Chapter 2
A Brief Introduction to the Calculus of Variations

The Lagrangian and Hamiltonian formalisms will be useful in the following chapters when the heat kernel will be computed using the path integral and geometric variational methods. In the following we shall present a brief overview of the variational theory needed in the sequel.

2.1 Lagrangian Mechanics

In classical mechanics a moving particle is completely described at any instance of time t by its *position* $x(t)$ and its *velocity* $\dot{x}(t)$. The position x belongs to the *coordinate space*, which is, in general, a Riemannian manifold with the metric defined by the kinetic energy. The space of the positions and velocities $(x, \dot{x})$ is called the *phase space*, and it is identified with the tangent bundle TM of the coordinate space M. The pair $(x, \dot{x})$ is called the *state* of the particle.

A real-valued function defined on the tangent bundle $L : TM \to \mathbb{R}$ is called *Lagrangian*. In classical mechanics the usual Lagrangian is given by the difference between the *kinetic energy* and the *potential energy* of the particle:

$$L(x, \dot{x}) = K(\dot{x}) - U(x),$$

where $K(\dot{x}) = \frac{1}{2}\sum_{i=1}^{n} \dot{x}_i^2$ and $U(x)$ is usually a polynomial function of x. The trajectory of a particle $x(t)$ in the coordinate space is a curve parameterized by the time parameter t. The Lagrangian $L(x, \dot{x}, t)$ describes the dynamics of the particle, in the sense that the particle moves on a trajectory $x(t)$ such that the following action integral

$$S(x_0, x, \tau) = \int_0^{\tau} L(x(t), \dot{x}(t), t)\, dt \tag{2.1.1}$$

is locally minimized under small variations of the path $x(t)$. We shall investigate this problem in the next few sections.

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2.1.1 The First Variation

For our study it would be sufficient to investigate the case of Lagrangians that do not depend explicitly on time t. Let $x(t)$ be a smooth curve joining $x_0 = x(0)$ and $x = x(\tau)$. The action along $x(t)$ is given by

$$S = S\big(x(t)\big) = \int_0^\tau L\big(x(s), \dot{x}(s)\big)\, ds.$$

The main problem of Lagrangian formalism is formulated below:

Given the fixed endpoints x_0 and x, find the path $x(t)$ for which the functional

$$x(t) \to S\big(x(t)\big)$$

(a) Has a "critical point"
(b) Has a minimum

Customarily, this problem is approached by considering a fixed path $x(t)$ and a variation

$$x_\epsilon(t) = x(t) + \epsilon\eta(t)$$

with fixed endpoints

$$x_\epsilon(0) = x(0) = x_0, \qquad x_\epsilon(\tau) = x(\tau) = x_0.$$

The vector field $\eta(t)$ defined on $[0, \tau]$ is an arbitrary *variation vector field* with homogeneous boundary conditions

$$\eta(0) = \eta(\tau) = 0. \tag{2.1.2}$$

Expanding S about the path $x(t)$ in powers of ϵ yields

$$\begin{aligned} S\big(x_\epsilon(t)\big) &= S\big(x(t)\big) + \epsilon \int_0^\tau \left(\left\langle \frac{\partial L}{\partial \dot{x}}, \dot{\eta} \right\rangle + \left\langle \frac{\partial L}{\partial x}, \eta \right\rangle \right) dt \\ &\quad + \frac{\epsilon^2}{2!} \int_0^\tau \left(\left\langle \frac{\partial^2 L}{\partial \dot{x}^2}\dot{\eta}, \dot{\eta} \right\rangle + 2\left\langle \frac{\partial^2 L}{\partial \dot{x}\partial x}\dot{\eta}, \eta \right\rangle + \left\langle \frac{\partial^2 L}{\partial x^2}\eta, \eta \right\rangle \right) dt + \mathcal{O}(\epsilon^3) \\ &= S + \epsilon\, \delta S + \frac{\epsilon^2}{2!}\, \delta^2 S + \mathcal{O}(\epsilon^3), \end{aligned}$$

The path $x(t)$ is a "critical point" for the action functional $S\big(x(t)\big)$ if and only if $\delta S = 0$. Integrating by parts and using the boundary conditions (2.1.2) yields

$$0 = \delta S = \int_0^\tau \left(\left\langle \frac{\partial L}{\partial \dot{x}}, \dot{\eta} \right\rangle + \left\langle \frac{\partial L}{\partial x}, \eta \right\rangle \right) dt = \int_0^\tau \left(\left\langle -\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} + \frac{\partial L}{\partial x}, \eta \right\rangle \right) dt.$$

Since the vector field η is arbitrary, we obtain the variational equations, which are the famous *Euler–Lagrange equations*

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = \frac{\partial L}{\partial x}, \tag{2.1.3}$$

where $\dot{x} = (\dot{x}_1, \ldots, \dot{x}_n)$ and $x = (x_1, \ldots, x_n)$ denote the velocity and position of the particle, respectively. A solution of (2.1.3) is called a *classical path* and will play a central role in the rest of the book.

2.1.2 The Second Variation

Assume $x(t)$ is a solution of the Euler–Lagrange equations; i.e., it is a classical path. If the second variation is positive definite along $x(t)$, i.e.,

$$\langle \delta^2 S\, \dot{\eta}(t), \eta(t) \rangle > 0, \qquad \forall t \in (0, \tau), \tag{2.1.4}$$

for any variation vector field $\eta(t)$ with $\eta(0) = \eta(\tau) = 0$, then the path $x(t)$ minimizes the action functional between x_0 and $x(\tau)$. In order to have relation (2.1.4) satisfied, it suffices to prove that

$$\min_{\eta}\{\langle \delta^2 S\, \dot{\eta}(t), \eta(t) \rangle,\ \forall t \in (0, \tau)\} > 0.$$

Let η be a variation vector field for which the previous minimum is reached. Then η will satisfy the Euler–Lagrange equations for the associated Lagrangian

$$\overline{L}(\eta, \dot{\eta}) = \langle \delta^2 S\, \dot{\eta}(t), \eta(t) \rangle,$$

which are given by

$$\frac{d}{dt}\left(\frac{\partial^2 L}{\partial \dot{x}^2}\dot{\eta}\right) + \left[\frac{d}{dt}\left(\frac{\partial^2 L}{\partial x \partial \dot{x}}\right) - \frac{\partial^2 L}{\partial x^2}\right]\eta + \left[\frac{\partial^2 L}{\partial \dot{x}\partial x} - \frac{\partial^2 L}{\partial x \partial \dot{x}}\right]\dot{\eta} = 0, \tag{2.1.5}$$

which is called the *Jacobi equation*. A solution $\eta(t)$ of (2.1.5) is called a *Jacobi vector field*. If there is a value $t_1 \in (0, \tau)$ such that a Jacobi vector field $\eta(t_1) = 0$, then inequality (2.1.4) fails at $t = t_1$. A well-known result of variational calculus states that as long as the Jacobi vector field doesn't vanish, the classical path is still minimizing the action. The classical path ceases to be a minimizer as soon as the Jacobi vector field vanishes the first time. The vanishing points of a Jacobi vector field are called *conjugate points*. This is equivalent to saying that the classical path is minimizing between two consecutive conjugate points and is no longer minimizing after that.

2.1.3 Geometrical Interpretation

Next we shall deal with the geometrical significance of the Jacobi vector fields. Consider the classical path starting at x_0 and all the neighboring, classical paths $x(p,t)$ starting at the same point and parameterized by their initial momenta p; this is $x(p,0) = x_0$; see Fig. 2.1. For the time being we neglect the fixed endpoint condition at $t = \tau$. The separation between two classical paths is given by

$$x(p+\epsilon,t) = x(p,t) + \epsilon J(p,t) + \mathcal{O}(\epsilon^2),$$

with $J(p,t) = \big(J_{ij}\big)(p,t)$, where

$$J_{ij}(p,t) = \frac{\partial x_i(p,t)}{\partial p_j}, \qquad i,j = 1,\ldots,n. \tag{2.1.6}$$

Since $x(p,t)$ are classical paths, the Euler–Lagrange equations are satisfied:

$$\frac{d}{dt}\Big(\frac{\partial L}{\partial \dot{x}_r}\Big) = \frac{\partial L}{\partial x_r}, \qquad r = 1,\ldots,n.$$

Using the chain rule

$$\begin{aligned}\frac{\partial L}{\partial p_k} &= \frac{\partial L}{\partial x_i}\frac{\partial x_i}{\partial p_k} + \frac{\partial L}{\partial \dot{x}_j}\frac{\partial \dot{x}_j}{\partial p_k} \\ &= \frac{\partial L}{\partial x_i} J_{ik} + \frac{\partial L}{\partial \dot{x}_j}\dot{J}_{jk}\end{aligned}$$

and differentiating in the Euler–Lagrange equations yields

$$\frac{d}{dt}\left[\frac{\partial^2 L}{\partial \dot{x}_r \partial \dot{x}_i} J_{ik}\right] + \left[\frac{d}{dt}\frac{\partial^2 L}{\partial \dot{x}_r \partial x_i} - \frac{\partial L}{\partial x_r \partial x_i}\right] J_{ik} + \left[\frac{\partial^2 L}{\partial \dot{x}_r \partial x_i} - \frac{\partial^2 L}{\partial x_r \partial \dot{x}_i}\right] \dot{J}_{ik} = 0. \tag{2.1.7}$$

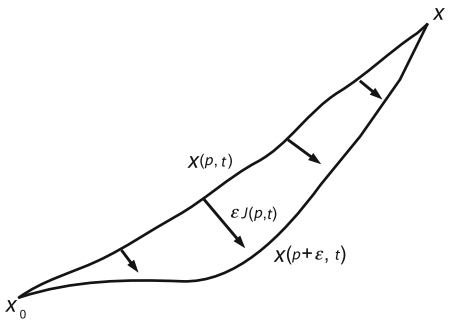

Fig. 2.1 The Jacobi vector field along a classical path between two conjugate points

A standard result of ODEs shows that the second-order-system (2.1.7) together with the following $2n^2$ initial conditions

$$J_{ik}(p,0) = \frac{\partial x_i(p,0)}{\partial p_k} = 0,$$
$$\dot{J}_{ik}(p,0) = \frac{\partial \dot{x}_i(p,0)}{\partial p_k} = \delta_{ik},$$

has a unique solution $J_{ij}(p,t) \neq 0$, for $t \in (0,\tau)$, with $\tau > 0$ small enough.

Let $p = \dot{x}(0)$ be fixed. For any vector $v = (v^1,\ldots,v^n) \neq 0$, we can define the vector field $\eta(t) = J(t)v$ along the classical path $x(t)$, by $\eta^i(t) = J_{ik}(t)v^k$. If there is a $T > 0$ such that $\eta(T) = 0$, then $\det J_{ik}(T) = 0$. The point $x(T)$ is conjugate with $x_0 = x(0)$, in the sense of the definition given in the previous section. This fact will be shown next.

Multiplying (2.1.7) by v^k and summing over k yields the equation

$$\frac{d}{dt}\left[\frac{\partial^2 L}{\partial \dot{x}_r \partial \dot{x}_i}\dot{\eta}^i\right] + \left[\frac{d}{dt}\frac{\partial^2 L}{\partial \dot{x}_r \partial x_i} - \frac{\partial^2 L}{\partial x_r \partial x_i}\right]\eta^i + \left[\frac{\partial^2 L}{\partial \dot{x}_r \partial x_i} - \frac{\partial^2 L}{\partial x_r \partial \dot{x}_i}\right]\dot{\eta} = 0,$$

which is exactly the Jacobi equation (2.1.5). The vector field $\eta(t)$ becomes a Jacobi vector field. Since J_{ik} is nondegenerate for $t \in (0,T)$, the set of Jacobi vectors forms an n-dimensional space at every point along the path $x(t)$. The first point where one Jacobi vector (and hence all of them) vanishes is a conjugate point with x_0. The classical path $x(t)$ minimizes the action as long as it does not pass through a conjugate point.

In the following we shall write the matrix J, which satisfies (2.1.7), in terms of the action S. Let x_0 and x be two fixed endpoints and let $x(t)$ be a classical path such that $x(0) = x_0$ and $x(\tau) = x$. The momentum along $x(t)$ at time t is denoted by $p(x_0,x;t)$. Let $\widetilde{x}(t)$ be the reverted curve defined by $\widetilde{x}(t) = x(\tau - t) = x(\tilde{t})$. The curves $\widetilde{x}(t)$ and $x(t)$ have the same endpoints, $x_0 = \widetilde{x}(\tau) = x(0)$ and $x = \widetilde{x}(0) = x(\tau)$. The following relation between the momenta along the curves $x(t)$ and $\widetilde{x}(t)$ holds:

$$p(x_0,x;t) = -p(x,x_0;\tau - t) = -p(x,x_0;\tilde{t}).$$

Using the well-known relation $\frac{\partial S}{\partial x} = p$ along $x(t)$ at instances t and τ yields

$$\frac{\partial S(x_0,x(t);t)}{\partial x(t)} = p(x_0,x(t);t), \qquad \frac{\partial S(x_0,x;\tau)}{\partial x} = p(x_0,x;\tau).$$

A similar argument for the curve $\widetilde{x}(t)$ yields

$$\frac{\partial S(x,x_0;\tilde{t})}{\partial x_0} = p(x,x_0;\tilde{t}) = -p(x_0,x;t).$$

Differentiating with respect to x yields

$$\frac{\partial S}{\partial x \partial x_0} = -\frac{\partial p(x_0, x; t)}{\partial x} = -\frac{1}{J(p, x)}. \tag{2.1.8}$$

This means that $\frac{\partial S}{\partial x^i \partial x_0^k}$ and $-J_{ik}$ are inverse matrices. Since at conjugate points $\det J_{ik} = 0$, it follows that at conjugate points

$$D = \det\Big(-\frac{\partial S}{\partial x \partial x_0}\Big) = \pm\infty.$$

One of the main properties of D is that it satisfies a *continuity equation* of the following type (see [54]):

$$\frac{\partial D}{\partial t} + \sum_k \frac{\partial}{\partial x_k}(\dot{x}_k\, D) = 0, \tag{2.1.9}$$

which means that D can be interpreted as a density of paths. This fact will be useful in the future chapters that deal with path integration, van Vleck's formula and the geometric method of computing heat kernels.

2.1.4 The Case of Riemannian Geometry

Consider the Lagrangian $L(x, \dot{x}) = \frac{1}{2}\sum_{i,j=1}^n g_{ij}(x)\dot{x}_i\dot{x}_j$, with g_{ij} a positive definite and non-degenerate matrix at each point $x \in \mathbb{R}^n$. This Lagrangian can also be considered on the tangent bundle of an n-dimensional Riemannian manifold (M, g). However, since we are studying local properties, we can make the simplifying assumption $M = \mathbb{R}^n$.

In this case the Euler–Lagrange equations become the familiar equations of geodesics

$$\ddot{x}_k(t) + \sum_{i,j} \Gamma_{ij}^k(x(t))\dot{x}_i(t)\dot{x}_j(t) = 0, \qquad k = 1, \ldots, n.$$

The classical paths are called geodesics and satisfy the following local result.

Theorem 2.1.1. *Given a point x_0 on a Riemannian manifold (M, g), there is a neighborhood $\mathcal{V}$ of x_0 such that for any $x \in \mathcal{V}$, there is a unique geodesic joining the points x_0 and x.*

The aforementioned result does not necessarily hold globally for any Riemannian manifold. However, it holds on compact manifolds, and in general on metrically complete manifolds, as the Hopf–Rinov theorem states; see [79].

Moreover, any geodesic is locally minimizing the action functional. The distance on the Riemannian manifold (M, g) is defined by

$$d(A, B) = \inf\{\ell(x) \mid \ x \text{ geodesic}, \ x(0) = A, x(\tau) = B\},$$

where the length of $x(t)$ is

$$\ell(x) = \int_0^\tau \sqrt{\sum_{i,j} g_{ij}(x(t))\dot{x}_i(t)\dot{x}_j(t)\, dt}.$$

The classical action in this case is given by the formula

$$S(x_0, x; t) = \frac{d^2(x_0, x)}{2t}.$$

Along a geodesic we have $\nabla S = \dot{x}(t)$, where ∇ is the gradient in the metric g:

$$g(U, \nabla S) = dS(U),$$

for any tangent vector field U; see [24].

The Jacobi equation (2.1.5) on Riemannian manifolds takes the form

$$\ddot{\eta}(t) = R\big(\eta(t)\dot{x}(t)\big)\dot{x}(t), \tag{2.1.10}$$

where R is the Riemannian curvature tensor induced by the Levi–Civita connection D:

$$R(U, V)W = D_{[U,V]}W - [D_U, D_V]W.$$

If the manifold has constant curvature K, then

$$R(U, V)W = K\big(g(W, U)V - g(W, V)U\big).$$

In this case, under the additional hypotheses that $x(t)$ is unit speed and the Jacobi vector field η is normal to the geodesic $x(t)$, the Jacobi equation (2.1.10) can be written in the suggestive form

$$\ddot{\eta}(t) = -K\eta(t), \tag{2.1.11}$$

with the initial condition $\eta(0) = 0$. Solving, we distinguish the following cases:

(1) Euclidean case: $K = 0$, $\eta(t) = ct$, c constant. See Fig. 2.2a.
(2) Elliptic case: $K = k^2 > 0$, $\eta(t) = c\sin(kt)$. See Fig. 2.2b.
(3) Hyperbolic case: $K = -k^2 < 0$, $\eta(t) = c\sinh(kt)$. See Fig. 2.2c.

In cases (1) and (3) there are no conjugate points, while in case (2) there are infinitely many conjugate points to $x(0)$ that occur at $t_n = n\pi/k$, $n = 1, 2, \ldots$.

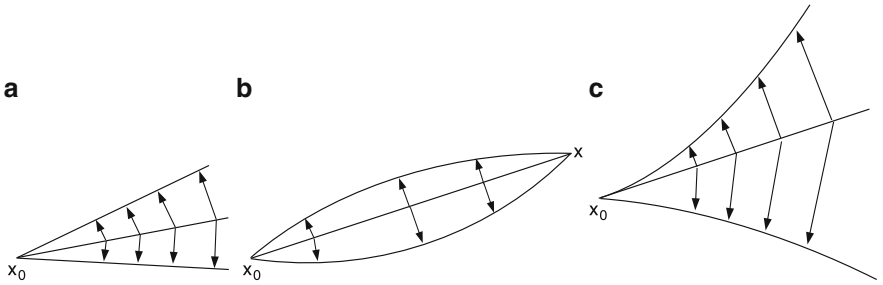

Fig. 2.2 (**a**) Euclidean case: $K = 0$; (**b**) elliptic case: $K > 0$; (**c**) hyperbolic case: $K < 0$

This behavior, for instance, occurs on a sphere. In general, all manifolds in situation (2) are compact. Just for the record, we include here a generalization of this case. Recall the notation for the diameter of a manifold as $\mathrm{diam}(M) = \sup\{d(p,q); p,q \in M\}$.

Theorem 2.1.2 (Myers). *Let (M,g) be a complete, connected n-dimensional Riemannian manifold. If there is a positive number $k > 0$ such that*

$$Ric \geq (n-1)k^2 g, \tag{2.1.12}$$

where Ric denotes the Ricci tensor of M, then the following relations hold:

(i) $diam(M) \leq \pi/k$
(ii) M is compact

As a special case of the previous theorem, we have

Corollary 2.1.3. *If (M,g) is a complete, connected n-dimensional Riemannian manifold with constant curvature K satisfying $K \geq k^2 > 0$, then*

(i) $diam(M) \leq \pi/k$
(ii) M is compact

References for Riemannian geometry and its variational methods are the books [24, 79, 94].

2.1.5 Examples of Lagrangian Dynamics

In the following examples we shall assume that the initial and final positions of the particle $x_0 = x(0)$ and $x = x(\tau)$ are given and we shall determine its trajectory between these endpoints.

Example 2.1.4 (The natural Lagrangian). Let $U(x)$ be a smooth potential, and consider the Lagrangian $L = \frac{1}{2}\dot{x}^2 - U(x)$. The Euler–Lagrange equation is

$$\ddot{x}(t) = -\frac{\partial U}{\partial x}. \tag{2.1.13}$$

Given the boundary conditions $x(0) = x_0$, $x(\tau) = x$, (2.1.13) might not always have a unique solution, regardless of how close the boundary points x_0 and x are: see [24]. If the potential is linear or quadratic, the aforementioned boundary value equation has a unique solution, and in this case the action is well defined. The Jacobi equation for the previous Lagrangian takes the form

$$\ddot{\eta}(t) = -\left.\frac{\partial^2 U(x)}{\partial x^2}\right|_{x(t)} \eta(t). \tag{2.1.14}$$

We note that if $U(x)$ is linear or quadratic in x, then the previous equation becomes similar to (2.1.11).

Example 2.1.5 (The free particle). If the Lagrangian is $L(\dot{x}, x) = \frac{1}{2}|\dot{x}|^2 = \frac{1}{2}\sum_j \dot{x}_j^2$, then the variational equation (2.1.13) is $\ddot{x}(t) = 0$, and the trajectories are the straight lines

$$x(t) = x_0 + \frac{t}{\tau}\big(x - x_0\big). \tag{2.1.15}$$

The Jacobi equation (2.1.14) is $\ddot{\eta}(t) = 0$. Using the initial conditions $\eta(0) = 0$, $\dot{\eta}(0) = 1$ yields the Jacobi vector field $\eta(t) = t$. The classical action is obtained by integrating the Lagrangian along the classical path:

$$S(x_0, x; \tau) = \int_0^\tau \frac{1}{2}\Big(\frac{x - x_0}{\tau}\Big)^2 dt = \frac{(x - x_0)^2}{2\tau}.$$

We recuperate formula (2.1.8) by taking the mixed derivative of the action

$$\frac{\partial^2 S}{\partial x \partial x_0} = -\frac{1}{\tau} = -\frac{1}{\eta(\tau)} \neq 0.$$

Hence there are no conjugate points to x_0 in this case. Next we shall check the continuity equation (2.1.9). We have $D = \frac{1}{t}$, $\dot{x}^k(t) = \frac{x^k - x_0^k}{t}$, and then

$$\begin{aligned}\frac{\partial D}{\partial t} + \sum_{k=1}^n \partial_{x_k}(v_k D) &= \frac{\partial}{\partial t}\frac{1}{t} + \sum_{k=1}^n \frac{\partial}{\partial x_k}\left(\frac{x^k - x_0^k}{t^2}\right) \\ &= -\frac{1}{t^2} + \frac{1}{t^2} = 0.\end{aligned}$$

Example 2.1.6 (Particle in constant gravitational field). The Lagrangian describing the dynamics of a free-falling particle under the action of a constant gravitational

force is given by $L(\dot{x}, x) = \frac{1}{2}\dot{x}^2 - kx$, $k > 0$. The trajectory $x(t)$ satisfies Galileo's equation $\ddot{x} = -k$ with the solution

$$x(t) = -\frac{k}{2}t^2 + (x - x_0)\frac{t}{\tau} + \frac{k}{2}t\tau + x_0.$$

Since the Jacobi equation is $\ddot{\eta}(t) = 0$ with the Jacobi vector field $\eta(t) = t \neq 0$, for $t > 0$, there are no conjugate points along the trajectory. We leave the computation of the classical action as an instructive exercise to the reader.

Example 2.1.7 (The linear oscillator). If $L(\dot{x}, x) = \frac{1}{2}\dot{x}^2 - \frac{k}{2}x^2$, $k > 0$, then the Euler–Lagrange equation is $\ddot{x}(t) = kx$, with the solution

$$x(t) = \big[x - x_0 \cosh(\sqrt{k}\tau)\big]\frac{\sinh(\sqrt{k}t)}{\sinh(\sqrt{k}\tau)} + x_0 \cosh(\sqrt{k}t).$$

This represents the trajectory of a particle under an elastic force $F(x) = kx$. The Jacobi equation (2.1.14) can be written as $\ddot{\eta}(t) = k\eta(t)$, and the Jacobi vector field is given by $\eta(t) = \frac{1}{\sqrt{k}}\sinh(\sqrt{k}t) \neq 0$, for $t > 0$. Then there are no conjugate points to x_0 along the classical path $x(t)$. A tedious computation shows that the classical action in this case is

$$S(x_0, x; \tau) = \frac{\sqrt{k}}{2\sinh(\sqrt{k}\,\tau)}\big[(x^2 + x_0^2)\cosh(\sqrt{k}\,\tau) - 2xx_0\big].$$

Differentiating yields

$$\frac{\partial^2 S}{\partial x \partial x_0} = -\frac{\sqrt{k}}{\sinh(\sqrt{k}\,\tau)} = -\frac{1}{\eta(t)},$$

which is (2.1.8).

Example 2.1.8 (The simple pendulum). The dynamics of a unit mass pendulum bob with unit length pendulum string under the action of the gravitational force is modeled by the Lagrangian $L(\dot{x}, x) = \frac{1}{2}\dot{x}^2 - k(1 - \cos x)$, $k > 0$. Its variational equation is given by the second-order differential equation $\ddot{x}(t) = -k \sin x$ that cannot be solved using elementary functions. A solution using elliptic functions can be found in [24], p. 38. In the case of small oscillations the dynamics is approximated by the linearized pendulum equation $\ddot{x}(t) = -kx$, with the solution

$$x(t) = \big[x - x_0 \cos(\sqrt{k}\,\tau)\big]\frac{\sin(\sqrt{k}\,t)}{\sin(\sqrt{k}\tau)} + x_0 \cos(\sqrt{k}\,t).$$

The Jacobi equation (2.1.14) becomes

$$\ddot{\eta}(t) = -k\eta(t).$$

Under the standard initial conditions, the Jacobi vector field is $\eta(t) = \frac{1}{\sqrt{k}} \sin(\sqrt{k}\, t)$. Hence the conjugate points to x_0 will occur along $x(t)$ at instances $t_n = n\pi/\sqrt{k}$, $n = 1, 2, \ldots$. The classical action is

$$S(x_0, x; \tau) = \frac{\sqrt{k}}{2\sin(\sqrt{k}\,\tau)}\big[(x^2 + x_0^2)\cos(\sqrt{k}\,\tau) - 2xx_0\big], \qquad \tau \notin \{n\pi/\sqrt{k}\}.$$

Example 2.1.9 (Particle in a constant electric field). The Lagrangian of a particle in a one-dimensional electric potential $U(x) = k/x$, $x > 0$, is $L(\dot{x}, x) = \frac{1}{2}\dot{x}^2 - k/x$, $k > 0$. The trajectories satisfy the equation $\ddot{x} = k/x^2$, which cannot be integrated using elementary functions. The same occurs for the Jacobi equation

$$\ddot{\eta} = -\frac{2k}{x^3}\eta.$$

2.2 Hamiltonian Mechanics

An alternate way of describing the dynamics of a particle is using the *Hamiltonian function*. A real-valued function defined on the cotangent bundle of the coordinate space T^*M is called a Hamiltonian function. There is an intimate relationship between the Lagrangian and the Hamiltonian associated with a moving particle. The Hamiltonian associated with a Lagrangian is obtained using Legendre's transform

$$H(x, p) = p\dot{x} - L(x, \dot{x}, t),$$

where $\dot{x}$ is a function of the momentum p obtained by solving the equation

$$p = \frac{\partial L}{\partial \dot{x}}. \tag{2.2.16}$$

For instance, if the Lagrangian $L(x, \dot{x}) = \frac{1}{2}\dot{x}^2 - x^m$, then the Hamiltonian is

$$H(x, p) = \frac{1}{2}p^2 + x^m.$$

The procedure works vice versa, i.e., for a given Hamiltonian, the associated Lagrangian can be obtained by

$$L(x, \dot{x}, t) = p\dot{x} - H(x, p),$$

with the momentum p given by (2.2.16).

The dynamics of the particle is described in the cotangent space by the Hamiltonian system of equations

$$\begin{aligned} \dot{x} &= \partial_p H, \\ \dot{p} &= -\partial_x H. \end{aligned}$$

A solution $\big(x(t), p(t)\big)$ of the aforementioned system is called a *bicharacteristic*.

If the Hamiltonian H does not depend explicitly on the time variable t, the system is said to be conservative, because in this case the Hamiltonian evaluated along the above solutions is constant. This can be verified by using the chain rule. If $\big(x(t), p(t)\big)$ is a bicharacteristic curve, then

$$\frac{d}{dt} H\big(x(t), p(t)\big) = \dot{x}(t)\, \partial_x H + \dot{p}(t)\, \partial_p H = 0.$$

The value of the Hamiltonian evaluated along the bicharacteristic is called the *total energy* of the particle. This is a first integral of motion.

If $(x(t), p(t))$ is a bicharacteristic curve, then the component $x(t)$ is a solution of the Euler–Lagrange equation. Conversely, if $x(t)$ is a solution of the Euler–Lagrange equations, then $\big(x(t), \frac{\partial L}{\partial \dot{x}}(t)\big)$ is a bicharacteristic curve, called the *lift* of $x(t)$.

2.3 The Hamilton–Jacobi Equation

The *classical action* associated with the Lagrangian $L(x, \dot{x}, t)$ is obtained by integrating the Lagrangian along the solution of the Euler–Lagrange equation

$$S_{cl}(x_0, x; \tau) = \int_0^\tau L\big(x(t), \dot{x}(t), t\big)\, dt. \tag{2.3.17}$$

This assumes that there is only one solution $x(t)$ satisfying the boundary conditions $x(0) = x_0$ and $x(\tau) = x$. The classical action is a solution of the following *Hamilton–Jacobi equation*:

$$\frac{\partial}{\partial \tau} S_{cl} + H(x, \partial_x S_{cl}) = 0. \tag{2.3.18}$$

Since the above equation is nonlinear, there might be more than one solution. In the case of a conservative system, if $E = E(x_0, x, \tau) = H$ denotes the energy along the solution, the equation becomes

$$\frac{\partial}{\partial \tau} S_{cl} = -E,$$

with the solution

$$S_{cl}(x_0, x, \tau) = -E(x_0, x, \tau)\tau + c(x_0, x), \tag{2.3.19}$$

where $c(x_0, x) = S_{cl}(x_0, x, 0)$ is the initial condition.

The action plays a very important role in the geometric methods of finding the heat kernel. To conclude our brief discussion, there are three ways of computing the action.

1. *Starting from the Lagrangian*. After solving the Euler–Lagrange equations, we integrate the Lagrangian along solutions using formula (2.3.17). This is a robust method and works as long as we are able to solve the Euler–Lagrange system of equations explicitly.

2. *Solving the Hamilton–Jacobi equation*. Substitute $p = \partial_x S$ in the expression of the Hamiltonian H and solve (2.3.18). Because it is nonlinear, there are no standard methods to solve the aforementioned equation. Depending on the problem, one may try different strategies. For instance, we can try to look for particular solutions of the type $S(x,t) = a(t) + b(x)$. Substituted in (2.3.18), the functions $a(t)$ and $b(x)$ satisfy the separable equation

$$a'(t) + H(x, \partial_x b) = 0,$$

so there is a constant C such that

$$\begin{aligned} a'(t) = -C \Longrightarrow a(t) &= -Ct + a(0), \\ H(x, \partial_x b) &= C. \end{aligned} \tag{2.3.20}$$

If the Hamiltonian H does not depend explicitly on the variable x, (2.3.20) can sometimes be reduced to an *eikonal equation*. For instance, if $H = \frac{1}{2}|p|^2$, then the function $b(x)$ satisfies

$$|\partial_x b|^2 = C/2, \qquad C > 0.$$

This equation has infinitely many solutions of the type

$$b(x) = \sqrt{\frac{2}{C}}|x - x_0| = \sqrt{\frac{2}{C}\sum_{i=1}^{n}(x_i - x_i^0)^2}, \qquad x_0 \in \mathbb{R}^n.$$

3. *The conservative Hamiltonian case*. If the Hamiltonian does not depend explicitly on the time parameter t, the action function is given by (2.3.19), where the energy should be expressed in terms of the endpoints $x(0)$ and $x(\tau)$.

Next we shall work out an example. The aforementioned methods will be used to find the action function for the *free particle case*; see Example 2.1.5. Differentiating in (2.1.15) yields

$$\dot{x} = \frac{1}{\tau}\big(x(\tau) - x(0)\big).$$

The Lagrangian along the solution is

$$L(x, \dot{x}) = \frac{1}{2}\dot{x}^2 = \frac{|x(\tau) - x(0)|^2}{2\tau^2},$$

and using (2.3.17) we obtain the action

$$S(x_0, x; \tau) = \int_0^\tau \frac{|x(\tau) - x(0)|^2}{2\tau^2}\, dt = \frac{|x(\tau) - x(0)|^2}{2\tau} = \frac{|x - x_0|^2}{2\tau}.$$

If we try to solve the Hamilton–Jacobi equation, using $\partial_x S = p = \frac{\partial L}{\partial \dot{x}} = \dot{x}$, (2.3.18) becomes

$$\frac{\partial}{\partial \tau} S + \frac{1}{2}|\dot{x}(t)|^2 = 0 \Longleftrightarrow \frac{\partial}{\partial \tau} S = -\frac{1}{2}\frac{|x - x_0|^2}{\tau^2} \Longleftrightarrow$$
$$\frac{\partial}{\partial \tau} S = \frac{\partial}{\partial \tau}\left(\frac{|x - x_0|^2}{2\tau}\right).$$

Integrating yields the aforementioned relation for the action.

The reader can find more advanced topics on the calculus of variations in [6, 24, 52].

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