Chapter 2
The Geometry of Hamiltonian Mechanics

In this chapter an introduction to Hamiltonian mechanics is given. Although, most of the textbooks devote one or more chapters to the Hamiltonian formulation of classical mechanics, only a few approach the subject from the theory of differential geometry [1, 3, 5]. The latter neatly exposes the geometrical properties of Hamiltonian mechanics. Modern analysis on manifolds [7] provides the means to develop the theory in a coordinate free way. However, numerical applications require the translation of the theory to specific coordinate systems. Hence, in this introductory chapter we follow both approaches to unveil the geometrical properties of Hamiltonian mechanics [4, 6]. This chapter must be read in parallel with the Appendix where some basic definitions and theorems from the calculus on manifolds are provided.

2.1 Configuration Manifolds and Coordinate Systems

2.1.1 Cartesian Coordinates

We consider a system of N particles whose configurations in a space fixed Cartesian coordinate system are described by N vectors of three components or with single vectors of $3N$ components. The Cartesian configuration space consists an ***Euclidean manifold*** (M) of dimension $3N$, $M \subset \mathbb{R}^{3N}$. The number of *degrees of freedom* for the system is $3N$. The positions of N particles with masses $m_\alpha, \alpha = 1, \ldots, N$, in our 3D world, are described by N vectors r^α

$$r^\alpha = x^\alpha \mathbf{i} + y^\alpha \mathbf{j} + z^\alpha \mathbf{k}, \quad \alpha = 1, \ldots, N. \tag{2.1}$$

$(\mathbf{i}, \mathbf{j}, \mathbf{k})$ denote the unit vectors along the (x, y, z)-axes, respectively.

The mechanical state of the system is defined by the coordinates of the particles and the rate of their change in time t, the velocities;

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$$v^\alpha = \frac{dr^\alpha}{dt} \equiv \dot{r}^\alpha = \frac{dx^\alpha}{dt}\mathbf{i} + \frac{dy^\alpha}{dt}\mathbf{j} + \frac{dz^\alpha}{dt}\mathbf{k}$$
$$\equiv \dot{x}^\alpha\mathbf{i} + \dot{y}^\alpha\mathbf{j} + \dot{z}^\alpha\mathbf{k}, \quad \alpha = 1, \dots, N. \tag{2.2}$$

Thus, the time evolution of the system is completely determined by the vectors, $[r^\alpha(t), v^\alpha(t)],\ \alpha = 1, \dots, N$.

The *kinetic energy* of the N-particle system is defined by the quadratic function in velocities

$$K = \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha (v^\alpha)^2$$
$$= \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha \left[(\dot{x}^\alpha)^2 + (\dot{y}^\alpha)^2 + (\dot{z}^\alpha)^2\right]. \tag{2.3}$$

The interactions among the particles are determined by the *potential energy*, $V(r^1, \dots, r^N)$, i.e., a function of the position vectors. The resultant *force* on particle α is the vector

$$F_\alpha = -\frac{\partial V(r)}{\partial r^\alpha} \equiv -\partial_\alpha V(r)$$
$$= -\frac{\partial V}{\partial x^\alpha}\mathbf{i} - \frac{\partial V}{\partial y^\alpha}\mathbf{j} - \frac{\partial V}{\partial z^\alpha}\mathbf{k}$$
$$= F_{x_\alpha}\mathbf{i} + F_{y_\alpha}\mathbf{j} + F_{z_\alpha}\mathbf{k}. \tag{2.4}$$

2.1.2 Curvilinear Coordinates

Because of some geometrical constraints or space-time symmetries which result in conservation laws, such as of the total energy, momentum and angular momentum, and the possible existence of other constants (integrals) of motion, the orbits of the particles are constrained in a configuration space with dimension less than $3N$. If there are k holonomic constraint equations[1]

$$\phi^i(r^1, \dots, r^N) = c^i, \quad i = 1, \dots, k, \tag{2.5}$$

that assign specific values to the associated quantities, geometrical or constants of motion, then, the number of degrees of freedom is $n = 3N - k$, and the configurations of the system form a ***smooth (differentiable) manifold*** Q of dimension n (see Appendix A), not necessarily Euclidean. The k constraint equations provide an implicit representation of the ***configuration manifold*** (see Appendix A.2).

[1] Holonomic constraints may contain the velocities $\phi^i(r^1, \dots, r^n, \dot{r}^1, \dots, \dot{r}^N) = c^i$, which however, can be integrated to equations without the velocities.

Taking into account possible constraint equations we may want to study the orbits of the system on the reduced dimension, n, configuration manifold Q. This may be an imperative step for extracting the underlying physics out of the dynamics of the system. Smooth manifolds can be covered by ***atlases of charts***, which locally define maps of open sets of the manifold to open sets of an Euclidean space. In this way we introduce generalized coordinates, $(q^1, \ldots, q^n)$, and apply ordinary calculus to study the dynamics of the system. However, it is worth emphasizing that global properties of manifolds may be studied without any reference to a local coordinate system. In principle and with the aid of the k constraint equations, one can find transformation equations from the n generalized coordinates to the $3N = n + k$ Cartesian coordinates

$$\begin{aligned} x^\alpha &= g_{x^\alpha}(q^1, \ldots, q^n, c^1, \ldots, c^k) \\ y^\alpha &= g_{y^\alpha}(q^1, \ldots, q^n, c^1, \ldots, c^k) \\ z^\alpha &= g_{z^\alpha}(q^1, \ldots, q^n, c^1, \ldots, c^k), \quad \alpha = 1, \ldots, N. \end{aligned} \tag{2.6}$$

The generalized velocities $(\dot{q}^1, \ldots, \dot{q}^n)$ are related to Cartesian velocities by the equations,

$$\begin{aligned} \dot{x}^\alpha &= \sum_{k=1}^{n} \frac{\partial g_{x^\alpha}}{\partial q^k} \dot{q}^k \\ \dot{y}^\alpha &= \sum_{k=1}^{n} \frac{\partial g_{y^\alpha}}{\partial q^k} \dot{q}^k \\ \dot{z}^\alpha &= \sum_{k=1}^{n} \frac{\partial g_{z^\alpha}}{\partial q^k} \dot{q}^k, \quad \alpha = 1, \ldots, N. \end{aligned} \tag{2.7}$$

Then, the kinetic energy (Eq. 2.3) in generalized coordinates will take the form,

$$K = \frac{1}{2} \sum_{i,k=1}^{n} \dot{q}^i g_{ik}(q, m) \dot{q}^k, \tag{2.8}$$

where, $g_{ik}(q, m)$ is the ***metric tensor*** and its components are functions of the masses, $m = (m_1, \ldots, m_\alpha, \ldots, m_N)$, and generalized coordinates, $q = (q^1, \ldots, q^n)^T$ [2] (see next section). The sum of kinetic and potential energy is the *total energy* of the system

$$E[q(t), \dot{q}(t)] = K[q(t), \dot{q}(t)] + V[q(t)]. \tag{2.9}$$

We must admit that the transformation equations from curvilinear to Cartesian coordinates and their inverses (Eq. 2.6) are not always easy to find. As a matter of

[2] The letter superscript (T) denotes a column vector and generally the transpose of a matrix.

fact, to determine the constants of motion for a dynamical system requires one to know the solutions of the equations of motion. The equations of motion take a simple form in Cartesian coordinates and can be solved numerically with modern computers for large systems with thousand of atoms. Combining, integration of equations of motion in Cartesian coordinates and transforming to specific curvilinear coordinates to describe the manifolds on which the trajectories lie is an appealing approach to illuminate Molecular Dynamics.

2.2 The Topological Map of Lagrangian and Hamiltonian Mechanics

Topological theories by not relying on specific coordinate systems have the advantage to reveal the general geometrical properties of physical systems, and thus, they are suitable for a qualitative analysis. In reverse, by knowing the topological structure of the system one can choose a suitable local coordinate system for computational work. Figure 2.1 portrays the topological structures of the two main formulations of Classical Mechanics, the Lagrangian and Hamiltonian. By considering the configuration space of a dynamical system as a smooth (differentiable) manifold, Q, there is always a ***chart*** (a local coordinate system), i.e., a homeomorphism (see Appendix A),

$$\phi : U \subset Q \to \phi(U) \subset \mathbb{R}^n, \tag{2.10}$$

of an open set U of Q onto an open set $\phi(U)$ of $\mathbb{R}^n$. Since, the map is on an Euclidean space ($\mathbb{R}^n$), we can also define a coordinate representation in $\mathbb{R}^n$

$$q^i = f^i \circ \phi \quad \text{or} \quad \phi(s) = (q^1(s), q^2(s), \ldots, q^n(s))^T \in \mathbb{R}^n, \tag{2.11}$$

for every point $s \in U$, and f^i are differentiable functions. The ***tangent space*** of Q (the space where the derivatives live) at a point $s \in Q$ ($T_s Q$) is a vector space (velocities belong to this space) and the union of all tangent spaces for all points s of Q form the ***tangent bundle*** (TQ) with Q the ***base space***

$$TQ = \bigcup_{s \in Q} T_s Q. \tag{2.12}$$

The tangent bundle contains both the manifold Q and its tangent spaces $T_s Q$ called the ***fibres*** and it is a smooth manifold of dimension $2n$. Since, TQ is also a smooth manifold a chart can be defined by the diffeomorphism

$$T\phi : TU \to \phi(U) \times \mathbb{R}^n \subset \mathbb{R}^n \times \mathbb{R}^n. \tag{2.13}$$

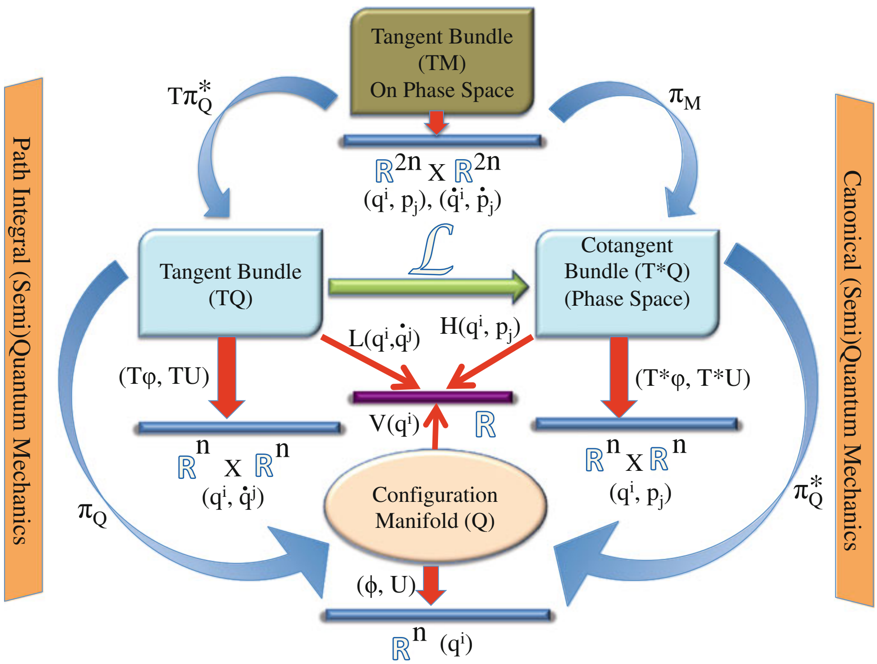

Fig. 2.1 Topological map of Lagrangian and Hamiltonian Mechanics. The tangent bundle (TQ) of the configuration manifold (Q) is a smooth manifold with charts defined by the generalized coordinates (q^i) and their corresponding velocities ($\dot{q}^j$). The Lagrangian, $L[q(t), \dot{q}(t)]$, is a function on the tangent bundle to real numbers. The dual space of TQ is the cotangent bundle ($M = T^*Q$), also named phase space. The phase space is a differentiable manifold of dimension $2n$ for which the tangent bundle, $TM \equiv T(T^*Q)$ of dimension ($2n \times 2n$), can also be defined with charts described by the generalized coordinates (q^i), the conjugate momenta (p_j) and their velocities ($\dot{q}^i, \dot{p}_j$). The potential function, $V(q)$, is a function on the configuration manifold to real numbers. The Hamiltonian, $H[q(t), p(t)]$, is a function on the phase space to real numbers obtained by a Legendre transform ($\mathbb{L}$) of the Lagrangian. We may consider that the Legendre transform generates a differentiable map between the tangent and cotangent bundles of Q, $F_{\mathbb{L}} : TQ \to T^*Q$. Then, the tangent mapping $TF_{\mathbb{L}}$ defines an isomorphism between the tangent of tangent bundle of Q (not shown) and the tangent bundle of phase space, $TF_{\mathbb{L}} : T(TQ) \to T(T^*Q)$. π_Q, π_Q^* and π_M are canonical projections. $T\pi_Q^*$ is the tangent mapping of π_Q^*. In Chap. 4 we discuss how the Lagrange formalism of classical mechanics leads to the path integral formulation of quantum mechanics and the Hamiltonian mechanics to canonical quantum mechanics

This is a linear map and each chart (ϕ, U) from the atlas of Q induces a chart $(T\phi, TU)$ for TQ. This chart is said to be the ***bundle chart*** associated with (ϕ, U).

The potential function V is a map of configuration manifold to real numbers $\mathbb{R}$, $V : Q \to \mathbb{R}$. On the tangent bundle we define the *state function*

$$L : TQ \to \mathbb{R}, \tag{2.14}$$

named *Lagrangian*. Having defined a chart the Lagrangian takes the form

$$L(q, \dot{q}) = K(q, \dot{q}) - V(q). \tag{2.15}$$

By using the Lagrangian we define the generalized momenta as

$$p_i(q, \dot{q}) = \frac{\partial L}{\partial \dot{q}^i}. \tag{2.16}$$

To extract the physical meaning of these derivatives we write the Lagrangian in Cartesian coordinates, Eq. 2.3.

$$L = K - V = \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha (v^\alpha)^2 - V(r), \;\; r = (r^1, \ldots, r^N). \tag{2.17}$$

The partial derivative of L with respect to the position vector of particle α, r_α, is the force acting on this particle, Eq. (2.4), whereas the partial derivative with respect to the velocity of particle α is

$$\frac{\partial L}{\partial v^\alpha} = m_\alpha v^\alpha. \tag{2.18}$$

The vector quantity

$$p_\alpha = m_\alpha v^\alpha = m_\alpha(\dot{x}^\alpha \mathbf{i} + \dot{y}^\alpha \mathbf{j} + \dot{z}^\alpha \mathbf{k}), \tag{2.19}$$

is the *momentum* of particle α.

Writing the Lagrangian in generalized coordinates,

$$L(q, \dot{q}) = \frac{1}{2}\sum_{i,j=1}^{n} \dot{q}^i g_{ij}(q, m)\dot{q}^j - V(q), \tag{2.20}$$

we define the component of the generalized force along the ith degree of freedom as

$$f_i = \frac{\partial L}{\partial q^i}, \tag{2.21}$$

and the component of the generalized momentum along the ith degree of freedom

$$p_i = \frac{\partial L}{\partial \dot{q}^i} = \sum_j g_{ij}\dot{q}^j. \tag{2.22}$$

The ***tangent*** and ***cotangent bundle*** (see Appendix A.8), TQ and T^*Q respectively, exist for any configuration manifold Q. If, however, we can define a metric on the manifold, i.e., Q is a Riemannian manifold, then, there is a diffeomorphism

$TQ \to T^*Q$ that sends the coordinate patch $(q, \dot{q})$ on the tangent space at a point s of Q to the coordinate patch (q, p) on the ***cotangent space***. Taking as a metric the covariant tensor rank-2, g_{ij}, that defines the kinetic energy, then, the momentum p_i is the ***covector*** of the velocity $\dot{q}^i$, and the velocity $\dot{q}^i$ can be obtained by the inverse tensor g^{ij}

$$\dot{q}^i = \sum_j g^{ij} p_j, \tag{2.23}$$

where $\sum_l g_{il} g^{lj} = \delta_i^j$.[3]

The metric tensor is a $2-$***form*** (see A.8), and thus, acts on two vectors of the tangent space to map them to a scalar. In other words, we can write

$$g_s(v, w) = \sum_{i=1}^{n} \sum_{j=1}^{n} v^i g_{ij} w^j, \tag{2.24}$$

where v^i and w^j are the components of the two vectors v and w of the tangent space, $T_s Q$, at the point s of the manifold Q, respectively in a local coordinate system. In a coordinate free interpretation of the metric, the kinetic energy is just the half of the metric, $K = \frac{1}{2} g_s(v, v)$. We may also consider the metric g_s to act only on one vector field, a mapping from TQ to T^*Q, i.e.,

$$g_s : TQ \to T^*Q : v \mapsto g_s(\bullet, v), \tag{2.25}$$

with $\bullet$ to denote a vacancy in the pair of vectors. Thus, $g_s(\bullet, v)$ is a $1-$***form***, which can act on another or the same vector in $T_s Q$ to yield a real number, $g_s(v, v)$. The metric assigns to each ***vector field*** $X \in \mathscr{X}(Q)$ the smooth $1-$form $g(\bullet, X) \in \mathscr{X}^*(Q)$, and vice versa. $\mathscr{X}(Q)$ is the set of vector fields on the configuration manifold Q and $\mathscr{X}^*(Q)$ the set of covectors. Therefore, we may conclude that, in charts the generalized momenta p_i, which is canonically conjugate to the coordinates q^i, is the $1-$form

$$p_i = \frac{\partial L}{\partial \dot{q}^i} = \sum_j g_{ij} \dot{q}^j \equiv g_s(\bullet, v), \tag{2.26}$$

which is a map from the tangent bundle (TQ) to the cotangent bundle (T^*Q). In fact, $(q, p) \equiv (q^1, \ldots, q^n, p_1, \ldots, p_n)$ are the local coordinates in the cotangent bundle which is called the *phase space* of the dynamical system.

The *Hamiltonian*, $H(q^i, p_j)$, is a function on the phase space to real numbers obtained by a *Legendre transform* ($\mathbb{L}$) of the Lagrangian

[3] The components of Kronecker delta tensor, δ_i^j, are equal to 1 for $i = j$ and 0 for $i \neq j$.

$$H(q, p) = \sum_{i=1}^{n} \dot{q}^i p_i - L(q, \dot{q}) = \sum_{i=1}^{n} \dot{q}^i \sum_{j=1}^{n} g_{ij}\dot{q}^j - L(q, \dot{q})$$
$$= \frac{1}{2}\sum_{ij} \dot{q}^i g_{ij}\dot{q}^j + V(q) = K + V. \quad (2.27)$$

The transformation equations in a new coordinate system in the configuration space lead to the following transformation equations for the velocities in the tangent space

$$Q^i = Q^i(q^1, \ldots, q^n), \quad i = 1, \ldots, n \quad (2.28)$$

$$\dot{q}^j = \sum_i \left(\frac{\partial q^j}{\partial Q^i}\right) \dot{Q}^i, \quad (2.29)$$

and the new momenta in the cotangent space

$$P_i = \frac{\partial L}{\partial \dot{Q}^i} = \sum_j \left(\frac{\partial L}{\partial \dot{q}^j}\right)\left(\frac{\partial \dot{q}^j}{\partial \dot{Q}^i}\right)$$
$$= \sum_j p_j \left(\frac{\partial q^j}{\partial Q^i}\right). \quad (2.30)$$

2.3 The Principle of Least Action

The function

$$S(q_a, q_b; t_a, t_b) = \int_{t_a}^{t_b} L[q(t), \dot{q}(t)]dt, \quad (2.31)$$

is called the *action* along the path that connects the configuration points q_a and q_b at the times t_a and t_b, respectively;

$$q_a = q(t_a), \quad q_b = q(t_b). \quad (2.32)$$

In mechanics we accept the *Principle of Least Action*; among the infinite number of paths between two fixed configuration points (q_a, q_b) and times t_a and t_b the system will follow that one which minimizes the action (Eq. 2.31),

$$S_0 = min\,[S(q_a, q_b; t_a, t_b)] = min \int_{t_a}^{t_b} L[q(t) + \delta q(t), \dot{q}(t) + \delta\dot{q}(t)]dt. \quad (2.33)$$

We assume the two end points fixed and we expand S in δq. The variation of S around an *extremum* q is

$$\delta S = \int_{t_a}^{t_b} L[q(t) + \delta q(t), \dot{q}(t) + \delta \dot{q}(t)]dt - \int_{t_a}^{t_b} L[q(t), \dot{q}(t)]dt$$
$$= \int_{t_a}^{t_b} \left(\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right) dt = 0. \tag{2.34}$$

Integrating by parts we have

$$\delta S = \int_{t_a}^{t_b} \left(\frac{\partial L}{\partial q} \delta q + \frac{d}{dt} \left[\frac{\partial L}{\partial \dot{q}} \delta q \right] - \frac{d}{dt} \left[\frac{\partial L}{\partial \dot{q}} \right] \delta q \right) dt$$
$$= \left[\frac{\partial L}{\partial \dot{q}} \delta q \right]_{t_a}^{t_b} + \int_{t_a}^{t_b} \left(\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right) \delta q dt = 0. \tag{2.35}$$

Since, $\delta q_a = \delta q_b = 0$ and δS is zero for any positive or negative variation of δq, we infer that

$$\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} = 0. \tag{2.36}$$

These are the *Euler–Lagrange equations*. Hence, according to the variational principle the equations of motion define the path for which the action takes a stationary value. Generally, for a system with n degrees of freedom is valid

$$\frac{\partial L}{\partial q^i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} = 0, \quad i = 1, \ldots, n. \tag{2.37}$$

For a Lagrangian written as in Eq. 2.17 the Euler–Lagrange equation (Eq. 2.37) takes the form

$$f_i = \dot{p}_i, \quad i = 1, \ldots, n, \tag{2.38}$$

i.e., *Newton's equations*. The importance of the Lagrangian stems from its utility to define the action along a path between two configuration points, (q_a, q_b). Hence, the action is a function of the initial and final configuration points as well as the time. The principle of the least action leads to the equations of motion, which involve the partial derivatives of the Lagrangian defined on the tangent space, TQ.

2.4 Hamiltonian Vector Fields

In Sect. 2.2 we introduced the Hamiltonian state function in phase space, the cotangent space of the tangent space of the configuration manifold. As we shall see, the Hamiltonian formalism of classical mechanics is the most appropriate to reveal intrinsic symmetries of the system, and the entrance to quantum and statistical mechanics. Thus, it is worth formulating classical mechanics in phase space. The Hamiltonian of a mechanical system in phase space, $H(q, p, t)$, is a function of coordinates, momenta and possibly of time. Then, the equations of motion can be inferred from the Principle of Least Action

$$\delta S(q_a, q_b; t_a, t_b) = \delta \left(\int_{t_a}^{t_b} \left(\sum_{i=1}^{n} p_i \dot{q}^i - H \right) dt \right) = 0, \tag{2.39}$$

with fixed end points. This equation is transformed to

$$\begin{aligned} \delta S &= \sum_{i=1}^{n} \int_{t_a}^{t_b} \left(\delta p_i \dot{q}^i + p_i \delta \dot{q}^i - \frac{\partial H}{\partial q^i} \delta q^i - \frac{\partial H}{\partial p_i} \delta p_i \right) dt \\ &= \sum_{i=1}^{n} \left[\int_{t_a}^{t_b} \delta p_i \left(\dot{q}^i - \frac{\partial H}{\partial p_i} \right) dt - \int_{t_a}^{t_b} \delta q^i \left(\dot{p}_i + \frac{\partial H}{\partial q^i} \right) dt + \left[p_i \delta q^i \right]_{t_a}^{t_b} \right] \\ &= 0. \end{aligned} \tag{2.40}$$

The last term evaluated at the end points is zero and the independent variations of δq_i and δp_i lead to *Hamilton's equations*

$$\begin{aligned} \dot{q}^i &= \frac{\partial H}{\partial p_i} \\ \dot{p}_i &= -\frac{\partial H}{\partial q^i}, \quad i = 1, \ldots, n. \end{aligned} \tag{2.41}$$

Equations 2.41 define the local ***flow*** of the *Hamiltonian vector field*. If we denote this vector field as $(X_H, \overline{(X_H)})^T$ to distinguish coordinates from momenta, then, the Hamiltonian vector field in local coordinates is written as

$$\begin{pmatrix} (X_H)^i \\ \overline{(X_H)_j} \end{pmatrix} = \begin{pmatrix} \partial H / \partial p_i \\ -\partial H / \partial q^j \end{pmatrix}, \quad i, j = 1, \ldots, n. \tag{2.42}$$

Hence, the principle of least action results in the Euler–Lagrange equations in the Lagrangian formalism, whereas in the Hamiltonian formalism of classical mechanics it gives Hamilton's equations. However, it is important to understand that in the

Lagrangian formalism the dynamics take place in the tangent of the tangent bundle of configuration manifold, $T(TQ)$, and in the Hamiltonian formalism in the tangent of the cotangent bundle of configuration manifold, $T(T^*Q)$. Since, the Lagrangian and Hamiltonian state functions are connected by a Legendre transform it can be proved that the two formulations of classical mechanics are equivalent.

Finally, if we consider the action as a function of the initial and final coordinates, not fixed but taking the path that minimizes the action, i.e., the generalized coordinates describe an integral solution of Hamilton's equations, then, the variation of the action is

$$\begin{aligned}\delta S(q_a, q_b) &= \sum_{i=1}^{n} \int_{t_a}^{t_b} \left(\delta p_i \dot{q}^i + p_i \delta \dot{q}^i - \frac{\partial H}{\partial q^i}\delta q^i - \frac{\partial H}{\partial p_i}\delta p_i \right) dt \\ &= \sum_{i=1}^{n} \left[\int_{t_a}^{t_b} \delta p_i \left(\dot{q}^i - \frac{\partial H}{\partial p_i} \right) dt - \int_{t_a}^{t_b} \delta q^i \left(\dot{p}_i + \frac{\partial H}{\partial q^i} \right) dt + \left[p_i \delta q^i \right]_{t_a}^{t_b} \right] \\ &= \sum_{i=1}^{n} \left[p_{ib}\delta q_b^i - p_{ia}\delta q_a^i \right], \end{aligned} \tag{2.43}$$

where a and b denote the end points of the path. Thus,

$$\begin{aligned}\frac{\partial S}{\partial q_a^i} &= -p_{ia} \\ \frac{\partial S}{\partial q_b^i} &= p_{ib}, \quad i = 1, \ldots, n. \end{aligned} \tag{2.44}$$

Similarly, if we consider the action as a function of the coordinates and time

$$\begin{aligned}\frac{d}{dt}S(q,t) = L &= \frac{\partial S}{\partial t} + \frac{\partial S}{\partial q}\dot{q} \\ &= \frac{\partial S}{\partial t} + p\dot{q}. \end{aligned} \tag{2.45}$$

Hence,

$$\frac{\partial S}{\partial t} = L - p\dot{q} = -H. \tag{2.46}$$

From the above equations we can write the total differential of action as

$$dS(q,t) = \sum_{i=1}^{n} p_i dq^i - H(q, p, t)dt. \tag{2.47}$$

2.5 The Canonical Equations Expressed with the Symplectic 2−Form

By replacing velocities with momenta not only second order differential equations (Euler–Lagrange) are replaced by the first order equations of Hamilton, but as we shall see, generalized coordinates and their conjugate momenta acquire equivalent significance and reveal the geometry of phase space. Let us first collect the generalized coordinates and their conjugate momenta of a dynamical system of n degrees of freedom to a single vector $x = (q^1, q^2, \ldots, q^n, p_1, p_2, \ldots, p_n)^T$ of $2n$-dimension. Then, Hamilton's equations are written in the form

$$\dot{x}(t) = J\partial H(x), \tag{2.48}$$

where ∂H is the gradient of Hamiltonian function, and J the *symplectic matrix*

$$J = \begin{pmatrix} 0_n & I_n \\ -I_n & 0_n \end{pmatrix}. \tag{2.49}$$

0_n and I_n are the zero and unit $n \times n$ matrices, respectively. It is proved that J satisfies the relations,

$$J^{-1} = -J = J^T \quad \text{and} \quad J^2 = -I_{2n}. \tag{2.50}$$

$X_{H_x} = J\partial H(x)$ is the Hamiltonian vector field as was defined by Eq. 2.42. In fact, as was discussed in Sect. 2.2 and from Fig. 2.1 (top) we can infer that x defines a chart in the tangent space (TM) of phase space M.

Let us denote with θ the 1−forms defined on the phase space manifold M

$$\theta : M \to T^*M : m \in M \mapsto \theta_m \in T^*_m M, \tag{2.51}$$

and with α the 1−forms on the configuration manifold Q

$$\alpha : Q \to T^*Q : r \in Q \mapsto \alpha_r \in T^*_r Q. \tag{2.52}$$

Since, α is a linear map from Q to M and θ an 1−form on M we can ***pull-back*** θ to Q to produce the 1−form $\alpha^*\theta$, which lives on the base manifold Q. Then, the **Canonical Poincaré** 1−**Form** is given by

$$\hat{\theta} = \sum_i p_i dq^i, \tag{2.53}$$

and satisfies the relation

$$\alpha^*\hat{\theta} = \alpha \quad \text{forall} \quad \alpha \in \mathscr{X}^*(Q). \tag{2.54}$$

$\hat{\theta}$ is invariant under coordinate transformations. This is proved by using Eq. 2.30. Indeed,

$$\begin{aligned}\hat{\theta} &= \sum_i p_i dq^i = \sum_i p_i \sum_j \frac{\partial q^i}{\partial Q^j} dQ^j \\ &= \sum_j \left(\sum_i p_i \frac{\partial q^i}{\partial Q^j} \right) dQ^j = \sum_j P_j dQ^j. \end{aligned} \tag{2.55}$$

The **Canonical Symplectic** 2− **Form** is extracted by taking the ***exterior derivative*** of $\hat{\theta}$

$$\hat{\omega} \equiv \overset{2}{\omega} = -d\hat{\theta}. \tag{2.56}$$

This is a ***closed*** 2−***form*** ($d\hat{\omega} = -d \circ d\hat{\theta} = 0$). In local coordinates (q, p), $\hat{\omega}$ is expressed by the ***wedge products*** (Darboux's theorem)

$$\hat{\omega}_r = \sum_i dq^i \wedge dp_i, \quad r \in M. \tag{2.57}$$

If we introduce $dx = (dq^1, \ldots, dq^n, dp_1, \ldots, dp_n)$, the symplectic 2−form (Eq. 2.57) is written

$$\hat{\omega} = \sum_{i=1}^{n} dx^i \wedge dx^{n+i}. \tag{2.58}$$

We can compute symplectic k−forms by taking the k−fold ***exterior products*** of $\hat{\omega}$

$$\begin{aligned} \hat{\omega}_r &= \sum_i dq^i \wedge dp_i, \\ \hat{\omega}_r \wedge \hat{\omega}_r &= -2! \sum_{i_1 < i_2} dq^{i_1} \wedge dq^{i_2} \wedge dp_{i_1} \wedge dp_{i_2}, \\ \hat{\omega}_r \wedge \hat{\omega}_r \wedge \hat{\omega}_r &= -3! \sum_{i_1 < i_2 < i_3} dq^{i_1} \wedge dq^{i_2} \wedge dq^{i_3} \wedge dp_{i_1} \wedge dp_{i_2} \wedge dp_{i_3}, \\ \cdots\cdots\cdots &= \cdots\cdots\cdots \end{aligned} \tag{2.59}$$

The largest $2n$−form is

$$\overbrace{\hat{\omega}_r \wedge \cdots \wedge \hat{\omega}_r}^{n-fold} = n!(-)^{[n/2]} dq^1 \wedge \cdots \wedge dq^n \wedge dp_1 \wedge \cdots \wedge p_n \tag{2.60}$$

and this defines the ***oriented volume*** form

$$\Omega_{\hat{\omega}} = \frac{(-)^{[n/2]}}{n!} \overbrace{\hat{\omega} \wedge \cdots \wedge \hat{\omega}}^{n-fold}. \tag{2.61}$$

$[n/2]$ is the largest integer smaller than or equal to $n/2$.

As is illustrated in the Appendix A.9.2, the geometric meaning of forms is that of an area or volume, objects, which are quite often introduced in chemical theories. For example, reaction rates are determined by the flux through a multidimensional dividing surface (transition state) and the evaluation of the density of states of reactant molecules, both requiring the calculation of phase space areas and volumes [2].

Summarizing, $\hat{\omega}$ is a symplectic form on a manifold M of even dimension $2n$ and it is non-degenerate, skew-symmetric, closed 2−form ($d\hat{\omega} = 0$). A pair $(M, \hat{\omega})$ is said to be a *symplectic manifold*. Those charts (coordinates) which satisfy Darboux's theorem, $\hat{\omega} = \sum_{i=1}^{n} dx^i \wedge dx^{n+i}$, are said to be *symplectic charts* and the local coordinates are called *canonical coordinates*. In the following we shall see that Hamiltonian mechanics and its geometrical properties can be formulated with $\hat{\omega}$.

2.5.1 Symplectic Transformations

The equations

$$X_i = F_i(x, t), \quad i = 1, \ldots, 2n, \tag{2.62}$$

define a transformation, which may involve both coordinates and their conjugate momenta, and do not change the equations of motion. These transformations are called *canonical* and the ***Jacobian matrix***, (DF), of the transformation, $(DF)_{ij} = \partial F_i/\partial x_j$, satisfies the *symplectic property*

$$(DF)^T J(DF) = J. \tag{2.63}$$

We can generalize the above transformations. A smooth map F that relates two symplectic manifolds $(M, \hat{\omega})$ and $(N, \hat{\tau})$ is said to be symplectic if $F^*\hat{\tau} = \hat{\omega}$, i.e., the pull-back of $\hat{\tau}$ yields $\hat{\omega}$. The symplectic maps are the canonical transformations of mechanics if the two manifolds (M, N) are identical

$$F^*\hat{\omega} = \hat{\omega}. \tag{2.64}$$

Let $(M, \hat{\omega})$ be a symplectic manifold of dimension $2n$ with $\hat{\omega}$ a canonical symplectic 2−form. The Hamiltonian function H is a smooth function on $M = T^*Q$. The Hamiltonian vector field, X_H, is then defined through the condition

$$i_{X_H}\hat{\omega} = \hat{\omega}(X_H, \bullet) = dH. \tag{2.65}$$

$i_{X_H}\hat{\omega}$ symbolizes ***interior product*** and the triple $(M, \hat{\omega}, X_H)$ is a *Hamiltonian system*.

Indeed, we have seen that Hamilton's equations can be written in the form

$$\dot{x}(t) = J\partial H[x(t)] = X_{H_x}, \tag{2.66}$$

where H is the Hamiltonian function and X_{H_x} the Hamiltonian vector field at x. Since, the Hamiltonian vector field in local coordinates is written as

$$\left((X_H)^i, \overline{(X_H)_j}\right)^T = \left(\frac{\partial H}{\partial p_i}, -\frac{\partial H}{\partial q^j}\right)^T,$$

the 2−form $\hat{\omega}$ with a vacant position $(\bullet)$ is transformed to

$$\begin{aligned}\hat{\omega}(X_H, \bullet) &= \sum_{i=1}^{n}\left(dq^i(X_H)dp_i - dp_i(X_H)dq^i\right),\\ &= \sum_{i=1}^{n}\left((X_H)^i dp_i - \overline{(X_H)_i}dq^i\right),\\ &= \sum_{i=1}^{n}\left(\frac{\partial H}{\partial p_i}dp_i + \frac{\partial H}{\partial q^i}dq_i\right),\\ &= dH.\end{aligned} \tag{2.67}$$

With every $Y \in \mathscr{X}(M)$ we can write

$$\hat{\omega}(X_H, Y) = dH(Y). \tag{2.68}$$

The integral curves of the Hamiltonian vector field X_H, $\Phi_t(x)$, are solutions of the canonical equations of motion Eq. 2.66. If the Hamiltonian does not have an explicit dependence on time, then, the energy is conserved. Indeed, the ***Lie derivative*** of the Hamiltonian is

$$\frac{d}{dt}H(x(t)) = dH(\dot{x}) = dH(X_{H_{x(t)}}) = \hat{\omega}(X_{H_{x(t)}}, X_{H_{x(t)}}) = 0. \tag{2.69}$$

We can also show this with charts.

$$\begin{aligned}\hat{\omega}(X_{H_{x(t)}}, X_{H_{x(t)}}) &= \sum_i dq^i \wedge dp_i(X_{H_{x(t)}}, X_{H_{x(t)}})\\ &= \sum_i \left[dq^i(X_{H_{x(t)}})dp_i(X_{H_{x(t)}}) - dp_i(X_{H_{x(t)}})dq^i(X_{H_{x(t)}})\right]\\ &= \sum_i \left[-\dot{q}^i\dot{p}_i + \dot{p}_i\dot{q}^i\right] = 0.\end{aligned} \tag{2.70}$$

Symplectic diffeomorphisms ($F^*\hat{\tau} = \hat{\omega}$) leave Hamilton's equations invariant. Using the properties of pull-back (Eq. A.89) we show

$$i_{X_{F^* H_\tau}} \hat{\omega} = d(F^* H_\tau) = F^* dH_\tau = F^* i_{X_{H_\tau}} \hat{\tau} = i_{F_*^{-1} X_{H_\tau}} F^* \hat{\tau} = i_{F_*^{-1} X_{H_\tau}} \hat{\omega}, \quad (2.71)$$

which implies $X_{F^* H_\tau} = F_*^{-1} X_{H_\tau}$. $F_*^{-1} X_{H_\tau}$ means push-forward the vector field X_{H_τ} which is related with $\hat{\tau}$ to the vector field $X_{F^* H_\tau}$ associated with the symplectic 2−form $\hat{\omega}$.[4]

---

[4] For time dependent Hamiltonians, $H(q, p, t)$, we can apply the same formalism of conservative Hamiltonians by introducing time as a new variable, $q^0 = t$, with conjugate momentum, p_0, and new Hamiltonian, $H_t = p_0 + H(q, p, t) = 0$. Thus, the extended phase space $M_t = T^* Q_t$ of the *extended configuration manifold*, $Q_t = (t, q^1, \ldots, q^n)^T$, is of $2(n+1)-$dimension and in its cotangent bundle we define the Canonical Poincaré 1−Form

$$\hat{\theta}_t = \sum_{i=0}^{n} p_i dq^i = p_0 dq^0 + \sum_{i=1}^{n} p_i dq^i = -H(q, p, t)dt + \hat{\theta}, \quad (2.72)$$

and symplectic 2−form

$$\hat{\omega}_t = -d\hat{\theta}_t = dH \wedge dt - d\hat{\theta} = -dt \wedge dH + \sum_{i=1}^{n} dq^i \wedge dp_i. \quad (2.73)$$

The new Hamiltonian vector field (X_{H_t}) is defined by the equation

$$\hat{\omega}_t(X_{H_t}, \bullet) = dH_t, \quad (2.74)$$

$$\begin{pmatrix} (X_{H_t})^0 \\ (X_{H_t})_0 \end{pmatrix} = \begin{pmatrix} 1 \\ -\partial H/\partial t \end{pmatrix}, \begin{pmatrix} (X_{H_t})^i \\ (X_{H_t})_i \end{pmatrix} = \begin{pmatrix} \partial H/\partial p_i \\ -\partial H/\partial q^i \end{pmatrix}, \quad i = 1, \ldots, n. \quad (2.75)$$

The Hamiltonian vector field lives in the tangent bundle of the extended phase space, $T(T^* Q_t)$, the base vector fields of which are

$$\left(\frac{\partial}{\partial t}, \frac{\partial}{\partial p_0}\right), \quad \left(\frac{\partial}{\partial q^i}, \frac{\partial}{\partial p_i}\right), \quad i = 1, \ldots, n. \quad (2.76)$$

$(M_t, \hat{\omega}_t, X_{H_t})$ is a Hamiltonian system and the Canonical Poincaré 1−Form, Eq. 2.72, is related to the total differential of action (Eq. 2.47). We can see, that with this formulation of time dependent systems the trajectories are projected at each time t in the physical phase space of the system of $2n-$dimension, $x = (q^1, \ldots, q^n, p_1, \ldots, p_n)^T$, and they are given by Hamilton's equations of motion with the time dependent Hamiltonian

$$\dot{x}(t) = J\partial H(x, t). \quad (2.77)$$

The symplectic maps of a symplectic vector space $(V, \hat{\sigma})$ onto itself

$$V : (V, \hat{\sigma}) \to (V, \hat{\sigma}), \quad F^{*}\hat{\sigma} = \hat{\sigma}, \tag{2.78}$$

form the *symplectic group* Sp_{2n}. Applying a symplectic transformation to the symplectic matrix J in local coordinate representation yields

$$(DF)^{T} J(DF) = J. \tag{2.79}$$

Theorem 1 (Liouville's Theorem)

If $(M, \hat{\omega}, X_H)$ *is a Hamiltonian system, and* Φ_t *the flow of the vector field* X_H $\left(\frac{d\Phi_t}{dt} = X_H\right)$*, then, for all times* t *the flow is symplectic, i.e.,* $\Phi_t^{*}\hat{\omega} = \hat{\omega}$*. From this, we conclude that the oriented volume* $\Omega_{\hat{\omega}}$ *(Eq. 2.61) is conserved* (Liouville's Theorem).

2.5.2 *Poisson Brackets*

f and g are two dynamical quantities acting on the Hamiltonian system $(M, \hat{\omega}, H)$. If X_f and X_g are vector fields assigned to the two dynamical quantities, then, they are defined by the equations

$$\hat{\omega}(X_f, \bullet) = df, \quad \hat{\omega}(X_g, \bullet) = dg, \tag{2.80}$$

which imply

$$X_f = \left(\frac{\partial f}{\partial p}, -\frac{\partial f}{\partial q}\right)^{T} \quad \text{and} \quad X_g = \left(\frac{\partial g}{\partial p}, -\frac{\partial g}{\partial q}\right)^{T}. \tag{2.81}$$

The Poisson bracket is defined as

$$\begin{aligned}
\hat{\omega}(X_f, X_g) &= df(X_g) \\
&= \sum_{i=1}^{n} \left[\frac{\partial f}{\partial q^i} dq^i(X_g) + \frac{\partial f}{\partial p_i} dp_i(X_g)\right] \\
&= \sum_{i=1}^{n} \left[\frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i} + \frac{\partial f}{\partial p_i}\left(-\frac{\partial g}{\partial q^i}\right)\right] \\
&= \sum_{i=1}^{n} \left[\frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q^i}\right] && (2.82) \\
&\equiv \{f, g\} = -\{g, f\}. && (2.83)
\end{aligned}$$

The Lie derivative of a dynamical quantity g with respect to a vector field X_f is defined as the directional derivative of g along the vector X_f

$$L_{X_f} g = dg(X_f) = \hat{\omega}(X_g, X_f). \tag{2.84}$$

So, to be consistent with the definition of Poisson brackets (Eq. 2.82) for a Hamiltonian vector field we take $L_{X_H} g = dg(X_H) = \hat{\omega}(X_g, X_H) = \{g, H\}$.

Some properties of Poisson brackets are:

P1: The Poisson bracket in terms of Lie derivative is written as

$$\{g, f\} = L_{X_f} g = dg(X_f) = -df(X_g) = -L_{X_g} f = -\{f, g\}. \tag{2.85}$$

P2: The quantity f (or g) is constant along the flow of X_g (X_f) if and only if $\{g, f\} = 0$.

P3: Let Φ_t be the flow of the Hamiltonian vector field X_H and g being a dynamical quantity, then, it is valid

$$\frac{d}{dt}(g \circ \Phi_t) = \frac{\partial}{\partial t}(g \circ \Phi_t) + \{g \circ \Phi_t, H\}. \tag{2.86}$$

P4: Poisson brackets defined on the set of smooth functions $\mathscr{F}(M)$ on M generate a Lie algebra, i.e.,

- $\{f, g\}$ is bilinear,
- $\{f, f\} = 0$, and
- $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\}$ (Jacobi identity).

P5: In a local symplectic chart with canonical coordinates (q^i, p_j) the following equations are true

$$\{q^i, q^j\} = 0 \tag{2.87}$$

$$\{p_i, p_j\} = 0 \tag{2.88}$$

$$\{q^i, p_j\} = \delta^i_j. \tag{2.89}$$

P6: F is diffeomorphism between two symplectic manifolds, $F : (M, \hat{\omega}) \to (N, \hat{\tau})$. This map is also symplectic if preserves the Poisson brackets of functions and/or $1-$forms, i.e.,

$$\{F^* f, F^* g\} = F^*\{f, g\} \text{ forall } \quad f, g \in \mathscr{F}(N). \tag{2.90}$$

Similarly to the previous section we can use the formalism of interior product to describe Lie derivatives and Poisson brackets. The Lie derivative of a form α is defined as (Cartan's magic formula)

$$L_X \alpha = i_X d\alpha + d i_X \alpha. \tag{2.91}$$

If α is a function (0−form) then

$$L_X \alpha = i_X d\alpha. \tag{2.92}$$

A differential form is conserved if

$$L_X \alpha = 0. \tag{2.93}$$

An example is the conservation of the canonical symplectic 2−form, $\hat{\omega}$, along a Hamiltonian vector field X_H

$$L_{X_H} \hat{\omega} = i_{X_H} d\hat{\omega} + d i_{X_H} \hat{\omega} = -i_{X_H} d \circ d\hat{\theta} + d \circ dH = 0. \tag{2.94}$$

The Poisson bracket is defined in terms of interior products as

$$\{g, f\} = L_{X_f} g = i_{X_f} dg = i_{X_f} i_{X_g} \hat{\omega}. \tag{2.95}$$

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