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Emmanuel Haven, and Andrei Khrennikov
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Part I

Physics concepts in social science? A discussion

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Classical, statistical, and quantum mechanics: all in one

This chapter provides for a very short course on classical (Newtonian as well as statistical) mechanics and quantum mechanics. Readers who have not been trained in physics will be able to gain basic knowledge of the main physical theories developed during the last 400 years, with the inclusion of some of the interpretational problems of these theories.

1.1 Newtonian mechanics

We discuss one of Newton's laws, namely Newton's second law: "the product of mass and acceleration is equal to the force" or in mathematical symbols:

$$ma = f. \quad (1.1)$$

We state that m is the mass of a particle, a is its acceleration, and f is the force acting on the particle.

Newton also introduced the notion of a continuous (infinitely divisible) physical space which was used to describe the dynamics of a particle. Here we can also mention the contribution of Leibniz. However, the rigorous mathematical formalization of the real continuum was done much later, at the end of the nineteenth century. Physical space was represented by the mathematical model \mathbb{R}^3 , the Cartesian product space $\mathbb{R} \times \mathbb{R} \times \mathbb{R}$ of three real lines. In this mathematical model, Newton's second law can be formalized in the following way. Let us introduce the following notations. Let $q = (x, y, z)$, be a three-dimensional vector, where x, y, z are the particle's coordinates:

$$v = \frac{dq}{dt} = \left(\frac{dx}{dt}, \frac{dy}{dt}, \frac{dz}{dt} \right) \quad (1.2)$$

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is the vector of velocity, and, finally:

$$a = \frac{dv}{dt} = \left(\frac{d^2x}{dt^2}, \frac{d^2y}{dt^2}, \frac{d^2z}{dt^2} \right) \quad (1.3)$$

is the vector of acceleration. The dynamics of a particle, $t \rightarrow q(t)$ (its trajectory in physical space), is described by the ordinary differential equation:

$$m \frac{d^2q(t)}{dt^2} = f(t, q(t)). \quad (1.4)$$

To find the particle's dynamics, we also have to know the initial conditions:

$$q(t_0) = q_0, v(t_0) = \frac{dq}{dt}(t_0) = v_0, \quad (1.5)$$

where q_0 and v_0 are respectively the particle's position and velocity at the initial instant of time t_0 .

An important class of forces is given by the so-called "conservative forces." We start with the one-dimensional model, a particle on the line: there is only one coordinate x . We state that a force $f(x)$ is called conservative if there exists a real valued function $V(x)$ (which is called the potential) such that:

$$f(x) = -\frac{dV}{dx}. \quad (1.6)$$

The potential $V(x)$ represents the potential energy of a particle (see for instance the next chapter for the use of such potential in a social science setting). To illustrate this notion, consider a basic example which also plays an important role in quantum mechanics. The harmonic oscillator is a well-known object in classical mechanics. The restoring force f which is proportional to the displacement of a particle from its equilibrium position is:

$$f(x) = -kx, \quad (1.7)$$

where k is a positive constant. This is a conservative force with the potential $V(x) = kx^2/2$. This is the equation of the standard parabola indicating the fact that the potential energy has its minimum at the point $x = 0$. Newton's second law for the system is:

$$m \frac{d^2x}{dt^2} = -kx. \quad (1.8)$$

Solving this ordinary differential equation, we find that the motion is described by the function:

$$x(t) = A \cos(2\pi vt + \phi), \quad (1.9)$$

where:

$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{m}} = \frac{1}{T}. \quad (1.10)$$

Remark that ν indicates the frequency expressed as the number of cycles per time unit. Clearly, as is intuitive, the force constant k and the mass m influence this frequency. The position $x(t)$ depends on this frequency ν but also on the amplitude A and phase ϕ . They can be found from the system of equations:

$$A \cos \phi = x_0, \quad A \sin \phi = -v_0/2\pi\nu. \quad (1.11)$$

In the case of a particle in the three-dimensional case, the force f is a vector $f = (f_x, f_y, f_z)$. It is called conservative if there exists a (real) potential $V(q)$, $q = (x, y, z)$, such that $f_x = -\frac{\partial V}{\partial x}$, $f_y = -\frac{\partial V}{\partial y}$, $f_z = -\frac{\partial V}{\partial z}$. We also recall the notion of the gradient of a function V . This is a vector composed of its partial derivatives and it is denoted as ∇V . Hence, a conservative force can be represented as the “negative gradient” of the potential:

$$f = -\nabla V. \quad (1.12)$$

Although in this book we try to minimize mathematical details as much as possible, we need to point out the theorem of the existence and uniqueness of the solution of the equation (1.4) with the initial conditions (1.5). Such a problem, i.e. an equation with initial conditions, is called the *Cauchy problem*. This is one of the basic mathematical problems of classical mechanics. The simplest version of the aforementioned theorem is that if the force is described by a smooth function f , i.e. differentiable and with continuous derivative, and the derivative is bounded, i.e. there exists a constant $c > 0$ such that, for every $q \in \mathbb{R}^3$, $|f'(q)| \leq c$, then, for any pair (q_0, v_0) , a unique solution of the Cauchy problem exists (1.4), (1.5). This mathematical theorem was the main source of the *causal deterministic viewpoint* to classical mechanics: if we know the position and velocity of a particle at $t = t_0$, then we can find them at any instant of time $t > t_0$: $q = q(t)$, $v = v(t) = \frac{dq(t)}{dt}$.

Consider the following quote by Laplace [1]:

We ought to regard the present state of the universe as the effect of its antecedent state and as the cause of the state that is to follow. An intelligence knowing all the forces acting in nature at a given instant, as well as the momentary positions of all things in the universe, would be able to comprehend in one single formula the motions of the largest bodies

as well as the lightest atoms in the world; provided that its intellect were sufficiently powerful to subject all data to analysis; to it nothing would be uncertain, the future as well as the past would be present to its eyes.

Later interpretations of quantum mechanics also leave the theoretical possibility of such a super intellect contested.

This is a good example of how pure mathematics generates fundamental philosophic principles. As it often happens in science, it is not easy to change philosophic principles which have been established on the basis of some special mathematical results and models. During Laplace's lifetime, the theory of differential equations had not yet been well developed. Nowadays, it is well known that the Cauchy problem (1.4), (1.5) may have a non-unique solution even for continuous forces. If f is smooth, then the solution is unique only locally, i.e. for a small neighborhood of the point (t_0, x_0) . However, globally it can be non-unique. Hence, modern mathematics does not imply determinism even in classical mechanics (see [2] for usage of this argument in classical non-deterministic biological dynamics). We also remark that if the dynamics of a particle is even deterministic, but unstable, then a small disturbance of initial conditions, can change crucially the trajectory of such a particle. In such a case, although the principle of determinism is formally valid, it has no usage in real practice, since it is impossible to determine initial conditions with infinite precision. This argument against the uncontrollable usage of the principle of determinism in classical mechanics was presented by Blohinzev [3] in his comparison of classical and quantum mechanics. In conclusion, we can see from the above that Laplace's causal determinism is indeed a mere prejudice.

Besides Laplace's prejudice, we can also mention the Kantian prejudice which says that physical space has to be identified with its Euclidean model [4]. This prejudice was based on two-thousand years of Euclidean geometry. The first blow to the Kantian views of physical space was given by Lobachevsky. However, the genius of Einstein was needed to establish modern views of the geometry of physical space.

The above discussion raises a reasonable recommendation: the reader may want to veer close to mathematics and instead steer away from general physical, meta-physical, and philosophic principles.

1.2 References

- [1] See <http://plato.stanford.edu/entries/determinism-causal> and the reference contained therein, cited as: Laplace, P. S. (1820). *Essai philosophique sur les probabilités* forming the introduction to his *Théorie analytique des probabilités*, Paris: V. Courcier repr. Truscott, F. W. and Emory, F. L. (1951). *A Philosophical Essay on Probabilities*. Dover, New York.

- [2] Conte, E., Federici, A., Khrennikov, A., and Zbilut, J. P. (2004). Is determinism the basic rule in dynamics of biological matter? *Proceedings of Quantum Theory: Reconsideration of Foundations. Series in Mathematical Modelling in Physics, Engineering and Cognitive Science*, 10, 639–678, Växjö University Press, Sweden.
- [3] Blochinzev, D. I. (1976). *Elementary Quantum Mechanics*. Nauka, Moscow (in Russian).
- [4] Kant, I. (2008). *The Critique of Pure Reason*. Penguin Classics, London.

1.3 The Hamiltonian formalism

To proceed from classical to quantum mechanics, one typically uses the Hamiltonian formalism for the description of the motion of classical particles. As usual, let us introduce the momentum $p = mv$ of a particle and consider *phase space* with coordinates (q, p) , where q is position. Points of the phase space are interpreted as states of classical particles. We state again that, by Newton's second law, to determine the trajectory of a particle it is necessary to know both initial position q_0 and the velocity v_0 . In particular, knowledge of only position is not sufficient. Therefore, it is natural to define the *particle's state* as the pair (q, v) . By scaling the velocity by the particle's mass, we introduce its momentum, p , and equivalently we represent the particle's state as a pair (q, p) .

We remark that the momentum's definition can be expressed in the form of an ordinary differential equation:

$$\frac{dq}{dt} = \frac{p}{m}. \quad (1.13)$$

Hence, Newton's second law, (1.4), can be written as:

$$\frac{dp}{dt} = -\frac{dV}{dq}. \quad (1.14)$$

Let us introduce the following function on the phase space:

$$\mathcal{H}(q, p) = \frac{p^2}{2m} + V(q). \quad (1.15)$$

$\mathcal{H}(\cdot, \cdot)$ is called the *Hamiltonian function*. This is the total energy of a particle which moves under the action of the force induced by the potential V and the kinetic energy $\frac{p^2}{2m}$. The system of equations (1.13), (1.14) can be written as:

$$\frac{dq}{dt} = \frac{\partial \mathcal{H}}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial \mathcal{H}}{\partial q}. \quad (1.16)$$

This is the system of Hamiltonian equations. It is easy to prove that the energy is preserved in the process of motion:

$$\mathcal{H}(q(t), p(t)) = \mathcal{H}(q(t_0), p(t_0)). \quad (1.17)$$

To prove this important fact (the law of energy conservation), it is sufficient to use the basic rule for the differentiation of a composition of functions and then to apply this rule to the system of Hamiltonian equations.

By using the Hamiltonian formalism, we can formulate a feature of classical mechanics, which can be called *locality*. Let us consider a system consisting of N particles with the three-dimensional coordinates $q_j = (x_j, y_j, z_j)$, $j = 1, \dots, N$ and corresponding momenta p_j . The Hamiltonian function of a system of N particles with masses m_j moving in the potential $V(q_1, \dots, q_N)$ has the form:

$$\mathcal{H}(q, p) = \sum_{j=1}^N \frac{p_j^2}{2m_j} + V(q), \quad (1.18)$$

where $q = (q_1, \dots, q_N)$, $p = (p_1, \dots, p_N)$. The above Hamiltonian gives the total energy of this system composed of N particles. The system of Hamiltonian equations describing the dynamics of this composite system can be written as:

$$\frac{dq_j}{dt} = \frac{\partial \mathcal{H}(q, p)}{\partial p_j}, \quad \frac{dp_j}{dt} = -\frac{\partial \mathcal{H}(q, p)}{\partial q_j}, \quad j = 1, \dots, N. \quad (1.19)$$

Within the potential V , the interaction between different particles is described by terms containing coordinates of a few particles. We can consider the interaction between particles by writing for instance terms of the form $q_i \dots q_N$ (various products of different coordinates). But let us consider now a potential which does *not* contain interaction terms, $V(q) = V_1(q_1) + \dots + V_N(q_N)$. The corresponding system of Hamiltonian equations is:

$$\frac{dq_j}{dt} = \frac{p_j}{m_j}, \quad \frac{dp_j}{dt} = -\frac{\partial V_j}{\partial q_j}, \quad j = 1, \dots, N. \quad (1.20)$$

This is a system of N -independent equations.

Hence, an important principle emerges from our discussion so far: *Hamiltonian mechanics is local, i.e. in the absence of interaction between particles, such particles move independently of each other.*

We remark that non-local motion, as is the case with for instance Bohmian mechanics (see Chapter 6), has the following (paradoxical from the viewpoint of our classical intuition) feature. In the absence of interaction, even for $V \equiv 0$, the dynamics of different particles are *dependent* on each other. Changing the state of one particle (q_j, p_j) induces changing the states (q_i, p_i) , $i \neq j$, of other particles. In the classical world, we have never seen such a behavior of physical systems.

Let us introduce a mathematical tool which has a key role in the Hamiltonian formalism. The *Poisson bracket* of two functions on the N -particle phase space,

$f(q, p), g(q, p)$, is defined as:

$$\{f, g\} = \sum_{j=1}^N \left(\frac{\partial f(q, p)}{\partial q_j} \frac{\partial g(q, p)}{\partial p_j} - \frac{\partial f(q, p)}{\partial p_j} \frac{\partial g(q, p)}{\partial q_j} \right). \quad (1.21)$$

As an example, consider functions $f(q, p) = q_j, g(q, p) = p_j$. Then:

$$\{q_j, p_j\} = 1, \{q_j, p_k\} = 0, j \neq k. \quad (1.22)$$

$$\{q_j, q_k\} = 0, \{p_j, p_k\} = 0. \quad (1.23)$$

By using the Poisson bracket, we rewrite the system of Hamiltonian equations as:

$$\frac{dq_j}{dt} = \{q_j, \mathcal{H}\}, \quad \frac{dp_j}{dt} = \{p_j, \mathcal{H}\}. \quad (1.24)$$

This form of the Hamiltonian dynamics will be used to proceed from classical Hamiltonian mechanics to quantum mechanics.

1.4 Statistical mechanics and the Liouville equation

In studying the dynamics of an ensemble of a huge number, say N particles, the presence of the system of Hamiltonian equations plays merely a methodological role. From as early as the nineteenth century until the 1960s, it was simply impossible to solve this system for large N and non-trivial potentials. Nowadays in principle one can solve it numerically and obtain millions of trajectories in the phase space. However, it is not clear how one can use or visualize the results of such computations. Already in the nineteenth century it was proposed that instead of studying the trajectories of individual particles, it would be better to consider the probability to find a particle in some domain, say W , of the phase space. Such an approach meant in effect a move away from the deterministic description of mechanics to a statistical description. Hence, the name *statistical mechanics* was coined to denote this particular area of study.

Let us consider the phase space of the system of N particles, \mathbb{R}^{2N} , with points (q, p) , where $q = (q_1, \dots, q_N), p = (p_1, \dots, p_N)$. What is the probability density function which indicates the probability to find the first particle at point q_1 with momentum p_1 , the second particle at point q_2 with momentum p_2, \dots , the N th particle at q_N with momentum p_N ? Since momenta are mass scalings of velocities, the question can be reformulated as: “What is the probability density function of the first particle at point q_1 with velocity v_1 , the second particle at point q_2 with velocity v_2, \dots , the N th particle at q_N with velocity v_N ?” We state that mathematically a probability density is a function $\rho(q, p)$ which is

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 non-negative and normalized by 1:

$$\int_{\mathbb{R}^{2N}} \rho(q, p) dq dp = 1. \quad (1.25)$$

The probability to find a particles at a point (q, p) from the domain W of the phase space is calculated with the aid of the probability density function:

$$P((q, p) \in W) = \int_W \rho(q, p) dq dp. \quad (1.26)$$

A fundamental problem now consists to describe the dynamics of the (time-dependent) probability density, $t \rightarrow \rho(t, q, p)$. Fortunately, the *Liouville equation* gives us the answer:

$$\frac{\partial \rho(t, q, p)}{\partial t} = \{\mathcal{H}(q, p), \rho(t, q, p)\}, \quad (1.27)$$

$$\rho(t_0, q, p) = \rho_0(q, p). \quad (1.28)$$

Here, we remark:

$$\{\mathcal{H}, \rho\} = \sum_{j=1}^N \left(\frac{\partial \mathcal{H}}{\partial q_j} \frac{\partial \rho}{\partial p_j} - \frac{\partial \mathcal{H}}{\partial p_j} \frac{\partial \rho}{\partial q_j} \right). \quad (1.29)$$

Hence, if the initial probability density function is known, then (by solving the Liouville equation) we can find the density at any instant of time. We remark that the usage of the probabilistic description of an ensemble of N particles does not contradict the existence of the deterministic Hamiltonian dynamics.

We do not provide the formal derivation of the Liouville equation. Instead of this, we present physical arguments which lie behind this equation. Consider the probability density function on a trajectory $(q(t), p(t))$ in the phase space $\rho(t, q(t), p(t))$. We calculate its total derivative with respect to time:

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \sum_{j=1}^N \left(\frac{\partial \rho}{\partial q_j} \frac{dq_j}{dt} + \frac{\partial \rho}{\partial p_j} \frac{dp_j}{dt} \right). \quad (1.30)$$

We now use the system of Hamiltonian equations (1.19) (this describes the trajectory in the phase space) to express the time derivatives of coordinates and momenta and obtain:

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \sum_{j=1}^N \left(\frac{\partial \rho}{\partial q_j} \frac{\partial \mathcal{H}(q, p)}{\partial p_j} - \frac{\partial \rho}{\partial p_j} \frac{\partial \mathcal{H}(q, p)}{\partial q_j} \right).$$

Then the Liouville equation is equivalent to the following statement: the distribution function is constant along any trajectory in phase space, i.e. $\frac{d\rho}{dt} = 0$.