain

$$H'(P_j(p_k, q_k), Q_j(p_k, q_k)) = \frac{p_1^2 + p_2^2}{2m} + \frac{\alpha}{\sqrt{q_1^2 + q_2^2}} = H(p_k, q_k) \qquad (68)$$

Not surprisingly, the function $H(p_j, q_j)$ is the same Hamiltonian we could have obtained directly from the Lagrangian L of Eq. 59. However, we emphasize that we have not obtained the expression for $H(p_j, q_j)$ given by Eq. 68 starting from the Lagrangian L, but rather from the change of canonical variables given by Eqs. 60 and 66. We could be given just the Hamiltonian $H'(P_j, Q_j)$, the change of variables $P_j(p_k, q_k), Q_j(p_k, q_k)$ and asked to substitute into H' to obtain a new function $H(p_j, q_j)$. We would find that, quite remarkably, H is the Hamiltonian that describes the evolution of the variables p_j, q_j.

The question is then: will any arbitrary change of variables

$$\begin{aligned} P_j &= P_j(p_k, q_k) \\ Q_j &= Q_j(p_k, q_k) \qquad (69) \end{aligned}$$

when substituted into a Hamiltonian $H(P_j, Q_j)$ lead to a new Hamiltonian $H'(p_j, q_j)$ which correctly describes the evolution of the variables p, q? The answer is absolutely not! This will happen only for a special class of transformations which are called "canonical transformations." Canonical transformations are changes of canonical variables with the property that they preserve the Hamiltionian equations of motion. Precisely the change of variables induces a change of the functional form of the Hamiltonian with the property that both the old and the new Hamiltonians correctly describe the evolution of the corresponding variables. The change of variables from Cartesian to polar coordinates which we derived above is a canonical transformation. But an arbitrary change of canonical variables would not be.

The procedure we followed to derive the canonical transformation from Cartesian to polar coordinates is such that the outcome had to be a canonical transformation. This is so because we started from a change of coordinates in the Lagrangian, derived the new Lagrangian, and derived the new momenta from the new Lagrangian. The passage to the Hamiltonian formalism was then bound to produce two Hamiltonians which correctly described the evolution of the two sets of canonical variables. Canonical transformations which are obtained by changing the coordinates $q_j \rightarrow Q_j = Q_j(q_k)$ and deriving then the change of momenta from the change of Lagrangian are called "contact transformations." They constitute a subclass of all possible canonical transformations. The wider class of canonical transformations contain transformations that cannot be derived starting from a change of coordinates only. We illustrate this point with a simple, but non-trivial example of a canonical transformation which is not a contact transformation.

Consider a harmonic oscillator moving in one dimension. Let the motion be along the x-axis and the energy be given by

$$E = \frac{m\dot{x}^2}{2} + \frac{kx^2}{2} \tag{70}$$

We take as generalized coordinate q the Cartesian coordinate x of the oscillator. (Since the system only has one degree we can dispense with the index of q.) The Lagrangian is

$$L = \frac{m\dot{q}^2}{2} - \frac{kq^2}{2} \tag{71}$$

and therefore the momentum and the Hamiltonian are

$$p = m\dot{q} \tag{72}$$

$$H = \frac{p^2}{2m} + \frac{kq^2}{2} \tag{73}$$

Let us introduce the new variables

$$\begin{aligned} P &= \frac{1}{2}\left(\frac{1}{\sqrt{mk}}p^2 + \sqrt{mk}q^2\right) \\ Q &= \arctan\frac{\sqrt{mk}\,q}{p} \end{aligned} \tag{74}$$

The inverse transformation is given by

$$\begin{aligned} p &= (mk)^{1/4}\sqrt{2P}\cos Q \\ q &= \frac{\sqrt{2P}}{(mk)^{1/4}}\sin Q \end{aligned} \tag{75}$$

Substituting into the Hamiltonian 73 we find

$$H(P,Q) = \sqrt{\frac{k}{m}}P \tag{76}$$

Hamilton's equation of motion are then

$$\begin{aligned}\dot{P} &= -\frac{\partial H}{\partial Q} = 0 \\ \dot{Q} &= \frac{\partial H}{\partial P} = \sqrt{\frac{k}{m}} \end{aligned} \tag{77}$$

with solution

$$\begin{aligned}P &= \text{const} \\ Q &= \sqrt{\frac{k}{m}}\, t + Q_0 = \omega t + Q_0 \end{aligned} \tag{78}$$

having defined $\omega = \sqrt{k/m}$.

If we go back to the original variables p, q, their time evolution can be obtained from the original Hamiltonian

$$H(p,q) = \frac{p^2}{2m} + \frac{kq^2}{2}$$

The evolution equations that follow from the Hamiltonian are

$$\begin{aligned}\dot{p} &= -\frac{\partial H}{\partial q} = -kq \\ \dot{q} &= \frac{\partial H}{\partial p} = \frac{p}{m} \end{aligned} \tag{79}$$

with solution

$$\begin{aligned}p &= A\cos(\omega t + \phi_0) \\ q &= A\frac{1}{\sqrt{mk}}\sin(\omega t + \phi_0) \end{aligned} \tag{80}$$

On the other hand, if we substitute into Eqs. 75 the solution we found for the new variables P, Q (Eqs. 78) we get

$$\begin{aligned}p &= (mk)^{1/4}\sqrt{2P}\cos(\omega t + Q_0) \\ q &= \frac{\sqrt{2P}}{(mk)^{1/4}}\sin(\omega t + Q_0) \end{aligned} \tag{81}$$

which coincides with the solution we obtained directly from the original Hamiltonian (Eqs. 80) with the identifications $A = (mk)^{1/4}\sqrt{2P}$ and $\phi_0 = Q_0$.

From these considerations we see that the change of variables defined by Eqs. 74, with the inverse given by Eqs. 75, is a canonical transformation because it preserves Hamilton's equations of motion: the original Hamiltonian and the new Hamiltonian one obtains with the change of variables give origin to the same evolution. On the other hand the change of variables of Eqs. 74 is not a contact transformation, i.e. a transformation induced by a change of coordinates in the Lagrangian. The new coordinate Q cannot be expressed as a function of q alone. It is intrinsically a function of p and q, and so is the new momentum P.

It is interesting to observe the simplicity of time evolution formulated in terms of the new variables P and Q: P, which has dimensions of an angular momentum, is a constant, and the energy is $E = \omega P$. Q, which is a dimensionless angular variable, evolves in time like ωt. The motion is periodic, a period being completed every time Q increases by 2π. The variables P, Q played an important role in the early development of quantum mechanics [4].

Canonical transformations and Poisson brackets.

We have observed that the time evolution of an observable can be expressed in terms of its Poisson bracket with the Hamiltonian, see Eq. 46:

$$\frac{dA}{dt} = [H, A] + \frac{\partial A}{\partial t}$$

In particular, Hamilton's equations of motion can be formulated in terms of the Poisson brackets of the Hamiltonian with the coordinates and momenta.

$$\begin{aligned} \dot{q}_j &= [H, q_j] \\ \dot{p}_j &= [H, p_j] \end{aligned} \tag{82}$$

---

[4] The first empirical rules of quantization assumed that, with a periodic motion, the integral of $P\,dQ$ over a period had to be a multiple of Planck's constant h. For the harmonic oscillator we considered here, the rule is $\oint P\,dQ = nh$. Since P is a constant and Q increases by 2π in a period, the condition is equivalent to $2\pi P = nh$ or $P = n\hbar$. (Note that both P and $\hbar$ have dimension of angular momentum.) Correspondingly the energy levels turn out to be $E_n = n\omega\hbar$. This empirical quantization misses the ground state energy $E_0 = \omega\hbar/2$, but otherwise reproduces the correct spacing of energy levels.

To be better convinced, we may verify the above equation by recalling the definition of the Poisson brackets:

$$\begin{aligned}
[H, q_j] &\equiv \sum_{j'} \left(\frac{\partial H}{\partial p_{j'}} \frac{\partial q_j}{\partial q_{j'}} - \frac{\partial H}{\partial q_{j'}} \frac{\partial q_j}{\partial p_{j'}} \right) = \frac{\partial H}{\partial p_j} = \dot{q}_j \\
[H, p_j] &\equiv \sum_{j'} \left(\frac{\partial H}{\partial p_{j'}} \frac{\partial p_j}{\partial q_{j'}} - \frac{\partial H}{\partial q_{j'}} \frac{\partial p_j}{\partial p_{j'}} \right) = -\frac{\partial H}{\partial q_j} = \dot{p}_j
\end{aligned} \tag{83}$$

If follows form this observation that if a transformation of the coordinates and momenta q_j, p_j to new coordinates and momenta $Q_j(q_k, p_k), P_j(q_k, p_k)$ preserves the Poisson brackets of the Hamiltonian with the observables, then the transformation will be a canonical transformation.

As a matter of fact, it is convenient to generalize the notion of canonical transformation. We will say that a transformation of coordinates and momenta

$$q_j, p_j \to Q_j(q_k, p_k), P_j(q_k, p_k) \tag{84}$$

is a "canonical transformation" if it preserves all Poisson brackets.

It follows, in particular, that a canonical transformation preserves the Hamiltonian equations of motion.

A very useful observation is if a change of canonical variables preserves the Poisson brackets of the canonical variables then it preserves all Poisson brackets. Thus we need only check that the Poisson brackets of the canonical variables are preserved to make sure that the transformation is canonical.

Let us make the meaning of "preserves the Poisson brackets of the canonical variables" totally clear. The new variables P_j, Q_j will be functions of the old ones p_j, q_j. We may than calculate the Poisson bracket of the functions $P_j(q_k, p_k), Q_j(q_k, p_k)$ by using their partial derivatives with respect to the old variables. For example, we should calculate $[P_j, Q_{j'}]$ as

$$[P_j, Q_{j'}]_{p,q} = \sum_k \left(\frac{\partial P_j}{\partial p_k} \frac{\partial Q_{j'}}{\partial q_k} - \frac{\partial P_j}{\partial q_k} \frac{\partial Q_{j'}}{\partial p_k} \right) \tag{85}$$

where we have appended the p, q subscript to the symbol of the Poisson bracket to make clear that it is calculated considering the p_k and q_k variables as the independent variables. Saying that the Poisson bracket is preserved implies that the result of the calculation should give

$$[P_j, Q_{j'}]_{p,q} = \delta_{j,j'} \tag{86}$$

as if the independent variables were P_j, Q_j (see Eq. 49). I.e.

$$[P_j, Q_{j'}]_{p,q} = [P_j, Q_{j'}]_{P,Q} \tag{87}$$

and similarly for all other Poisson brackets of the Ps and Qs.

The proof that a transformation that preserves the Poisson brackets of the canonical variables preserves all Poisson brackets is straightforward, but rather lengthy and tedious. We offer it here anyway.

Let us consider the Poisson bracket of two functions $A(P,Q)$ and $B(P,Q)$ of the new variables taken with respect to the old variables:

$$[A, B]_{p,q} = \sum_j \left[\frac{\partial A}{\partial p_j}\frac{\partial B}{\partial q_j} - \frac{\partial A}{\partial q_j}\frac{\partial B}{\partial p_j} \right] \tag{88}$$

In the r.h.s. of this equation we must express the new variables as functions of the old variables. We obtain

$$\frac{\partial A}{\partial p_j} = \sum_i \left(\frac{\partial A}{\partial P_i}\frac{\partial P_i}{\partial p_j} + \frac{\partial A}{\partial Q_i}\frac{\partial Q_i}{\partial p_j} \right) \tag{89}$$

and similarly for all other partial derivatives appearing in Eq. 88.

With a little patience we can put all terms together getting

$$\begin{aligned}
[A,B]_{p,q} = \sum_{i,j,k} \Bigg[& \frac{\partial A}{\partial P_i}\frac{\partial P_i}{\partial p_j}\frac{\partial B}{\partial P_k}\frac{\partial P_k}{\partial q_j} + \frac{\partial A}{\partial P_i}\frac{\partial P_i}{\partial p_j}\frac{\partial B}{\partial Q_k}\frac{\partial Q_k}{\partial q_j} \\
& + \frac{\partial A}{\partial Q_i}\frac{\partial Q_i}{\partial p_j}\frac{\partial B}{\partial P_k}\frac{\partial P_k}{\partial q_j} + \frac{\partial A}{\partial Q_i}\frac{\partial Q_i}{\partial p_j}\frac{\partial B}{\partial Q_k}\frac{\partial Q_k}{\partial q_j} \\
& - \frac{\partial A}{\partial P_i}\frac{\partial P_i}{\partial q_j}\frac{\partial B}{\partial P_k}\frac{\partial P_k}{\partial p_j} - \frac{\partial A}{\partial P_i}\frac{\partial P_i}{\partial q_j}\frac{\partial B}{\partial Q_k}\frac{\partial Q_k}{\partial p_j} \\
& - \frac{\partial A}{\partial Q_i}\frac{\partial Q_i}{\partial q_j}\frac{\partial B}{\partial P_k}\frac{\partial P_k}{\partial p_j} - \frac{\partial A}{\partial Q_i}\frac{\partial Q_i}{\partial q_j}\frac{\partial B}{\partial Q_k}\frac{\partial Q_k}{\partial p_j} \Bigg] \\
= \sum_{i,k} \Bigg[& \frac{\partial A}{\partial P_i}\frac{\partial B}{\partial P_k}\sum_j \left(\frac{\partial P_i}{\partial p_j}\frac{\partial P_k}{\partial q_j} - \frac{\partial P_i}{\partial q_j}\frac{\partial P_k}{\partial p_j} \right) \\
& + \frac{\partial A}{\partial P_i}\frac{\partial Q}{\partial P_k}\sum_j \left(\frac{\partial P_i}{\partial p_j}\frac{\partial Q_k}{\partial q_j} - \frac{\partial P_i}{\partial q_j}\frac{\partial Q_k}{\partial p_j} \right) + \\
& \frac{\partial A}{\partial Q_i}\frac{\partial B}{\partial P_k}\sum_j \left(\frac{\partial Q_i}{\partial p_j}\frac{\partial P_k}{\partial q_j} - \frac{\partial Q_i}{\partial q_j}\frac{\partial P_k}{\partial p_j} \right) \\
& + \frac{\partial A}{\partial Q_i}\frac{\partial B}{\partial Q_k}\sum_j \left(\frac{\partial Q_i}{\partial p_j}\frac{\partial Q_k}{\partial q_j} - \frac{\partial Q_i}{\partial q_j}\frac{\partial Q_k}{\partial p_j} \right) \Bigg] \\
= \sum_{i,k} \Bigg(& \frac{\partial A}{\partial P_i}\frac{\partial B}{\partial P_k}[P_i, P_k]_{p,q} + \frac{\partial A}{\partial P_i}\frac{\partial B}{\partial Q_k}[P_i, Q_k]_{p,q} \\
& + \frac{\partial A}{\partial Q_i}\frac{\partial B}{\partial P_k}[Q_i, P_k]_{p,q} + \frac{\partial A}{\partial Q_i}\frac{\partial B}{\partial Q_k}[Q_i, Q_k]_{p,q} \Bigg)
\end{aligned} \tag{90}$$

If the Poisson brackets of the new variables with respect to the old ones are preserved, so that $[P_i, P_k]_{p,q} = [Q_i, Q_k]_{p,q} = 0$ and $[P_i, Q_k]_{p,q} = -[Q_i, P_k]_{p,q} = \delta_{i,k}$ then Eq. 90 reduces to

$$[A,B]_{p,q} = \sum_i \left[\frac{\partial A}{\partial P_i}\frac{\partial B}{\partial Q_i} - \frac{\partial A}{\partial Q_i}\frac{\partial B}{\partial P_i} \right] = [A,B]_{P,Q} \tag{91}$$

as we wanted to prove.

To conclude this section let us verify that the change of canonical variables for the harmonic oscillator of Eq. 74 preserves the Poisson brackets of the new canonical variables. We recall the form of the transformation:

$$\begin{aligned} P &= \frac{1}{2}\left(\frac{1}{\sqrt{mk}}p^2 + \sqrt{mk}q^2\right) \\ Q &= \arctan\frac{\sqrt{mk}\,q}{p} \end{aligned}$$

We only need to check that $[P,Q]_{p.q} = 1$, since $[P,P] = [Q,Q] = 0$. We have

$$\begin{aligned} \frac{\partial P}{\partial p} &= \frac{p}{\sqrt{mk}} \\ \frac{\partial P}{\partial q} &= \sqrt{mk}q \\ \frac{\partial Q}{\partial p} &= -\frac{\sqrt{mk}q}{p^2 + mkq^2} \\ \frac{\partial Q}{\partial q} &= \frac{\sqrt{mk}p}{p^2 + mkq^2} \end{aligned} \tag{92}$$

and thus

$$[P,Q]_{p,q} = \frac{\partial P}{\partial p}\frac{\partial Q}{\partial q} - \frac{\partial P}{\partial q}\frac{\partial Q}{\partial p} =$$
$$\frac{p}{\sqrt{mk}}\frac{\sqrt{mk}p}{(p^2 + mkq^2)} + \sqrt{mk}q\frac{\sqrt{mk}q}{(p^2 + mkq^2)} = \frac{p^2 + mkq^2}{p^2 + mkq^2} = 1 \tag{93}$$

showing that the transformation does indeed preserve the Poisson brackets of the canonical variables.

Generators of symmetry transformations.

An obvious question is “What is the most general form of a canonical transformation?”, or “How can one make a change of canonical variables in such a way that the resulting transformation is canonical?” There are ways of defining changes of canonical variables such that the resulting transformation is canonical, but we will not pursue this matter here. Rather we will focus our attention on the so-called “infinitesimal transformations” and their “generators.”

A transformation of variables is called "infinitesimal" if the changes it induces in the variables are infinitesimal. The concept is most easily explained by an example. Consider the transformation induced by a rotation in the $x - y$ plane which sends an object of coordinates x, y into a new position x', y':

$$\begin{aligned} x &\rightarrow x' = x\cos\phi - y\sin\phi \\ y &\rightarrow y' = x\sin\phi + y\cos\phi \end{aligned} \tag{94}$$

If we take the angle ϕ to be an infinitesimal quantity $\phi = \epsilon$ and expand up to first order in ϵ we obtain an infinitesimal rotation

$$\begin{aligned} x &\rightarrow x' = x - \epsilon y \\ y &\rightarrow y' = y + \epsilon x \end{aligned} \tag{95}$$

Note that this can also be written in matrix form

$$\mathbf{r} \rightarrow \mathbf{r}' = \mathbf{r} + \epsilon\mathbf{\Omega}\mathbf{r} \tag{96}$$

with

$$\mathbf{r} = \begin{pmatrix} x \\ y \end{pmatrix} \qquad \mathbf{\Omega} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{97}$$

$\mathbf{\Omega}$ is called the "generator" of the transformation. Infinitesimal transformations are in a sense more basic than finite transformations, because a finite transformation can be obtained by exponentiating its infinitesimal generator. Indeed, in the example above it is easy to check that the finite rotation of Eq. 94 is given by

$$\mathbf{r} \rightarrow \mathbf{r}' = e^{\mathbf{\Omega}\phi}\mathbf{r} \tag{98}$$

We will be interested in infinitesimal canonical transformations and we will state, without proof, the following important proposition:

The most general infinitesimal canonical transformation is of the form

$$\begin{aligned} p_j &\rightarrow p'_j = p_j + \epsilon[f(p_k, q_k), p_j] \\ q_j &\rightarrow q'_j = q_j + \epsilon[f(p_k, q_k), q_j] \end{aligned} \tag{99}$$

where $f(p_k, q_k)$ can be an arbitrary function of the canonical variables.

From Eq. 99 we see that we can consider the Poisson bracket $[f(p_k, q_k), \quad]$ as the generator of the infinitesimal transformation. We will just say, however, that the generator of the infinitesimal transformation is the function f. By writing the explicit form of the Poisson brackets in Eq. 99 we see that the infinitesimal transformation can also be written as

$$\begin{aligned} p_j &\rightarrow p'_j = p_j - \epsilon\tfrac{\partial f}{\partial q_j} \\ q_j &\rightarrow q'_j = q_j + \epsilon\tfrac{\partial f}{\partial p_j} \end{aligned} \tag{100}$$

As stated above, we will not give a proof that Eq. 99 represents the most general infinitesimal canonical transformation, but we will prove here that the transformation given by Eqs. 99 or 100 preserves the Poisson brackets of the canonical variables and is therefore a canonical transformation. Let us check that this is the case for $[p_j, q_{j'}]$. Using equation 100 we find

$$[p_j, q_{j'}] \rightarrow \left[p_j - \epsilon\frac{\partial f}{\partial q_j}, q_{j'} + \epsilon\frac{\partial f}{\partial p_{j'}}\right] = [p_j, q_{j'}] + \epsilon\left[p_j, \frac{\partial f}{\partial p_{j'}}\right] - \epsilon\left[\frac{\partial f}{\partial q_j}, q_{j'}\right] \tag{101}$$

But, from the definition of Poisson brackets, we have

$$\left[p_j, \frac{\partial f}{\partial p_{j'}}\right] = \frac{\partial}{\partial q_j}\frac{\partial f}{\partial p_{j'}} = \frac{\partial^2 f}{\partial q_j \partial p_{j'}} \tag{102}$$

and

$$\left[\frac{\partial f}{\partial q_j}, q_{j'}\right] = \frac{\partial}{\partial p_{j'}}\frac{\partial f}{\partial q_j} = \frac{\partial^2 f}{\partial p_{j'} \partial q_j} \tag{103}$$

Since

$$\frac{\partial^2 f}{\partial q_j \partial p_{j'}} = \frac{\partial^2 f}{\partial p_{j'} \partial q_j} \tag{104}$$

the last two terms in Eq. 101 cancel and under the transformation $[p_j, q_{j'}] \rightarrow [p_j, q_{j'}]$ as we wanted to prove.

Another very important consequence of Eq. 100 is that all observables transform by

$$A(p_j, q_j) \rightarrow A'(p_j, q_j) = A(p_j, q_j) + \epsilon[f(p_k, q_k), A(p_j, q_j)] \tag{105}$$

i.e. that $[f, \quad]$ is the generator of the infinitesimal transformation of all observables, not just of the p's and q's. Indeed, under the transformation

$$A(p_j, q_j) \rightarrow A'(p_j, q_j) = A\left(p_j - \epsilon\frac{\partial f}{\partial q_j}, q_j + \epsilon\frac{\partial f}{\partial p_j}\right) =$$

$$A(p_j, q_j) - \epsilon\sum_j\left(\frac{\partial A}{\partial p_j}\frac{\partial f}{\partial q_j} - \frac{\partial A}{\partial q_j}\frac{\partial f}{\partial q_j}\right) = A(p_j, q_j) + \epsilon[f, A] \tag{106}$$

Generators of symmetry transformations. Conservation laws.

We will conclude this set of lecture notes illustrating the transformations which are generated with by two important observables, namely the total momentum and the angular momentum.

Let us consider is the total momentum $\vec{P}$ of a multi-body system. Let us imagine that the system consists of N elementary components which we label by an index $k = 1, \ldots N$. We denote by m_k the mass of the k^{th} component and by $x_{i,k},\ i = 1,2,3$ its Cartesian coordinates. Let us denote by X_i the coordinates of the center of mass of the system

$$X_i = \frac{\sum_{k=1}^{N} m_k x_{i,k}}{\sum_{k=1}^{N} m_k} \tag{107}$$

and by $x'_{i,k}$ the relative coordinates of the system's components with respect to its center of mass

$$x'_{i,k} = x_{i,k} - X_i \tag{108}$$

Let us take the center of mass coordinates as the first three generalized coordinates

$$q_i \equiv X_i \quad i = 1,2,3 \tag{109}$$

and let us denote by $q_j,\ j = 4, \ldots K$ the remaining generalized coordinates. For example, if the system is a solid object, q_4, q_5, q_6 could be the three angles which are needed to specify its orientation. The relative coordinates $x'_{i,k}$ will only depend on $q_4, \ldots q_K$ and thus we will have

$$x_{i,k} = q_i + x'_{i,k}(q_j,\ j = 4, \ldots K) \quad i = 1,2,3 \tag{110}$$

The kinetic energy separates into the kinetic energy associated to the motion of the center of mass and the energy associated to the relative motion:

$$K = \frac{M \sum_{j=1}^{3} \dot{q}_j^2}{2} + K' \tag{111}$$

where we denoted by $M = \sum_{k=1}^{N} m_k$ the total mass of the system. It is clear from Eq. 110 that K' will only depend on $q_j, \dot{q}_j$ with $j \geq 4$ and therefore, for $j = 1,2,3$ we will have

$$p_j = \frac{\partial K}{\partial \dot{q}_j} = M\dot{q}_j = M\dot{X}_j \tag{112}$$

i.e. the first three conjugate momenta will be the three components of the total momentum of the system. To make clearer what follows, let us focus on one of these momenta, for example p_1. From Eq. 110 we derive the following expressions for the Poisson brackets of p_1 with the coordinates of the system's components:

$$\begin{aligned} [p_1, x_{1,k}] &= 1 \quad k = 1, \dots N \\ [p_1, x_{2,k}] &= 0 \quad k = 1, \dots N \\ [p_1, x_{3,k}] &= 0 \quad k = 1, \dots N \end{aligned} \tag{113}$$

Thus the infinitesimal transformation generated by p_1 is a translation of all the system in the direction of the first coordinate axis

$$\begin{aligned} x_{1,k} &\to x_{1,k} + \epsilon[p_1, x_{1,k}] = x_{1,k} + \epsilon \\ x_{2,k} &\to x_{2,k} + \epsilon[p_1, x_{2,k}] = x_{2,k} \\ x_{3,k} &\to x_{3,k} + \epsilon[p_1, x_{3,k}] = x_{3,k} \end{aligned} \tag{114}$$

And similarly p_2 and p_3 generate infinitesimal translations along the second and third coordinate axes.

On the other hand, Poisson brackets are left unchanged by canonical transformations, so Eqs. 114 will be true irrespective of the choice of canonical variables, even if the components of the total momentum are not among the canonical variables chosen to describe the system. The components total momentum of a system are always the generators of infinitesimal translations along the coordinate axes.

To illustrate the above statement let us consider a system of N interacting monoatomic molecules. The simplest canonical coordinates to use are the $3N$ positions of the molecules $x_{i,k}$ (we dispense here with the q_j notation). The conjugate momenta are then the actual momenta of the molecules $p_{i,k} = m_k \dot{x}_{i,k}$. The components of the total momentum

$$P_i = \sum_{k=1}^{N} p_{i,k} \tag{115}$$

are not among the canonical variables. Yet, if for definiteness we consider again P_1, we clearly have

$$[P_1, x_{i,k}] = \sum_{k'=1}^{N} [p_{1,k'}, x_{i,k}] = [p_{1,k}, x_{i,k}] = \delta_{1,i} \tag{116}$$

and we see that the infinitesimal canonical transformation generated by P_1

$$x_{i,k} \to x_{i,k} + \epsilon[P_1, x_{i,k}] = x_{i,k} + \epsilon\delta_{1,i} \tag{117}$$

is still an infinitesimal translation of all molecules' positions along the first axis.

A very important consequence of the fact that the total momentum of a system is the generator of (infinitesimal) translations is that, if a system is invariant under translations, its total momentum is conserved. Indeed, if a system is invariant under translations, its Hamiltonian must be left unchanged by a translation, and thus in particular by an infinitesimal translation. But the change of of any observable O induced by the the transformation generated by P_i is given by

$$O \to O' = O + \epsilon[P_i, O] \tag{118}$$

and in particular

$$H \to H' = H + \epsilon[P_i, H] \tag{119}$$

Thus, if H is left invariant, i.e. if $H' = H$, we must have

$$[P_i, H] = 0 \tag{120}$$

On the other hand the time evolution of P_i is given by

$$\frac{dP_i}{dt} = [H, P_i] \tag{121}$$

(see Eq. 46) and thus, if $[P_i, H] = -[H, P_i] = 0$, then $dP_i/dt = 0$ and the total momentum is conserved.

This relation is quite general: If the infinitesimal transformation induced by an observable O leaves the system invariant, then the observable O is conserved (assuming that O has no explicit time dependence.)

Another generator of important transformations is the angular momentum of a system. It is the generator of infinitesimal rotations. Without going into as much generality as we have done for the total momentum, let us consider just one point-like object of mass m and coordinates x_i. The conjugate moment are the components of the object's momentum $p_i = m\dot{x}_i$. Let us consider for definiteness the third component ℓ_3 of the object's angular momentum:

$$\ell_3 = x_1 p_2 - x_2 p_1 \tag{122}$$

The infinitesimal transformations induced by ℓ_3 are

$$\begin{aligned} x_1 &\rightarrow x_1' = x_1 + \epsilon[\ell_3, x_1] = x_1 - \epsilon[x_2 p_1, x_1] = x_1 - \epsilon x_2 \\ x_2 &\rightarrow x_2' = x_2 + \epsilon[\ell_3, x_1] = x_2 + \epsilon[x_1 p_2, x_2] = x_2 + \epsilon x_1 \\ x_3 &\rightarrow x_3' = x_3 + \epsilon[\ell_3, x_3] = x_3 \end{aligned} \tag{123}$$

and we recognize in the transformation the infinitesimal rotation of Eq. 95. It is easy to show that the momenta transform in the same way.

We conclude, in particular, that if a system is invariant with respect to rotations around an axis, then the corresponding component of its angular momentum is conserved.