Chapter 1
Analytical Mechanics

1.1 Introduction

The differential equations that govern the dynamical problems can be derived from variational principles, upon which the theories of Euler and Lagrange, and those of Hamilton and Jacobi, are based. Apart from being the source of the greatest intellectual enjoyment, these theories have the definite advantage of generality. Their concepts can in fact be extended to cases where the Newtonian equation of dynamics does not apply. Among such cases there are the equations governing the electromagnetic field and those related to the quantum description of the particles' motion.

The invariance property of the Lagrange equations with respect to a change of coordinates gives origin to the concept of generalized coordinates and conjugate momenta; in turn, the introduction of the Hamilton equations provides a picture in which the intrinsic symmetry of the roles of coordinates and momenta becomes apparent. Basing on the concept of conjugate coordinates, the time evolution of a particle or of a system of particles is described in the phase space instead of the coordinate space. This chapter and the next one illustrate the basic principles of Analytical Mechanics. Their purpose is to introduce a number of concepts that are not only useful *per se*, but also constitute a basis for the concepts of Quantum Mechanics that are introduced in later chapters. A third chapter devoted to Analytical Mechanics describes a number of important examples, that will be applied to later developments illustrated in the book.

As the velocity of particles within a semiconductor device is small with respect to that of light, the non-relativistic form of the mechanical laws is sufficient for the purposes of this book. The relativistic form is used only in a few paragraphs belonging to the chapter devoted to examples, to the purpose of describing a specific type of collision between particles. This chapter starts with the description of the Lagrangian function and the Lagrange equations, that are derived as a consequence of the variational calculus, followed by the derivation of the Hamiltonian function and Hamilton equations. Next, the Hamilton–Jacobi equation is derived after discussing the time–energy conjugacy. The chapter continues with the definition of the Poisson

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brackets and the derivation of some properties of theirs, and concludes with the description of the phase space and state space.

1.2 Variational Calculus

Consider a real function $w(\xi)$ defined in the interval $\xi \in [a, b]$ and differentiable in its interior at least twice. The first two derivatives will be indicated with $\dot{w}$ e $\ddot{w}$. Now, define the integral

$$G[w] = \int_a^b g(w, \dot{w}, \xi)\, \mathrm{d}\xi, \tag{1.1}$$

where the form of the function $g(w, \dot{w}, \xi)$ is prescribed. If (1.1) is calculated for any function w fulfilling the requisites stated above, with a and b fixed, the result is some real number G whose value depends on the choice of w. By this procedure, (1.1) establishes a correspondence $G[w]$ between a set of functions and a set of numbers. Such a correspondence is called *functional*.

It is interesting to extend to the case of functionals some concepts and procedures that apply to functions proper; among these it is important the concept of extremum. In fact, one defines the *extremum function* of a functional by a method similar to that used for defining the extremum point of a function: some w is an extremum of G if a variation $\mathrm{d}w$ in (1.1) produces a variation $\mathrm{d}G$ that is infinitesimal of an order higher than that of $\mathrm{d}w$. The procedure by which the extremum functions are calculated is called *variational calculus*.

To proceed it is necessary to define the variation $\mathrm{d}w$. For this one lets $\delta w = \alpha\eta$, with $\eta(\xi)$ an arbitrary function defined in $[a, b]$ and differentiable in its interior, and α a real parameter. The function δw thus defined is the finite variation of w. The sum $w + \delta w$ tends to w in the limit $\alpha \to 0$. As a consequence, such a limit provides the infinitesimal variation $\mathrm{d}w$. For simplicity it is convenient to restrict the choice of η to the case $\eta(a) = \eta(b) = 0$, so that $w + \delta w$ coincides with w at the integration boundaries for any value of α.

Now, replacing w with $w + \alpha\eta$ in (1.1) makes G a function of α, whose derivative is

$$\frac{\mathrm{d}G}{\mathrm{d}\alpha} = \int_a^b \left[\frac{\partial g}{\partial(w + \alpha\eta)}\, \eta + \frac{\partial g}{\partial(\dot{w} + \alpha\dot{\eta})}\, \dot{\eta} \right] \mathrm{d}\xi. \tag{1.2}$$

According to the definition given above, if w is an extremum function of G then it must be $\lim_{\alpha\to 0} \mathrm{d}G/\mathrm{d}\alpha = 0$; in this case, in fact, the first-order term in the power expansion of G with respect to α vanishes, and the variation of G becomes second order in α or higher. In conclusion, one proceeds by imposing that the right hand side of (1.2) vanishes for $\alpha = 0$. Then, integrating by parts the second term in brackets yields

$$\int_a^b \frac{\partial g}{\partial w} \eta \mathrm{d}\xi + \left[\frac{\partial g}{\partial \dot{w}} \eta \right]_a^b = \int_a^b \left(\frac{\mathrm{d}}{\mathrm{d}\xi} \frac{\partial g}{\partial \dot{w}} \right) \eta \mathrm{d}\xi \tag{1.3}$$

where, in turn, the integrated part vanishes because $\eta(a) = \eta(b) = 0$. This makes the two integrals in (1.3) equal to each other. On the other hand, such an equality must hold for any choice of η due to the arbitrariness of the latter. It follows that the integrands must be equal to each other, namely,

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\frac{\partial g}{\partial \dot{w}} = \frac{\partial g}{\partial w}. \tag{1.4}$$

The relation (1.4) thus found is a second-order differential equation in the unknown w, whose explicit form is easily calculated:

$$\frac{\partial^2 g}{\partial \dot{w}^2}\,\ddot{w} + \frac{\partial^2 g}{\partial w \partial \dot{w}}\,\dot{w} + \frac{\partial^2 g}{\partial \xi \partial \dot{w}} = \frac{\partial g}{\partial w}. \tag{1.5}$$

Its solution provides the extremum function w sought. To actually find a solution one must associate to (1.4) suitable boundary conditions, e.g., $w(a) = w_a$, $\dot{w}(a) = \dot{w}_a$, or $w(a) = w_a$, $w(b) = w_b$, and so on. As g does not contain $\ddot{w}$, (1.4) is linear with respect to $\ddot{w}$. It is also worth noting that, consistently with what happens in the case of functions proper, the above calculation does not provide in itself any information about w being a minimum or maximum of G. Such an information must be sought through additional calculations.

The analysis above is easily extended to the case where g depends on several functions $w_1, w_2, \ldots$ and the corresponding derivatives. Introducing the vectors $\mathbf{w}(\xi) = (w_1, w_2, \ldots, w_n)$, $\dot{\mathbf{w}}(\xi) = (\dot{w}_1, \dot{w}_2, \ldots, \dot{w}_n)$ one finds that the set of n extremum functions $w_i(\xi)$ of functional

$$G[\mathbf{w}] = \int_a^b g(\mathbf{w}, \dot{\mathbf{w}}, \xi)\,\mathrm{d}\xi \tag{1.6}$$

is the solution of the set of differential equations

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\frac{\partial g}{\partial \dot{w}_i} = \frac{\partial g}{\partial w_i}, \qquad i = 1, \ldots, n, \tag{1.7}$$

supplemented with suitable boundary conditions. Equations (1.7) are called *Euler equations* of the functional G.

Each equation (1.7) is homogeneous with respect to the derivatives of g and does not contain g itself. As a consequence, the differential equations (1.7) are invariant when g is replaced with $A\,g + B$, where $A, B \neq 0$ are constants. As the boundary conditions of w_i are not affected by that, the solutions w_i are invariant under the transformation. Moreover, it can be shown that the solutions are invariant under a more general transformation. In fact, consider an arbitrary function $h = h(\mathbf{w}, \xi)$ and let $g' = g + \mathrm{d}h/\mathrm{d}\xi$, this transforming (1.6) into

$$G'[\mathbf{w}] = A \int_a^b g(\mathbf{w}, \dot{\mathbf{w}}, \xi)\,\mathrm{d}\xi + h(\mathbf{w}_b, \xi_b) - h(\mathbf{w}_a, \xi_a). \tag{1.8}$$

When each w_i is replaced with $w_i + \mathrm{d}w_i$, the terms involving h do not vary because the variations vanish at the boundaries of the integration domain. Thus, the variation of

G' equals that of the integral, namely, it is of a higher order than $\mathrm{d}w_i$. In conclusion, the extremum functions of G are also extremum functions of G'. This means that the solutions $w_i(\xi)$ are invariant under addition to g of the total derivative of an arbitrary function that depends on $\mathbf{w}$ and ξ only. This reasoning does not apply if h depends also on the derivatives $\dot{\mathbf{w}}$, because in general the derivatives of the variations do not vanish at the boundaries.

1.3 Lagrangian Function

In many cases the solution of a physical problem is achieved by solving a set of second-order differential equations of the form $\ddot{w}_i = \ddot{w}_i(\mathbf{w}, \dot{\mathbf{w}}, \xi)$. For instance, for non-relativistic velocities the law of motion of a particle of constant mass m is Newton's law $\mathbf{F} = m\mathbf{a}$ which, in a Cartesian frame, takes the form

$$m\,\ddot{x}_i = F_i(\mathbf{r}, \dot{\mathbf{r}}, t), \qquad i = 1, 2, 3. \tag{1.9}$$

In (1.9), $\mathbf{r}(t) = (x_1, x_2, x_3)$ is the particle's position vector[1] at t. In the following the particle's velocity will be indicated with $\mathbf{u} = \dot{\mathbf{r}}$.

Equations (1.9) and (1.7) have the same form, as is easily found by observing that t is the analogue of ξ and x_i is that of w_i. As a consequence, one may argue that (1.9) could be deduced as Euler equations of a suitable functional. This problem is in fact the inverse of that solved in Sect. 1.2: there, the starting point is the function g, whose derivatives provide the coefficients of the differential equations (1.7); here, the coefficients of the differential equation are given, while the function g is to be found. For the inverse problem the existence of a solution is not guaranteed in general; if a solution exists, finding the function g may be complicated because the process requires an integration. In other terms, the direct problem involves only the somewhat "mechanical" process of calculating derivatives, whereas the inverse problem involves the integration which is, so to speak, an art.

When dealing with the dynamics of a particle or of a system of particles, the function g, if it exists, is called *Lagrangian function* and is indicated with L. The equations corresponding to (1.7) are called *Lagrange equations*. The expression of the Lagrangian function depends on the form of the force F_i in (1.9). Some examples are given in the following. It is important to note that by "system of particles" it is meant a collection of particles that interact with each other. If there were no interactions it would be possible to tackle the dynamics of each particle separately; in other terms, each particle would constitute a system in itself, described by a smaller number of degrees of freedom.

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[1] The units in (1.9) are: $[m] = \mathrm{kg}$, $[\mathbf{r}] = \mathrm{m}$, $[\dot{\mathbf{r}}] = \mathrm{m\,s^{-1}}$, $[\ddot{x}_i] = \mathrm{m\,s^{-2}}$, $[F_i] = \mathrm{N}$, where "N" stands for Newton.

1.3.1 Force Deriving from a Potential Energy

Consider the case of a force deriving from a potential energy, namely $\mathbf{F} = -\mathrm{grad} V$ with $V = V(\mathbf{r}, t)$, so that (1.9) becomes

$$m\dot{u}_i = -\frac{\partial V}{\partial x_i}. \tag{1.10}$$

Using the replacements $\xi \leftarrow t$, $w_i \leftarrow x_i$, $g \leftarrow L$ and equating (1.7) and (1.10) side by side yields

$$\frac{\partial L}{\partial x_i} = -\frac{\partial V}{\partial x_i}, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial u_i} = \frac{\mathrm{d}}{\mathrm{d}t}(m u_i), \qquad i = 1, 2, 3. \tag{1.11}$$

The first of (1.11) shows that the sum $T = L + V$ does not depend on the coordinates x_i. Inserting $L = T - V$ into the second of (1.11) and taking $i = 1$ shows that the difference $\Phi = \partial T/\partial u_1 - m u_1$ does not depend on time either, so it depends on the u_i components at most. Integrating Φ with respect to u_1 yields $T = m u_1^2/2 + T_1(u_2, u_3, t)$, with T_1 yet undetermined. Differentiating this expression of T with respect to u_2, and comparing it with the second of (1.11) specified for $i = 2$, yields $T = m\,(u_1^2 + u_2^2)/2 + T_2(u_3, t)$, with T_2 undetermined. Repeating the procedure for $i = 3$ finally provides $T = m\,(u_1^2 + u_2^2 + u_3^2)/2 + T_0(t)$, with T_0 an undetermined function of time only. The latter, in turn, can be viewed as the time derivative of another function h. Remembering the invariance property discussed at the end of Sect. 1.2 with reference to (1.8), one lets $T_0 = 0$. In conclusion, indicating with u the modulus of $\mathbf{u}$ it is $T = m u^2/2$, and the Lagrangian function reads

$$L = \frac{1}{2} m u^2 - V. \tag{1.12}$$

The derivation of (1.12) may appear lengthy. However, the procedure is useful because it is applicable to forces of a more complicated form.

1.3.2 Electromagnetic Force

Consider a charged particle subjected to an electromagnetic field and let m, e be its mass and charge, respectively. The particle's velocity $\mathbf{u}$ is assumed to be non-relativistic. The electromagnetic field acts on the particle with the *Lorentz force* (Sect. 4.11) [2]

$$\mathbf{F} = e\,(\mathbf{E} + \mathbf{u} \wedge \mathbf{B}), \tag{1.13}$$

[2] The units in (1.13) are: $[\mathbf{F}] = \mathrm{N}$, $[e] = \mathrm{C}$, $[\mathbf{E}] = \mathrm{V\,m^{-1}}$, $[\mathbf{u}] = \mathrm{m\,s^{-1}}$, $[\mathbf{B}] = \mathrm{V\,s\,m^{-2}} = \mathrm{Wb\,m^{-2}} = \mathrm{T}$, where "N", "C", "V", "Wb", and "T" stand for Newton, Coulomb, Volt, Weber, and Tesla, respectively. The coefficients in (1.13) differ from those of [4] because of the different units adopted there. In turn, the units in (1.14) are: $[\varphi] = \mathrm{V}$, $[\mathbf{A}] = \mathrm{V\,s\,m^{-1}} = \mathrm{Wb\,m^{-1}}$.

where the electric field $\mathbf{E}$ and the magnetic induction $\mathbf{B}$ are in turn expressed through the scalar potential $\varphi = \varphi(\mathbf{r}, t)$ and the vector potential $\mathbf{A} = \mathbf{A}(\mathbf{r}, t)$ as (Sect. 4.5)

$$\mathbf{E} = -\mathrm{grad}\varphi - \frac{\partial \mathbf{A}}{\partial t}, \qquad \mathbf{B} = \mathrm{rot}\mathbf{A}. \tag{1.14}$$

Letting $i = 1$ in (1.9) one finds from (1.13) $m\dot{u}_1 = e\,(E_1 + u_2\,B_3 - u_3\,B_2)$. Using for E_1, B_3, B_2 the expressions extracted from (1.14) yields

$$m\dot{u}_1 + e\left(\frac{\partial A_1}{\partial t} + u_2\,\frac{\partial A_1}{\partial x_2} + u_3\,\frac{\partial A_1}{\partial x_3}\right) = e\left(-\frac{\partial \varphi}{\partial x_1} + u_2\,\frac{\partial A_2}{\partial x_1} + u_3\,\frac{\partial A_3}{\partial x_1}\right). \tag{1.15}$$

Now, using $u_i = \dot{x}_i$ transforms the term in parentheses at the left hand side of (1.15) into $\mathrm{d}A_1/\mathrm{d}t - u_1\,\partial A_1/\partial x_1$, which gives (1.15) the more compact form

$$\frac{\mathrm{d}}{\mathrm{d}t}\,(m u_1 + e A_1) = \frac{\partial}{\partial x_1}\,(e\mathbf{u}\cdot\mathbf{A} - e\varphi)\,. \tag{1.16}$$

Similar expressions are found for $i = 2, 3$. Comparing with (1.7) in the same manner as in Sect. 1.3.1 yields

$$\frac{\partial L}{\partial x_i} = \frac{\partial}{\partial x_i}\,(e\mathbf{u}\cdot\mathbf{A} - e\varphi)\,, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial u_i} = \frac{\mathrm{d}}{\mathrm{d}t}\,(m u_i + e A_i)\,, \qquad i = 1, 2, 3. \tag{1.17}$$

Note that (1.17) reduce to (1.11) when $\mathbf{A} = 0$, with $e\varphi = V$. The first of (1.17) shows that the sum $T = L + e\varphi - e\mathbf{u}\cdot\mathbf{A}$ does not depend on the coordinates x_i. Inserting $L = T - e\varphi + e\mathbf{u}\cdot\mathbf{A}$ into the second of (1.17) transforms the latter into $\mathrm{d}(\partial T/\partial u_i)/\mathrm{d}t = \mathrm{d}(m u_i)/\mathrm{d}t$. Like in Sect. 1.3.2 the procedure eventually yields $T = m u^2/2$. In conclusion, the Lagrangian function of a particle subjected to the Lorentz force (1.13) is

$$L = \frac{1}{2}\,m u^2 - e\varphi + e\mathbf{u}\cdot\mathbf{A}. \tag{1.18}$$

It is shown in Sect. 4.5 that the $\mathbf{E}$ and $\mathbf{B}$ fields are invariant under the *gauge transformation*

$$\varphi \leftarrow \varphi - \frac{\partial h}{\partial t}, \qquad \mathbf{A} \leftarrow \mathbf{A} + \mathrm{grad}h, \tag{1.19}$$

where $h(\mathbf{r}, t)$ is an arbitrary function. Using (1.19) in (1.18) transforms the terms containing the potentials as

$$-e\varphi + e\mathbf{u}\cdot\mathbf{A} \leftarrow -e\varphi + e\mathbf{u}\cdot\mathbf{A} + e\,\frac{\mathrm{d}h}{\mathrm{d}t}, \tag{1.20}$$

namely, the transformed Lagrangian function differs from the original one by the total derivative of an arbitrary function that depends on position and time only. As a consequence, the solutions $x_i(t)$ are invariant under the gauge transformation (1.19). This is easily understood by observing that the invariance of the $\mathbf{E}$ and $\mathbf{B}$ fields makes the Lorentz force (1.13) invariant as well. As a consequence, the particle's dynamics is not influenced by the gauge transformation.

1.3.3 Work

The elementary work exerted by a force $\mathbf{F}$ acting on a particle of mass m during the time $\mathrm{d}t$ is $\mathbf{F} \cdot \mathrm{d}\mathbf{r}$, where $\mathbf{r}$ is the particle's position at t in a Cartesian frame and $\mathrm{d}\mathbf{r} = \mathbf{u}\mathrm{d}t$ the elementary displacement. Let $P = \mathbf{r}(t = a)$, $Q = \mathbf{r}(t = b)$ be the boundaries of the particle's trajectory. The work exerted from P to Q is found by integrating $\mathbf{F} \cdot \mathrm{d}\mathbf{r}$ over the trajectory, namely,

$$\int_P^Q \mathbf{F} \cdot \mathrm{d}\mathbf{r} = m \int_a^b \dot{\mathbf{u}} \cdot \mathbf{u}\mathrm{d}t = \frac{1}{2} m \int_a^b \frac{\mathrm{d}u^2}{\mathrm{d}t} \mathrm{d}t = T(b) - T(a), \tag{1.21}$$

where the relation $T = mu^2/2$ has been used. The exerted work is then equal to the variation of T, which is the same quantity that appears in (1.12, 1.18) and is called *kinetic energy* of the particle.

If a system having n degrees of freedom is considered instead of a single particle, the work exerted by the forces is defined as the sum of terms of the form (1.21). As a consequence, the kinetic energy of the system is the sum of the kinetic energies of the individual particles. The expression of the system's kinetic energy in Cartesian coordinates is

$$T = \sum_{i=1}^{n} \frac{1}{2} m_i\, u_i^2 = \sum_{i=1}^{n} \frac{1}{2} m_i\, \dot{x}_i^2, \tag{1.22}$$

that is, a positive-definite quadratic form in the velocities. The masses in (1.22) take the same value when they are referred to the same particle. When other types of coordinates are used, the kinetic energy is still a second-degree function of the velocities, however the function's coefficients may depend on the coordinates (an example is given in Sect. 2.8).

When a force deriving from a potential energy $V = V(\mathbf{r}, t)$ is considered, like that of Sect. 1.3.1, the integrand of (1.21) becomes $-\mathrm{grad}V \cdot \mathrm{d}\mathbf{r}$. To calculate the integral it is necessary to account for the explicit dependence of V on t by using mutually consistent values of $\mathbf{r}$ and t; in other terms, the integral in (1.21) can actually be calculated only after determining the function $\mathbf{r}(t)$. An exception occurs when V has no explicit dependence on time; in this case one finds

$$\int_P^Q \mathbf{F} \cdot \mathrm{d}\mathbf{r} = -\int_P^Q \mathrm{grad}V \cdot \mathrm{d}\mathbf{r} = -\int_P^Q \mathrm{d}V = V(P) - V(Q), \tag{1.23}$$

namely, to calculate the integral it suffices to know the boundaries of the trajectory. Moreover, when $V = V(\mathbf{r})$ the Lagrangian function (1.12) does not depend explicitly on time either. It is shown in Sect. 1.6 that in this case also the sum $T + V$ of the kinetic and potential energies is independent of time. A dynamical property that does not depend on time is called *constant of motion*. A force field that makes $T + V$ a constant of motion is called *conservative*.

When a force of the form $\mathbf{F} = e\,(\mathbf{E} + \mathbf{u} \wedge \mathbf{B})$ is considered, like that of Sect. 1.3.2, the scalar multiplication by $\mathrm{d}\mathbf{r} = \mathbf{u}\,\mathrm{d}t$ shows that the second term of the force does not contribute to the work because $\mathbf{u} \wedge \mathbf{B} \cdot \mathbf{u} = 0$ (Sect. A.7). Remembering the first of (1.14), the integral corresponding to that of (1.23) reads

$$\int_P^Q \mathbf{F} \cdot \mathrm{d}\mathbf{r} = -e \int_P^Q \left(\mathrm{grad}\varphi + \frac{\partial \mathbf{A}}{\partial t} \right) \cdot \mathrm{d}\mathbf{r}. \tag{1.24}$$

If the electromagnetic field is independent of time, the calculation is the same as in (1.23) and the exerted work is $e\varphi(P) - e\varphi(Q)$.

1.3.4 Hamilton Principle—Synchronous Trajectories

From the analysis of Sect. 1.2 it follows that the solutions $x_i(t)$ of the motion equations (1.9) are the extremum functions of the functional

$$S[\mathbf{r}] = \int_a^b L(\mathbf{r}, \dot{\mathbf{r}}, t)\,\mathrm{d}t. \tag{1.25}$$

On the other hand, $\mathbf{r}(t)$ describes the particle's trajectory. The latter is also called *natural trajectory* to distinguish it from the $\mathbf{r} + \delta\mathbf{r}$ trajectories that are obtained through a variation. In summary, the natural trajectory of the particle is the extremum function of (1.25). This statement is called *Hamilton principle*.

The integration boundaries in (1.25) determine a time interval $b - a$ that measures the motion's duration between the initial and final position of the particle, $\mathbf{r}(a)$ and $\mathbf{r}(b)$ respectively. The duration is the same also for the $\mathbf{r} + \delta\mathbf{r}$ trajectories. In fact, remembering the derivation of Sect. 1.2, the variation $\delta\mathbf{r}$ vanishes at the integration boundaries, so that any trajectory obtained through a variation has the same initial and final positions as the natural one at the same instants a and b. Moreover, any position $\mathbf{r} + \delta\mathbf{r}$ between $\mathbf{r}(a)$ and $\mathbf{r}(b)$ is considered at the same instant as the position $\mathbf{r}$ of the natural trajectory. For this reason the $\mathbf{r} + \delta\mathbf{r}$ trajectories of the functional (1.25) are called *synchronous*.

1.4 Generalized Coordinates

The extremum functions are calculated as shown in Sect. 1.3 also when a system of N particles, instead of a single particle, is considered. The starting point is still (1.9), where a new index is introduced to distinguish the masses. The number of coordinates that describe the motion of all particles in the system is not necessary equal to $3\,N$; in fact, a number of constraints may exist that limit the relative positions of the particles. As a consequence, letting $n \le 3\,N$ indicate the number of degrees of freedom of the system, the set $x_1(t), \ldots, x_n(t)$ suffices to determine the positions of the particles at time t.

Depending on the problem in hand it may be more convenient to use a new set of coordinates $q_1(t), \dots, q_n(t)$ instead of the Cartesian set $x_1(t), \dots, x_n(t)$. For this, it is necessary to extend the calculation of the extremum functions to the case where the new set is used. Let the relation between the old and new coordinates be

$$\begin{cases} q_1 &= q_1(x_1, \dots, x_n, t) \\ &\vdots \\ q_n &= q_n(x_1, \dots, x_n, t) \end{cases} \qquad \begin{cases} x_1 &= x_1(q_1, \dots, q_n, t) \\ &\vdots \\ x_n &= x_n(q_1, \dots, q_n, t) \end{cases} \tag{1.26}$$

The coordinates q_i, whose units are not necessarily a length, are called *generalized coordinates*. Their time derivatives $\dot{q}_i = \mathrm{d}q_i/\mathrm{d}t$ are called *generalized velocities*. The explicit dependence on time in (1.26) is present if a relative motion of the two frames exists: e.g., the relations $q_1 = x_1 - v_0 t$, $q_2 = x_2$, $q_3 = x_3$ transform the $x_1 x_2 x_3$ set into the $q_1 q_2 q_3$ set, that moves with respect to the former one with the velocity v_0 along the first axis.

Differentiating q_i twice with respect to time and using the first of (1.26) provides a relation of the form $\ddot{q}_i = \ddot{q}_i(x_1, \dot{x}_1, \ddot{x}_1, \dots, x_n, \dot{x}_n, \ddot{x}_n, t)$. The above, after eliminating the second derivatives $\ddot{x}_1, \dots, \ddot{x}_n$ through (1.9), becomes $\ddot{q}_i = \ddot{q}_i(x_1, \dot{x}_1, \dots, x_n, \dot{x}_n, t)$. Finally, replacing $x_1, \dot{x}_1, \dots, x_n, \dot{x}_n$ extracted from the second of (1.26) yields

$$\ddot{q}_i = \ddot{q}_i(\mathbf{q}, \dot{\mathbf{q}}, t), \qquad i = 1, \dots, n, \tag{1.27}$$

where $\mathbf{q}$ indicates the set $q_1, \dots, q_n$, and $\dot{\mathbf{q}}$ indicates the corresponding derivatives. Equations (1.27) have the same form as (1.9), hence they must be deducible as the extremum functions of a functional. To show this, one starts from (1.25) by writing the Lagrangian function in the new set of coordinates. A rather lengthy calculation based on the chain-differentiation rule yields

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i}, \qquad i = 1, \dots, n, \tag{1.28}$$

that is, the Lagrange equations written in the q_i coordinates. Specifically, (1.28) turn out to be the Lagrange equations of the functional

$$S[\mathbf{q}] = \int_a^b L(\mathbf{q}, \dot{\mathbf{q}}, t)\, \mathrm{d}t. \tag{1.29}$$

This result is very important because it shows that the Lagrange equations are invariant under a change of coordinates of the type (1.26).

The solution of (1.28) provides the time evolution of the coordinates q_i describing the particles' motion. As (1.28) are n second-order equations, to determine their solution it is necessary to specify at $t = a$ the values of the n functions q_i and of the correspondent derivatives $\dot{q}_i$, namely, a total of $2n$ constants. The function

$p_i = \partial L/\partial \dot{q}_i$ is called *generalized momentum* or *conjugate momentum* of q_i. From this definition and from (1.28) it follows

$$p_i = \frac{\partial L}{\partial \dot{q}_i}, \qquad \dot{p}_i = \frac{\partial L}{\partial q_i}, \qquad i = 1, \dots, n. \tag{1.30}$$

The derivative $\dot{p}_i$ is called *generalized force*. Due to the definitions (1.30), the generalized momentum and force depend on the same coordinates as the Lagrangian function, namely, $p_i = p_i(\mathbf{q}, \dot{\mathbf{q}}, t)$, $\dot{p}_i = \dot{p}_i(\mathbf{q}, \dot{\mathbf{q}}, t)$.

1.5 Hamiltonian Function

From (1.30) one derives the following expression of the total derivative with respect to time of the Lagrangian function:

$$\frac{\mathrm{d}L}{\mathrm{d}t} = \frac{\partial L}{\partial t} + \sum_{i=1}^{n} \left(\frac{\partial L}{\partial q_i}\, \dot{q}_i + \frac{\partial L}{\partial \dot{q}_i}\, \ddot{q}_i \right) = \frac{\partial L}{\partial t} + \sum_{i=1}^{n} \left(\dot{p}_i\, \dot{q}_i + p_i\, \ddot{q}_i \right). \tag{1.31}$$

The quantity in parentheses in (1.31) is the time derivative of $p_i\, \dot{q}_i$, so that

$$\frac{\partial L}{\partial t} = -\frac{\mathrm{d}H}{\mathrm{d}t}, \qquad H = \sum_{i=1}^{n} p_i\, \dot{q}_i - L. \tag{1.32}$$

The quantity H defined by (1.32) is called *Hamiltonian function*. Remembering the derivation of the Lagrangian function one observes that L, H, and $p_i \dot{q}_i$ have the units of an energy. In turn, the product energy $\times$ time is called *action*. In particular, the functional (1.29) is called *action integral* [42, Chap. 8]. From the above observation it follows that $q_i\, p_i$ has the units of an action in all coordinate sets.

By way of example one takes the single-particle Lagrangian functions (1.12) and (1.18), where the Cartesian coordinates are used. The momentum conjugate to x_i is given, respectively, by

$$L = \frac{1}{2}\, m u^2 - V \to\ p_i = m u_i, \quad L = \frac{1}{2}\, m u^2 - e\varphi + e\mathbf{u} \cdot \mathbf{A} \to\ p_i = m u_i + e A_i. \tag{1.33}$$

The expression of H is found from (1.32) after introducing the vector $\mathbf{p} = (p_1, p_2, p_3)$ and indicating its modulus with p. For the case $L = m u^2/2 - V$ one finds

$$H = \frac{1}{2}\, m u^2 + V = \frac{1}{2m}\, p^2 + V, \tag{1.34}$$

while the case $L = m u^2/2 - e\varphi + e\mathbf{u} \cdot \mathbf{A}$ yields

$$H = \frac{1}{2}\, m u^2 + e\varphi = \frac{1}{2m}\, |\mathbf{p} - e\mathbf{A}|^2 + e\varphi. \tag{1.35}$$

Still using the Cartesian coordinates, (1.34) is readily extended to the case of a system of particles having n degrees of freedom. The force acting on the ith degree of freedom at time t is given by a generalization of (1.10),

$$m_i \dot{u}_i = -\frac{\partial V}{\partial x_i}, \tag{1.36}$$

where the time derivative is calculated at t and the $x_1, \ldots, x_n$ coordinates appearing in V are calculated at t as well. For the sake of simplicity the coordinate index i is also used to distinguish the masses in (1.36). It is implied that the same value of m_i must be applied to the indices associated with the same particle. The Lagrangian function is calculated in the same manner as in Sect. 1.3 and reads

$$L = \sum_{i=1}^{n} \frac{1}{2} m_i u_i^2 - V(\mathbf{r}, t), \qquad p_i = m_i u_i, \tag{1.37}$$

whence

$$H = \sum_{i=1}^{n} \frac{1}{2} m_i u_i^2 + V(\mathbf{r}, t) = \sum_{i=1}^{n} \frac{1}{2m_i} p_i^2 + V(\mathbf{r}, t). \tag{1.38}$$

Comparing the two forms of H shown in (1.38), one notes that the second of (1.37) is exploited to express the Hamiltonian function in terms of the $\mathbf{r}$, $\mathbf{p}$ sets instead of the $\mathbf{r}$, $\mathbf{u}$ sets. This procedure is generalized in Sect. 1.6.

1.6 Hamilton Equations

As the Lagrangian function depends on $\mathbf{q}$, $\dot{\mathbf{q}}$, and t, the generalized momentum p_i defined by (1.30) depends on the same variables at most. It is useful to consider also the inverse relations, where the generalized velocities $\dot{q}_i$ are expressed in terms of $\mathbf{q}$, $\mathbf{p}$, and t. The two sets of relations are

$$\begin{cases} p_1 = p_1(q_1, \dot{q}_1, \ldots, q_n, \dot{q}_n, t) \\ \quad\vdots \\ p_n = p_n(q_1, \dot{q}_1, \ldots, q_n, \dot{q}_n, t) \end{cases} \qquad \begin{cases} \dot{q}_1 = \dot{q}_1(q_1, p_1, \ldots, q_n, p_n, t) \\ \quad\vdots \\ \dot{q}_n = \dot{q}_n(q_1, p_1, \ldots, q_n, p_n, t) \end{cases} \tag{1.39}$$

A simple example is given by the two cases of (1.33). Letting $q_i = x_i$, $\dot{q}_i = u_i$, the first case gives (1.39) the form $p_i = m\,\dot{q}_i$ and $\dot{q}_i = p_i/m$, while the second one gives (1.39) the form $p_i = m\,\dot{q}_i + e\,A_i(\mathbf{q}, t)$ and $\dot{q}_i = [p_i - e\,A_i(\mathbf{q}, t)]/m$.

Introducing the second of (1.39) into the definition (1.32) of the Hamiltonian function expresses the latter in terms of $\mathbf{q}$, $\mathbf{p}$, and t. The derivatives of the Hamiltonian function with respect to the new variables q_i, p_i are very significant. In fact, for any index r one finds

$$\frac{\partial H}{\partial q_r} = \sum_{i=1}^{n} p_i \frac{\partial \dot{q}_i}{\partial q_r} - \left(\frac{\partial L}{\partial q_r} + \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}_i} \frac{\partial \dot{q}_i}{\partial q_r} \right) = -\frac{\partial L}{\partial q_r} = -\dot{p}_r. \tag{1.40}$$

The two sums in (1.40) cancel each other thanks to the first of (1.30), while the last equality is due to the second of (1.30). The derivative with respect to p_r is found by the same token,

$$\frac{\partial H}{\partial p_r} = \left(\dot{q}_r + \sum_{i=1}^{n} p_i \frac{\partial \dot{q}_i}{\partial p_r} \right) - \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}_i} \frac{\partial \dot{q}_i}{\partial p_r} = \dot{q}_r. \tag{1.41}$$

The results of (1.40, 1.41) are condensed in the *Hamilton equations*

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \qquad i = 1, \ldots, n, \tag{1.42}$$

that provide a set of $2n$ differential equations of the first order in the $2n$ independent unknowns $q_1, \ldots, q_n$, $p_1, \ldots, p_n$. It is important to note that from (1.42) one readily derives the following:

$$\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} = \frac{\partial^2 H}{\partial q_i \partial p_i} - \frac{\partial^2 H}{\partial p_i \partial q_i} = 0. \tag{1.43}$$

The Hamilton equations (1.42) provide the time evolution of the generalized coordinates q_i; as a consequence, they are equivalent to the Lagrange equations (1.28). Another way of obtaining the Hamilton equations is to derive them as the extremum equations of a suitable functional. This is shown in Sect. 1.7.

In contrast to the Lagrange equations (1.28), that are n second-order differential equations, the Hamilton equations (1.42) are $2n$, first-order differential equations. To determine the solution of the latter it is necessary to prescribe the values of the $2n$ unknowns $q_1, \ldots, q_n$, $p_1, \ldots, p_n$ at the initial time $t = a$, that is, $2n$ constants. Therefore, the number of constants to be prescribed is the same as for the Lagrange equations. The independent functions $q_1, \ldots, q_n$, $p_1, \ldots, p_n$ are called *canonical coordinates*. For each index i the functions q_i, p_i are called *conjugate coordinates*.

Thanks to (1.42) the total derivative of H reads

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\partial H}{\partial t} + \sum_{i=1}^{n} \left(\frac{\partial H}{\partial p_i} \dot{p}_i + \frac{\partial H}{\partial q_i} \dot{q}_i \right) = \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}, \tag{1.44}$$

where the last equality derives from the first of (1.32). If the Lagrangian function does not depend explicitly on time it follows $\mathrm{d}H/\mathrm{d}t = 0$, namely, H is a constant of motion. Its value is fixed by the values of the canonical coordinates at the initial time $t = a$. From (1.44) it also follows that $\mathrm{d}H/\mathrm{d}t = 0$ is equivalent to $\partial H/\partial t = 0$. In other terms, the Hamiltonian function is a constant of motion if it does not depend explicitly on time, and vice versa.

If the Lagrangian function does not depend on one of the coordinates, say, q_r, the latter is called *cyclic* or *ignorable*. From the second of (1.30) it follows that, if q_r is cyclic, its conjugate momentum p_r is a constant of motion. Moreover, due to the second of (1.42) it is $\partial H/\partial q_r = 0$, namely, the Hamiltonian function does not depend on q_r either.

1.7 Time–Energy Conjugacy—Hamilton–Jacobi Equation

Equations (1.42) can also be derived as the extremum equations of a functional. To show this it suffices to replace the Lagrangian function taken from the second of (1.32) into the functional (1.29), this yielding

$$S = \int_a^b \left(\sum_{i=1}^n p_i \dot{q}_i - H \right) \mathrm{d}t. \tag{1.45}$$

Using in (1.45) the expressions of the generalized velocities given by the second of (1.39), the integrand becomes a function of q_i, p_i, and t. Then, the extremum equations are found by introducing the variations in the coordinates, that become $q_i + \alpha_i \eta_i$. Like in the case of (1.1) it is assumed that η_i vanishes at a and b. Similarly, the conjugate momenta become $p_i + \beta_i \zeta_i$. Differentiating (1.45) with respect to α_i or β_i yields, respectively,

$$\frac{\partial S}{\partial \alpha_i} = \int_a^b \left[(p_i + \beta_i \zeta_i)\, \dot{\eta}_i - \frac{\partial H}{\partial (q_i + \alpha_i \eta_i)} \eta_i \right] \mathrm{d}t, \tag{1.46}$$

$$\frac{\partial S}{\partial \beta_i} = \int_a^b \left[(\dot{q}_i + \alpha_i \dot{\eta}_i)\, \zeta_i - \frac{\partial H}{\partial (p_i + \beta_i \zeta_i)} \zeta_i \right] \mathrm{d}t. \tag{1.47}$$

Letting $\alpha_1 = \ldots = \beta_n = 0$ in (1.46, 1.47), integrating by parts the term containing $\dot{\eta}_i$, and using the condition $\eta_i(a) = \eta_i(b) = 0$ provides

$$\left(\frac{\partial S}{\partial \alpha_i} \right)_0 = - \int_a^b \left(\dot{p}_i + \frac{\partial H}{\partial q_i} \right) \eta_i \, \mathrm{d}t, \qquad \left(\frac{\partial S}{\partial \beta_i} \right)_0 = \int_a^b \left(\dot{q}_i - \frac{\partial H}{\partial p_i} \right) \zeta_i \, \mathrm{d}t. \tag{1.48}$$

As in Sect. 1.2 the equations for the extremum functions are found by letting $(\partial S/\partial \alpha_i)_0 = 0$, $(\partial S/\partial \beta_i)_0 = 0$. Such equations coincide with (1.42). It is worth observing that, as no integration by part is necessary for obtaining the second of (1.48), the derivation of (1.42) does not require any prescription for the boundary conditions of ζ_i. On the other hand, considering that in the Hamilton equations q_i and p_i are independent variables, one can add the prescription $\zeta_i(a) = \zeta_i(b) = 0$. Although the latter is not necessary here, it becomes useful in the treatment of the canonical transformations, as shown in Sect. 2.2.

In the coordinate transformations discussed so far, time was left unchanged. This aspect is not essential: in fact, within the coordinate transformation one can replace t with another parameter that depends single-valuedly on t. This parameter, say, $\theta(t)$, is equally suitable for describing the evolution of the particles' system; proceeding in this way transforms (1.45) into

$$S = \int_{\theta(a)}^{\theta(b)} \left(\sum_{i=1}^{n} p_i \dot{q}_i \frac{\mathrm{d}t}{\mathrm{d}\theta} - H \frac{\mathrm{d}t}{\mathrm{d}\theta} \right) \mathrm{d}\theta = \int_{\theta(a)}^{\theta(b)} \left(\sum_{i=1}^{n} p_i q_i' - H\, t' \right) \mathrm{d}\theta, \tag{1.49}$$

where the primes indicate the derivatives with respect to θ. Now, letting $q_{n+1} = t$, $p_{n+1} = -H$, the Lagrangian function is recast in the more compact form $L = \sum_{i=1}^{n+1} p_i q_i'$. Remembering the definition (1.30) of the conjugate momenta, it follows that the latter becomes $p_i = \partial L / \partial q_i'$. In conclusion, the negative Hamiltonian function is the momentum conjugate to θ. This result is not due to any particular choice of the relation $\theta(t)$, hence it holds also for the identical transformation $\theta = t$; in other terms, $-H$ is the momentum conjugate to t.

If the upper limit b in the action integral S (Eq. (1.29)) is considered as a variable, the Langrangian is found to be the total time derivative of S. Letting $b \leftarrow t$, from the (1.45) form of S one derives its total differential

$$\mathrm{d}S = \sum_{i=1}^{n} p_i \mathrm{d}q_i - H \mathrm{d}t. \tag{1.50}$$

As a consequence it is $p_i = \partial S / \partial q_i$, $H = -\partial S / \partial t$. Remembering that H depends on the generalized coordinates and momenta, and on time, one may abridge the above findings into the relation

$$\frac{\partial S}{\partial t} + H \left(q_1, \dots, q_n, \frac{\partial S}{\partial q_1}, \dots, \frac{\partial S}{\partial q_n}, t \right) = 0, \qquad p_i = \frac{\partial S}{\partial q_i}, \tag{1.51}$$

that is, a partial-differential equation in the unknown function S. The former is called *Hamilton–Jacobi equation*, while the latter in this context is called *Hamilton's principal function*. As (1.51) is a first-order equation in the $n + 1$ variables $q_1, \dots, q_n$, t, the solution S contains $n + 1$ integration constants. One of them is an additive constant on S, as is easily found by observing that (1.51) contains the derivatives of S, not S itself. For this reason the additive constant is irrelevant and can be set to zero, so that the integration constants reduce to n. It is shown in Sect. 2.2 that (1.51) provides the time evolution of the generalized coordinates q_i. As a consequence it is equivalent to the Lagrange equations (1.28) and to the Hamilton equations (1.42) for describing the system's dynamics.

1.8 Poisson Brackets

Let ρ, σ be arbitrary functions of the canonical coordinates, differentiable with respect to the latter. The *Poisson bracket* of ρ and σ is defined as the function[3]

$$[\rho, \sigma] = \sum_{i=1}^{n} \left(\frac{\partial \rho}{\partial q_i} \frac{\partial \sigma}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial \sigma}{\partial q_i} \right). \tag{1.52}$$

From (1.52) it follows $[\rho, \sigma] = -[\sigma, \rho]$, $[\rho, \rho] = 0$. Also, due to (1.42) it is

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + [\rho, H]. \tag{1.53}$$

Letting $\rho = H$ shows that (1.44) is a special case of (1.53). If ρ is a constant of motion, then

$$\frac{\partial \rho}{\partial t} + [\rho, H] = 0. \tag{1.54}$$

If ρ does not depend explicitly on time, (1.53) yields

$$\frac{d\rho}{dt} = [\rho, H] \tag{1.55}$$

where, in turn, the right hand side is equal to zero if ρ is a constant of motion, while it is different from zero in the other case. Special cases of the Poisson bracket are

$$\left[q_i, q_j\right] = 0, \qquad \left[p_i, p_j\right] = 0, \qquad \left[q_i, p_j\right] = \delta_{ij}, \tag{1.56}$$

with δ_{ij} the Kronecker symbol (A.18). Other interesting expressions are found by introducing the $2\,n$-dimensional vectors **s**, **e** defined as

$$\mathbf{s} = \begin{bmatrix} q_1 \\ \vdots \\ q_n \\ p_1 \\ \vdots \\ p_n \end{bmatrix}, \qquad \mathbf{e} = \begin{bmatrix} \partial H/\partial p_1 \\ \vdots \\ \partial H/\partial p_n \\ -\partial H/\partial q_1 \\ \vdots \\ -\partial H/\partial q_n \end{bmatrix}. \tag{1.57}$$

Using the definitions (1.57) one finds

$$\dot{\mathbf{s}} = \mathbf{e}, \qquad \mathrm{div}_{\mathbf{s}}\, \dot{\mathbf{s}} = \sum_{i=1}^{n} \left(\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} \right) = 0, \tag{1.58}$$

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[3] The definition and symbol (1.52) of the Poisson bracket conform to those of [42, Sect. 9–5]. In [67, Sect. 42], instead, the definition has the opposite sign and the symbol $\{\rho, \sigma\}$ is used. In [110, Sect. 11] the definition is the same as that adopted here, while the symbol $\{\rho, \sigma\}$ is used.

the first of which expresses the Hamilton equations (1.42) in vector form, while the second one derives from (1.43). The symbol $\mathrm{div}_{\mathbf{s}}$ indicates the divergence with respect to all the variables that form vector $\mathbf{s}$ (Sect. A.3). Now, taking an arbitrary function ρ like that used in (1.53) and calculating the divergence of the product $\rho\,\dot{\mathbf{s}}$ yields, thanks to (1.58) and to (A.16, A.12),

$$\mathrm{div}_{\mathbf{s}}(\rho\,\dot{\mathbf{s}}) = \rho\,\mathrm{div}_{\mathbf{s}}\,\dot{\mathbf{s}} + \dot{\mathbf{s}}\cdot\mathrm{grad}_{\mathbf{s}}\rho = \sum_{i=1}^{n}\left(\frac{\partial\rho}{\partial q_i}\,\dot{q}_i + \frac{\partial\rho}{\partial p_i}\,\dot{p}_i\right) = [\rho, H]. \tag{1.59}$$

1.9 Phase Space and State Space

Given a system of particles having n degrees of freedom it is often convenient to describe its dynamical properties by means of a geometrical picture. To this purpose one introduces a $2n$-dimensional space whose coordinates are $q_1, \dots, q_n, p_1, \dots, p_n$. This space has no definite metrical structure, one simply assumes that q_i and p_i are plotted as Cartesian coordinates of an Euclidean space [65, Chap. 6-5]. Following Gibbs, the space thus defined is often called *phase space*. However, it is convenient to better specify the terminology by using that of Ehrenfest, in which the term γ-*space* is used for this space (the citations of Gibbs and Ehrenfest are in [110, Sect. 17]). At some instant t the whole set of canonical coordinates $q_1, \dots, q_n,\ p_1, \dots, p_n$ corresponds to a point of the γ-space. Such a point is called *phase point*. In turn, the *state* of a mechanical system at some instant t is defined as the set of its canonical coordinates at that instant. It follows that the phase point represents the dynamical state of the system at t. As time evolves, the phase points representing the state at different instants provide a curve of the γ-space called *phase trajectory*.

A generalization of the γ-space is obtained by adding the time t as a $(2n+1)$th coordinate. The $(2n+1)$-dimensional space thus obtained is called *state space* [65, Chap. 6–5]. The curve of the state space describing the system's dynamics is called *state trajectory*. Consider two systems governed by the same Hamiltonian function and differing only in the initial conditions. The latter are represented by two distinct points of the $2n$-dimensional section of the state space corresponding to $t = 0$. The subsequent time evolution of the two systems provides two state trajectories that never cross each other. In fact, if a crossing occurred at, say, $t = \bar{t}$, the canonical coordinates of the two Hamiltonian functions would be identical there, this making the initial conditions of the subsequent motion identical as well. As a consequence, the two state trajectories would coincide for $t \ge \bar{t}$. However, the same reasoning holds when considering the motion backward in time ($t \le \bar{t}$). Thus, the two trajectories should coincide at all times, this contradicting the hypothesis that the initial conditions at $t = 0$ were different.

A similar reasoning about the crossing of trajectories is possible in the γ-space. The conclusion is that the phase trajectories do not cross each other if the Hamiltonian function does not depend explicitly on time. Instead, they may cross each other if the Hamiltonian function depends on time; the crossing, however, occurs at different times (in other terms, the set of canonical coordinates of the first system calculated at $t = t_1$ may coincide with the set of canonical coordinates of the second system calculated at $t = t_2$ only in the case $t_2 \neq t_1$).

Despite of the larger number of dimensions, the adoption of the state space is convenient for the geometrical representation of the system's dynamics, because a trajectory is uniquely specified by the initial point and no crossing of trajectories occurs. With the provision stated above, this applies also to the γ-space. In contrast, consider a geometrical picture of the Lagrangian type, in which the generalized coordinates $q_1, \dots, q_n$ only are used. The latter may be considered as the Cartesian coordinates of an n-dimensional Euclidean space called *configuration space*. To specify a trajectory in such a space it is necessary to prescribe the position $q_1, \dots, q_n$ and velocity $\dot{q}_1, \dots, \dot{q}_n$ of the system at $t = 0$. If one considers two or more systems differing only in the initial conditions, the motion of each system could start from every point of the configuration space and in every direction. As a consequence, it would be impossible to obtain an ordered picture of the trajectories, which will inevitably cross each other.

As mentioned above, the γ-space for a system having n degrees of freedom is a $2n$-dimensional space whose coordinates are $q_1, \dots, q_n, \; p_1, \dots, p_n$. It is sometimes convenient to use a different type of phase space whose dimension is twice the number of degrees of freedom possessed by each of the system's particles. To specifiy this issue, consider the case of a system made of N point-like particles, with no constraints. In this case each particle (say, the jth one) has three degrees of freedom and its dynamical state at the time t is determined by the six canonical coordinates $\bar{q}_{1j}, \bar{q}_{2j}, \bar{q}_{3j}, \; \bar{p}_{1j}, \bar{p}_{2j}, \bar{p}_{3j}$. Together, the latter identify a point X_j of a six-dimensional phase space called μ-*space*[4]. At the time t the system as a whole is represented in the μ-space by the set of N points $X_1, \dots, X_N$.

1.10 Complements

1.10.1 Higher-Order Variational Calculus

The variational calculus described in Sect. 1.2 can be extended to cases were the function g in (1.1) depends on derivatives of a higher order than the first. Consider for instance the functional

$$G[w] = \int_a^b g(w, \dot{w}, \ddot{w}, \xi)\, \mathrm{d}\xi. \tag{1.60}$$

Following the procedure of Sect. 1.2 and assuming that the derivative $\dot{\eta}$ vanishes at a and b, yields the following differential equation for the extremum functions of (1.60):

$$-\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\frac{\partial g}{\partial \ddot{w}} + \frac{\mathrm{d}}{\mathrm{d}\xi}\frac{\partial g}{\partial \dot{w}} = \frac{\partial g}{\partial w}. \tag{1.61}$$

[4] The letter "μ" stands for "molecule", whereas the letter "γ" in the term "γ-space" stands for "gas".

1.10.2 Lagrangian Invariance and Gauge Invariance

It is shown in Sect. 1.2 that the extremum functions $w_i(\xi)$ are invariant under addition to g of the total derivative of an arbitrary function h that depends on $\mathbf{w}$ and ξ only (refer to Eq. (1.8)). Then, it is mentioned in Sect. 1.3.2 that the $\mathbf{E}$ and $\mathbf{B}$ fields are invariant under the gauge transformation (1.19), where $h(\mathbf{r}, t)$ is an arbitrary function. These two properties have in fact the same origin, namely, the description based upon a Lagrangian function. In fact, as shown in Sect. 4.2, a Lagrangian description is possible also in the case of a system having a continuous distribution of the degrees of freedom like, for instance, the electromagnetic field.

1.10.3 Variational Calculus with Constraints

In several problems it is required that the function w, introduced in Sect. 1.2 as the extremum function of functional (1.1), be able to fulfill one or more constraints. By way of example consider the constraint

$$G_0 = \int_a^b g_0(w, \dot{w}, \xi)\, \mathrm{d}\xi, \tag{1.62}$$

where the function g_0 and the number G_0 are prescribed. A typical case where (1.62) occurs is that of finding the maximum area bounded by a perimeter of given length (*Dido's problem*). For this reason, extremum problems having a constraint like (1.62) are called *isoperimetric* even when they have no relation with geometry [115, Par. 4-1].

To tackle the problem one extends the definition of the variation of w by letting $\delta w = \alpha_1 \eta_1 + \alpha_2 \eta_2$, where $\eta_1(\xi)$, $\eta_2(\xi)$ are arbitrary functions that are differentiable in the interior of $[a, b]$ and fulfill the conditions $\eta_1(a) = \eta_1(b) = 0$, $\eta_2(a) = \eta_2(b) = 0$.

If w is an extremum function of G that fulfills (1.62), replacing w with $w + \delta w$ transforms (1.1, 1.62) to a pair of functions of the α_1, α_2 parameters, namely,

$$G = G(\alpha_1, \alpha_2), \qquad G_0(\alpha_1, \alpha_2) = G_0(0, 0) = \text{const.} \tag{1.63}$$

The first of (1.63) has an extremum at $\alpha_1 = \alpha_2 = 0$, while the second one establishes a relation between α_1 and α_2. The problem is thus reduced to that of calculating a constrained extremum, and is solved by the method of the *Lagrange multipliers*.

For this, one considers the function $G_\lambda = G(\alpha_1, \alpha_2) + \lambda\, G_0(\alpha_1, \alpha_2)$, with λ an indeterminate parameter, and calculates the free extremum of G_λ by letting

$$\left(\frac{\partial G_\lambda}{\partial \alpha_1}\right)_0 = 0, \qquad \left(\frac{\partial G_\lambda}{\partial \alpha_2}\right)_0 = 0, \tag{1.64}$$

where index 0 stands for $\alpha_1 = \alpha_2 = 0$. The rest of the calculation is the same as in Sect. 1.2; the two relations (1.64) turn out to be equivalent to each other and provide the same Euler equation. More specifically, from the definition of G and G_0 as integrals of g and g_0 one finds that the Euler equation of this case is obtained from that of Sect. 1.2 by replacing g with $g_\lambda = g + \lambda g_0$:

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\frac{\partial g_\lambda}{\partial \dot{w}} = \frac{\partial g_\lambda}{\partial w}. \tag{1.65}$$

As (1.65) is a second-order equation, its solution w contains two integration constants. The λ multiplier is an additional indeterminate constant. The three constants are found from the constraint (1.62) and from the two relations provided by the boundary or initial conditions of w.

1.10.4 An Interesting Example of Extremum Equation

Consider the Hamilton–Jacobi Eq. (1.51) for a single particle of mass m. Using the Cartesian coordinates and a Hamiltonian function of the form

$$H = \frac{p^2}{2m} + V(x_1, x_2, x_3, t), \qquad p^2 = p_1^2 + p_2^2 + p_3^2, \tag{1.66}$$

the Hamilton–Jacobi equation reads

$$\frac{\partial S}{\partial t} + \frac{|\mathrm{grad} S|^2}{2m} + V(x_1, x_2, x_3, t) = 0, \qquad p_i = \frac{\partial S}{\partial q_i}. \tag{1.67}$$

If V is independent of time, then $H = E$ and the separation $S = W - E\,t$ (Sect. 2.4) yields $\partial S/\partial t = -E$, $\mathrm{grad} S = \mathrm{grad} W = \mathbf{p}$. It follows

$$\frac{|\mathrm{grad} W|^2}{2m} + V(x_1, x_2, x_3) = E. \tag{1.68}$$

Both Hamilton's principal (S) and characteristic (W) functions have the dimensions of an action and are defined apart from an additive constant. Also, the form of $|\mathrm{grad} W|$ is uniquely defined by that of $V - E$. In turn, E is prescribed by the initial conditions of the particle's motion.

Consider now the case where $E \geq V$ within a closed domain Ω whose boundary is $\partial\Omega$. As $\mathrm{grad} W$ is real, the motion of the particle is confined within Ω, and $\mathrm{grad} W$ vanishes at the boundary $\partial\Omega$. The Hamilton–Jacobi equation for W (1.68) is recast in a different form by introducing an auxiliary function w such that

$$w = w_0 \exp(W/\mu), \tag{1.69}$$

with μ a constant having the dimensions of an action. The other constant w_0 is used for prescribing the dimensions of w. Apart from this, the choice of w_0 is arbitrary due to the arbitrariness of the additive constant of W. Taking the gradient of (1.69) yields $\mu\,\mathrm{grad} w = w\,\mathrm{grad} W$, with $w \neq 0$ due to the definition. As $\mathrm{grad} W$ vanishes at the boundary, grad$w$ vanishes there as well. As a consequence, w is constant over the boundary. Inserting (1.69) into (1.68) yields

$$\frac{\mu^2}{2m}\,\frac{|\mathrm{grad} w|^2}{w^2} + V(x_1, x_2, x_3) = E, \tag{1.70}$$

which determines $|\mathrm{grad} w/w|$ as a function of $V - E$. Rearranging the above and observing that $\mathrm{div}(w\,\mathrm{grad} w) = w\nabla^2 w + |\mathrm{grad} w|^2$ (Sect. A.1) provides

$$\frac{\mu^2}{2m}\left[\mathrm{div}(w\,\mathrm{grad} w) - w\nabla^2 w\right] + (V - E)\,w^2 = 0. \tag{1.71}$$

Integrating (1.71) over Ω and remembering that grad$w$ vanishes at the boundary,

$$\int_\Omega w\left[-\frac{\mu^2}{2m}\nabla^2 w + (V - E)\,w\right] \mathrm{d}\Omega = 0. \tag{1.72}$$

The term in brackets of (1.72) does not necessarily vanish. In fact, the form of w is such that only the integral as a whole vanishes. On the other hand, by imposing that the term in brackets vanishes, and replacing μ with the reduced Planck constant $\hbar$, yields

$$-\frac{\hbar^2}{2m}\nabla^2 w + (V - E)\,w = 0, \tag{1.73}$$

namely, the Schrödinger equation independent of time (7.45). This result shows that the Schrödinger equation derives from a stronger constraint than that prescribed by the Hamilton–Jacobi equation.

An immediate consequence of replacing the integral relation (1.72) with the differential Eq. (1.73) is that the domain of w is not limited any more by the condition $E \ge V$, but may extend to infinity.

Another consequence is that, if the boundary conditions are such that w vanishes over the boundary (which, as said above, may also be placed at infinity), then (1.73) is solvable only for specific values of E, that form its spectrum of eigenvalues. Moreover it can be demonstrated, basing on the form of the Schrodinger equation, that the condition $E \ge V_{\min}$ must be fulfilled (Sect. 8.2.3).

It is interesting to note another relation between the Schrödinger and the Hamilton–Jacobi equations. For the sake of simplicity one takes the one-dimensional case of the Hamilton–Jacobi equation expressed in terms of w (1.70):

$$\frac{\mu^2}{2m}(w')^2 + V(x)\,w^2 = E\,w^2, \tag{1.74}$$

where the prime indicates the derivative with respect to x. The left hand side of the equation may be considered the generating function $g = g(w, w', x)$ of a functional G, defined over an interval of the x axis that may extend to infinity:

$$G[w] = \int_a^b \left[\frac{\mu^2}{2m}(w')^2 + V\,w^2\right] \mathrm{d}x. \tag{1.75}$$

One then seeks the extremum function w of G that fulfills the constraint

$$G_0[w] = \int_a^b w^2 \, \mathrm{d}x = 1. \tag{1.76}$$

The problem is solved by the method of Sect. 1.10.3, namely, by letting $g_0 = w^2$, $g_E = g - E\, g_0$, and applying the Euler equation to g_E:

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial g_E}{\partial w'} = \frac{\mathrm{d}}{\mathrm{d}x}\frac{\mu^2}{m} w' = \frac{\mu^2}{m} w'', \qquad \frac{\partial g_E}{\partial w} = 2\,(V - E)\, w, \tag{1.77}$$

showing that the Schrödinger equation is actually the Euler equation of the functional G subjected to the constraint G_0, with the eigenvalue E provided by the Lagrange multiplier. This result holds also in the higher-dimensional cases, and is in fact the method originally used by Schrödinger to determine the time-independent equation [94, Eqs. (23, 24)].

1.10.5 Constant-Energy Surfaces

Consider the γ-space for a system having n degrees of freedom (Sect. 1.9). If the system is conservative, the relation $H(q_1, \dots, q_n,\ p_1, \dots, p_n) = E$ introduces a constraint among the canonical coordinates. Due to this, at each instant of time the latter must belong to the $(2n-1)$-dimensional surface $H = E$ of the phase space, that is called *constant-energy surface*. As E is prescribed by the initial conditions, the phase point of a conservative system always belongs to the same constant-energy surface.

For a system having one degree of freedom the relation describing the constant-energy surface reduces to $H(q, p) = E$, that describes a curve in the $q\,p$ plane. The corresponding state trajectory is a curve of the three-dimensional $q\,p\,t$ space.

Problems

1.1 In the xy plane find the geodesic $y = y(x)$ through the points $A \equiv (a, y_a)$, $B \equiv (b, y_b)$, $A \neq B$.

1.2 Given the Hamiltonian function $H = p^2/(2\,m) + (c/2)\,x^2$, $m, c > 0$ (that describes the *linear harmonic oscillator*, Sect. 3.3), find the constant-energy curves of the xp plane corresponding to different values of the total energy E.

1.3 Given the Hamiltonian function of the harmonic oscillator of the general form $H = p^2/(2\,m) + (c/s)\,|x|^s$, $m, c, s > 0$, find the constant-energy curves of the xp plane corresponding to a fixed total energy E and to different values of parameter s.