

# Survey of Classical Physics

In this first chapter and in the following one, the fundamentals of classical and quantum physics will be reviewed. Obviously, the purpose is not to provide an exhaustive (or even partial) treatment of these subjects: the readers are supposed to be already familiar with them. We simply intend to recall the main concepts and to define the symbols that will be used in the rest of the book. Many excellent textbooks have been written on classical and quantum physics. We may refer, for example, to Goldstein [168] and Jackson [202] for the former, and to Messiah [306], Schiff [398] or Greiner [172] for the latter.

## 1.1 Newton Dynamics

### Linear Momentum

The fundamental law of nonrelativistic classical mechanics is *Newton second law of motion* for a particle of mass  $m$  subject to a force  $\mathbf{F}$ :

$$\boxed{\frac{d\mathbf{p}}{dt} = \mathbf{F} = m \frac{d^2\mathbf{r}}{dt^2}} \quad (1.1)$$

where  $\mathbf{p}$  is the linear momentum, or simply the momentum, of the particle:

$$\mathbf{p} = m\mathbf{v} \ , \quad \mathbf{v} = \frac{d\mathbf{r}}{dt}.$$

Here,  $\mathbf{r}(t)$  and  $\mathbf{v}(t)$  are the position and velocity of the particle at time  $t$ .

If a system is composed of many particles, a total linear momentum is defined as the sum over the particles

$$\mathbf{P} = \sum_i \mathbf{p}_i,$$

where  $\mathbf{p}_i$  is the momentum of the  $i$ -th particle. In such a case, the force acting on each particle is the sum of the forces external to the system and those due to other particles. According to *Newton third law of motion*, the forces that two particles exert on each other are equal and opposite and lie along the line joining the two particles. As a result,

$$\frac{d\mathbf{P}}{dt} = \mathbf{F}^{(e)},$$

where  $\mathbf{F}^{(e)}$  is the sum of the external forces acting on all the particles of the system.

### Angular Momentum

The angular momentum  $\mathbf{L}$  of a particle with linear momentum  $\mathbf{p}$  with respect to point  $\mathbf{O}$  is defined as

$$\mathbf{L} = \mathbf{r} \times \mathbf{p},$$

where  $\mathbf{r}$  is the vector from  $\mathbf{O}$  to the particle position. In the same way, if a force  $\mathbf{F}$  is applied to a particle in  $\mathbf{r}$ , the momentum  $\mathbf{T}$  of this force (or torque) with respect to point  $\mathbf{O}$  is defined as

$$\mathbf{T} = \mathbf{r} \times \mathbf{F}. \quad (1.2)$$

Observing that  $\mathbf{v} \times \mathbf{p} = \mathbf{v} \times m\mathbf{v} = 0$ , from Newton second law it follows immediately that

$$\frac{d\mathbf{L}}{dt} = \mathbf{T}. \quad (1.3)$$

If a system is composed of many particles, a total angular momentum is defined as the sum over the particles

$$\mathbf{L} = \sum_i \mathbf{L}_i,$$

where  $\mathbf{L}_i$  is the angular momentum of the  $i$ -th particle. The application of Newton second and third laws yields

$$\frac{d\mathbf{L}}{dt} = \mathbf{T}^{(e)},$$

where  $\mathbf{T}^{(e)}$  is the total momentum of the external forces acting on the system.

## 1.2 Work and Energy

The kinetic energy of a particle with mass  $m$  and velocity  $\mathbf{v}$  is defined as

$$T = \frac{1}{2}mv^2.$$

This is a scalar quantity and should not be confused with the torque  $\mathbf{T}$  in (1.2), which is a vector quantity.

If  $\mathbf{F}(\mathbf{r})$  is the force acting on a particle in  $\mathbf{r}$ , and the particle moves from  $\mathbf{r}_1$  to  $\mathbf{r}_2$  following a path  $\mathbf{s}$ , the work performed by the force on the particle along  $\mathbf{s}$  is defined as

$$W = \int_{\mathbf{s}} \mathbf{F} \cdot d\mathbf{r}.$$

From Newton second law, it follows immediately that the work performed over a particle produces an equal change of its kinetic energy:

$$W = T_2 - T_1.$$

If a particle is moving in a force field such that the work performed along any close trajectory is zero,

$$W = \oint \mathbf{F} \cdot d\mathbf{r} = 0,$$

then the force field is said to be conservative, and a potential-energy field  $V(\mathbf{r})$  can be defined such that

$$\mathbf{F} = -\nabla V.$$

In this case, the total energy of the particle

$$\epsilon = T + V \tag{1.4}$$

is constant.

In a many-particle system, the kinetic energy is the sum of the kinetic energies of all the particles,

$$T = \sum_i T_i = \sum_i \frac{1}{2} m_i v_i^2.$$

If both the applied (external) forces that act on the particles and the forces due to particle interactions (internal) are conservative, then the total potential energy of the system is given by:

$$V = \sum_i V_i + \frac{1}{2} \sum_{i \neq j} V_{ij},$$

where  $V_i$  is the potential energy of the  $i$ -th particle due to the external forces, and  $V_{ij}$  is the potential interaction energy of the pair of particles  $i$  and  $j$ . The factor 1/2 is inserted since each pair of particles is present twice in the sum. Energy conservation, given by (1.4) for a single particle, still holds for the many-particle system.

### 1.3 Hamiltonian Formulation of Dynamics

In a system composed of  $n$  particles that can move separately, even though interacting with each other, the number of coordinates necessary to describe the configuration of the system is  $3n$ . These quantities are not enough to indicate how the system will evolve, since the differential equations of motion are of second order with respect to time, as shown in (1.1). Thus, also the velocities of the particles must be assigned. This situation is described by saying that the state of the system is defined by the positions and velocities of all its particles.

If, however, the particle positions are subject to given constraints, as it happens, for example, in rigid bodies where the distances between all the particles are fixed, then the number of *degrees of freedom* of the system is reduced. In such a case, the configuration of the system is described by a certain number of parameters  $q_i$ , called *generalized coordinates*. The number of independent generalized coordinates necessary to describe the configuration of the system is the number of its degrees of freedom.

The positions of all particles of the system are functions of the generalized coordinates, so that the state of the system is described by the values of all the  $q_i$  and their time derivatives  $\dot{q}_i$ . The dynamical equations of motion in terms of such variables are known as the Lagrange equations. For a conservative system, the Lagrangian function is defined as the difference between the kinetic and the potential energy of the system:

$$L(q_i, \dot{q}_i) = T(q_i, \dot{q}_i) - V(q_i),$$

and the Lagrange equations of motion are

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0. \quad (1.5)$$

The Lagrange equations can be written also for a nonconservative system if a generalized potential function  $U(q_i, \dot{q}_i, t)$  can be defined such that the forces applied to the system are given by

$$Q_i = -\frac{\partial U}{\partial q_i} + \frac{d}{dt} \left( \frac{\partial U}{\partial \dot{q}_i} \right). \quad (1.6)$$

In this case, the Lagrangian function is defined as

$$L = T - U,$$

and the equations of motion are still the Lagrange equations (1.5).

The *momenta*  $p_i$ , *conjugate to the generalized coordinates*  $q_i$ , are defined by means of the Lagrangian function, as

$$p_i = \frac{\partial L(q_i, \dot{q}_i, t)}{\partial \dot{q}_i}. \quad (1.7)$$

The Hamiltonian function of the system is then defined as

$$H(q_i, p_i, t) = \sum_i \dot{q}_i p_i - L(q_i, \dot{q}_i, t). \quad (1.8)$$

As can be seen from the l.h.s. of the above equation,  $H$  is defined as function of the generalized coordinates  $q_i$  and their conjugate momenta  $p_i$ . Thus, in the functions on the r.h.s.,  $\dot{q}_i$  must be replaced with its expression in terms of the  $q_i$  and  $p_i$  obtained from (1.7).

It may be important to note that the analytical forms of the Lagrangian and Hamiltonian functions are their crucial properties in the theory, rather than their particular numerical values.

In general, the Hamiltonian of a system coincides with its energy, but this is not always necessarily true (see [168] Sect. 7-3).

At this point, we are in the position to write the Hamilton dynamical equations,

$$\boxed{\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}} \quad (1.9)$$

For purely mechanical systems, they are equivalent to Newton laws, but they can also be derived, along with Lagrange equations, from some variational principles that may be used in more general physical systems [168].

In the Hamiltonian formulation of classical physics, the state of a system with  $N$  degrees of freedom is described by the set of  $2N$  values  $(q_i, p_i)$ . These may be considered as the coordinates of a point representative of the state of the system in a  $2N$ -dimensional space called the *phase-space* of the system.

## 1.4 Canonical Transformations

The generalized coordinates and their conjugate momenta which describe the state of a physical system are not unique. Given a set of  $q_i$  and  $p_i$  a transformation may be considered to new variables  $q'_i$  and  $p'_i$  defined by the functions

$$q'_i = q'_i(q_j, p_j, t), \quad p'_i = p'_i(q_j, p_j, t). \quad (1.10)$$

Such a transformation is said to be canonical, and it is of interest, if the new variables are canonical, i.e., if a function  $K$  exists such that the equations of motion in the new set are the Hamilton equations:

$$\dot{q}'_i = \frac{\partial K}{\partial p'_i}, \quad \dot{p}'_i = -\frac{\partial K}{\partial q'_i}.$$

The function  $K(q'_i, p'_i, t)$  plays the role of the Hamiltonian function in the new set of variables.

It can be shown [168] that the transformation from the values of the Hamilton coordinates at time  $t$  to the same variables at time  $t'$ ,

$$q'_i(t) = q'_i(q_j(t), p_j(t), t) = q_i(t'), \quad p'_i(t) = p'_i(q_j(t), p_j(t), t) = p_i(t')$$

is a canonical transformation. In particular, this is true for the transformation that associates with the  $q_i$  and  $p_i$  at time  $t$  their initial values. Thus, the state of the system can be described by the values of the set of  $q_{i0}$  and  $p_{i0}$  at the initial time,

$$q'_i(t) = q_i(t_0) = q_{i0}, \quad p'_i(t) = p_i(t_0) = p_{i0}. \quad (1.11)$$

If the value of a physical quantity  $A$  at time  $t$  is needed, the inverse transformation must be used:

$$A(q_i(t), p_i(t)) = A(q_i(q_{j0}, p_{j0}, t), p_i(q_{j0}, p_{j0}, t)). \quad (1.12)$$

Note that while in the original description the state of the system is described by time-varying canonical coordinates and the physical quantities are given functions of such coordinates, after the canonical transformation in (1.11) the state of the system is defined by a set of constant canonical coordinates, while the physical quantities (including  $p_i(t)$  and  $q_i(t)$ ), are given by functions of these coordinates that depend explicitly on time as effect of the dynamics. A similar situation exists in connection with the Schrödinger and Heisenberg pictures of quantum mechanics (see Sect. 2.2).

## 1.5 Small Oscillations

A system is in a stable equilibrium state when its generalized coordinates have values  $q_i^{(e)}$  corresponding to a minimum of its potential energy and the kinetic energy is zero. If the system is slightly displaced from that position and then left alone, it will perform small oscillations about the equilibrium position. A set of generalized coordinates can be found, called *normal coordinates*, such that the dynamics described in terms of these coordinates, correspond to  $n$  independent harmonic oscillators, if  $n$  is the number of degrees of freedom of the system. In fact, if the potential energy is expanded around the equilibrium configuration  $q_i^{(e)}$ , it is given, to second order, by

$$V(q_1, \dots, q_n) \approx V(q_1^{(e)}, \dots, q_n^{(e)}) + \sum_i \left( \frac{\partial V}{\partial q_i} \right)_{(e)} \theta_i + \frac{1}{2} \sum_{ij} \left( \frac{\partial^2 V}{\partial q_i \partial q_j} \right)_{(e)} \theta_i \theta_j,$$

where

$$\theta_i = q_i - q_i^{(e)}$$

are the deviations of the coordinates from their equilibrium values. The first term in the above equation represents the value of the potential energy at the equilibrium configuration. Since  $V$  is defined with an arbitrary zero, this value can be made to vanish. The first derivatives in the second term are zero owing to the condition of minimum potential energy, so that we are left with the quadratic term

$$V = \frac{1}{2} \sum_{ij} v_{ij} \theta_i \theta_j,$$

where  $v_{ij} = (\partial^2 V / \partial q_i \partial q_j)_{(e)}$ . Similarly, the kinetic energy can be put in the form

$$T = \frac{1}{2} \sum_{ij} t_{ij} \dot{\theta}_i \dot{\theta}_j.$$

Both matrices  $v_{ij}$  and  $t_{ij}$  are symmetric and it can be shown [168] that with a suitable canonical transformation of the generalized coordinates they can be put simultaneously in a diagonal form. In the new *normal coordinates*  $\eta_i$ , the Lagrangian is given by

$$L = T - V = \frac{1}{2} \sum_i \mu_i \dot{\eta}_i^2 - \frac{1}{2} \sum_i \beta_i \eta_i^2,$$

where  $\mu_i$  and  $\beta_i$  are the diagonal elements of the matrices  $v_{ij}$  and  $t_{ij}$  transformed into the normal coordinates. The conjugate momenta, according to (1.7), are given by

$$\pi_i = \frac{\partial L(\eta_i, \dot{\eta}_i, t)}{\partial \dot{\eta}_i} = \mu_i \dot{\eta}_i,$$

and, according to (1.8), the Hamiltonian is then given by

$$H(\eta_i, \pi_i) = \sum_i \dot{\eta}_i \pi_i - L(\eta_i, \dot{\eta}_i) = \frac{1}{2} \sum_i \frac{1}{\mu_i} \pi_i^2 + \frac{1}{2} \sum_i \beta_i \eta_i^2.$$

This Hamiltonian is the sum of separate Hamiltonians for each normal coordinate and its conjugate momentum. This means that each normal coordinate follows its own dynamics, which, moreover, is the dynamics of a harmonic oscillator. In fact, Hamilton equations yield

$$\dot{\eta}_i = \frac{\partial H}{\partial \pi_i} = \frac{\pi_i}{\mu_i},$$

already known, and

$$\dot{\pi}_i = -\frac{\partial H}{\partial \eta_i} = -\beta_i \eta_i.$$

These equations are the dynamical equations of a harmonic oscillator: by substitution of the time derivative of the first into the second one, we obtain

$$\ddot{\eta}_i = -\frac{\beta_i}{\mu_i} \eta_i,$$

with solution

$$\eta_i(t) = A_i \cos(\omega_i t + \phi_i), \quad \omega_i = \sqrt{\frac{\beta_i}{\mu_i}}.$$

Each normal coordinate evolves as an independent harmonic oscillator.

## 1.6 Maxwell Equations

The electric field  $\mathbf{E}$  and the magnetic induction field  $\mathbf{B}$  are defined through the force (*Lorentz force*) they exert on a test charge  $q$ :

$$\mathbf{F} = q[\mathbf{E} + \mathbf{v} \times \mathbf{B}] \quad (1.13)$$

This expression must be considered in the limit of a test charge so small that the sources of the electric and magnetic fields are not altered by its presence. Here, as in general in this book, we use the International System of Units (SI), recommended by the *Conférence Générale des Poids et Mesures* since 1960.

Sources of the electromagnetic fields are charges and currents. The dynamics of electric and magnetic fields, or electrodynamics, is described by Maxwell equations. If we assume a charge density  $\rho(\mathbf{r}, t)$  and a current density  $\mathbf{j}(\mathbf{r}, t)$  in vacuum, i.e., in otherwise empty space, Maxwell equations are

$$\begin{aligned} \nabla \cdot \mathbf{B} &= 0 \\ \nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} &= 0 \\ \varepsilon_0 \nabla \cdot \mathbf{E} &= \rho \\ \frac{1}{\mu_0} \nabla \times \mathbf{B} - \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} &= \mathbf{j} \end{aligned} \quad (1.14)$$

where  $\varepsilon_0$  and  $\mu_0$  are the electric permittivity and the magnetic permeability of free space, respectively. If these equations are considered inside a material,  $\rho$  and  $\mathbf{j}$  contain also charges and currents induced in the medium by the external applied fields. If a polarization field  $\mathbf{P}$  is defined as the dipole moment per unit volume inside the medium, and a magnetization field  $\mathbf{M}$  is defined as the magnetic moment per unit volume inside the medium, a polarization charge is generated as

$$\rho_P = -\nabla \cdot \mathbf{P},$$

and a magnetization current is generated as

$$\mathbf{j}_M = \nabla \times \mathbf{M}.$$

These charges and currents are added to the external  $\rho$  and  $\mathbf{j}$  and the last two Maxwell equations in (1.14) become

$$\nabla \cdot \mathbf{D} = \rho, \quad (1.15)$$



$$\nabla \times \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} = \mathbf{j}, \quad (1.16)$$

where  $\mathbf{D}$  and  $\mathbf{H}$  are the electric induction field and the magnetic field, respectively:<sup>1</sup>

$$\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P}, \quad \mathbf{H} = \frac{1}{\mu_0} \mathbf{B} - \mathbf{M}. \quad (1.17)$$

The polarization  $\mathbf{P}$ , the magnetization  $\mathbf{M}$ , and the current density  $\mathbf{j}$  are induced by the applied fields. Their dependences upon the applied fields are characteristic of each material and are described by the so-called *constitutive equations*. In the simplest case of linear materials, the following equations hold:

$$\mathbf{P} = \chi_e \varepsilon_0 \mathbf{E}, \quad \mathbf{M} = \chi_m \mathbf{H}, \quad \mathbf{j} = \sigma \mathbf{E}. \quad (1.18)$$

The proportionality coefficients  $\chi_e$ ,  $\chi_m$ , and  $\sigma$  are called *electric susceptibility*, *magnetic susceptibility*, and *electric conductivity*, respectively. If the above equations (1.18) are used in the definition (1.17) of  $\mathbf{D}$  and  $\mathbf{H}$ , linear relations result between  $\mathbf{D}$  and  $\mathbf{E}$  and between  $\mathbf{H}$  and  $\mathbf{B}$ :

$$\mathbf{D} = \varepsilon \mathbf{E} = \varepsilon_r \varepsilon_0 \mathbf{E}, \quad \mathbf{B} = \mu \mathbf{H} = \kappa_m \mu_0 \mathbf{H}.$$

Here  $\varepsilon$  is the permittivity or dielectric constant of the material;  $\varepsilon_r$  is the relative dielectric constant;  $\mu$  is the magnetic permeability, and  $\kappa_m$  the relative permeability. In a linear homogeneous medium, Maxwell equations can then be rewritten as

$$\nabla \cdot \mathbf{B} = 0, \quad (1.19)$$

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0, \quad (1.20)$$

$$\varepsilon \nabla \cdot \mathbf{E} = \rho, \quad (1.21)$$

$$\frac{1}{\mu} \nabla \times \mathbf{B} - \varepsilon \frac{\partial \mathbf{E}}{\partial t} = \mathbf{j}. \quad (1.22)$$

These equations are very similar to the original “microscopic” Maxwell equations (1.14) with the electric permittivity and the magnetic permeability of free space substituted by equivalent quantities of the material.

## 1.7 Electromagnetic Potentials and Gauge Transformations

It is often convenient to reduce the four first-order differential Maxwell equations to two second-order equations by the introduction of the *electromagnetic potentials*. Since the divergence of the curl of any vector field is zero, the first

<sup>1</sup> In different systems of units, not only the electromagnetic units change, but also the equations of the present section are formally different (see, e.g., [202]).

Maxwell equation is automatically verified if we define a vector field  $\mathbf{A}(\mathbf{r}, t)$ , called *vector potential*, such that

$$\boxed{\mathbf{B}(\mathbf{r}, t) = \nabla \times \mathbf{A}(\mathbf{r}, t)} \quad (1.23)$$

With this position, the second homogeneous Maxwell equation in (1.14) becomes

$$\nabla \times \left[ \mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} \right] = 0$$

and is again automatically satisfied if we define a scalar field  $\phi(\mathbf{r}, t)$ , called *scalar potential*, such that

$$\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} = -\nabla \phi(\mathbf{r}, t),$$

since the curl of the gradient of any scalar field is zero. In terms of the electromagnetic potentials  $\mathbf{A}$  and  $\phi$ , the electric field is then given by

$$\boxed{\mathbf{E} = -\nabla \phi(\mathbf{r}, t) - \frac{\partial \mathbf{A}}{\partial t}} \quad (1.24)$$

The electromagnetic potentials are not uniquely defined. In fact,  $\mathbf{E}$  and  $\mathbf{B}$  are left unchanged by the following transformations, called gauge transformations:

$$\mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} + \nabla \Lambda, \quad \phi \rightarrow \phi' = \phi - \frac{\partial \Lambda}{\partial t}, \quad (1.25)$$

where  $\Lambda$  is an arbitrary function of  $\mathbf{r}$  and  $t$ .

The freedom implied by the gauge transformations can be used to prescribe that the potentials satisfy the Lorentz condition

$$\nabla \cdot \mathbf{A} + \varepsilon \mu \frac{\partial \phi}{\partial t} = 0. \quad (1.26)$$

We can still perform a gauge transformation (1.25) and preserve the Lorentz condition if we request that the function  $\Lambda$  verifies the condition

$$\nabla^2 \Lambda - \varepsilon \mu \frac{\partial^2 \Lambda}{\partial t^2} = 0.$$

The electric and magnetic fields given by the electromagnetic potentials in (1.23) and (1.24) satisfy already the first two homogeneous Maxwell equations. If they are introduced in the last two Maxwell equations, they yield:

$$\boxed{\begin{aligned} \nabla^2 \phi - \varepsilon \mu \frac{\partial^2 \phi}{\partial t^2} &= -\frac{1}{\varepsilon} \rho \\ \nabla^2 \mathbf{A} - \varepsilon \mu \frac{\partial^2 \mathbf{A}}{\partial t^2} &= -\mu \mathbf{j} \end{aligned}} \quad (1.27)$$

where use has been made of the Lorentz condition. These are the wave equations that in free space predict a velocity of electromagnetic waves given by

$$c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}}.$$

## 1.8 Hamiltonian of a Charged Particle in an Electromagnetic Field

A charged particle in an electromagnetic field is subject to the Lorentz force (1.13). This force depends on the particle velocity, so that, to write a Lagrangian, it is necessary to find a suitable function  $U$  such that (1.6) is satisfied. It is easy to verify that such a function is

$$U = q(\phi - \mathbf{A} \cdot \mathbf{v}).$$

The Lagrangian is then

$$L = T - U = \frac{1}{2}mv^2 - q\phi + q\mathbf{A} \cdot \mathbf{v}.$$

Following the procedure indicated in Sect. 1.3, we have the canonical momenta

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = mv_i + qA_i, \quad (1.28)$$

and the corresponding Hamiltonian, from (1.8), is

$$H = \frac{1}{2m} (\mathbf{p} - q\mathbf{A})^2 + q\phi \quad (1.29)$$

This Hamiltonian will be used to study the dynamics of a charged particle in a crystal subject to an electromagnetic field.