

# Introduction to Classical and Quantum Mechanics

We formulate the equations of motion of a particle according to classical and quantum mechanics.

**Introduction to classical mechanics.** We consider a particle of mass  $m$  subjected to a conservative force field  $F(x)$ . A conservative force field is given by minus the gradient of a potential function  $V(x)$ . Suppose that the particle is moving in  $d$ -dimensional Euclidean space, called the configuration space. Then  $V(x)$  is a real-valued function of  $x \in \mathbb{R}^d$  and the force acting at the point  $x$  is given by

$$F(x) = -\nabla V(x).$$

Suppose that at time  $t_0$  the particle is at the position  $x_0$  with velocity  $v_0$ . Then according to **Newton's law**, the position  $x(t)$  of the particle at time  $t$  is determined by the initial value problem

$$\begin{aligned} m\ddot{x} &= -\nabla V(x), \\ x(t_0) &= x_0, \\ \dot{x}(t_0) &= v_0. \end{aligned}$$

Newton's equation can be formulated in Hamiltonian form. We define the **momentum**  $p$  of the particle by

$$p = m\dot{x}.$$

In Hamiltonian mechanics, the state of the particle is represented by a point  $(x, p)$  in the space  $\mathbb{R}^d \times \mathbb{R}^d$ , called the **phase space**. Using the variables  $x$  and  $p$ , we can rewrite Newton's equation as a first order system called Hamilton's equations:

$$\begin{aligned} \dot{x} &= \frac{1}{m}p, \\ \dot{p} &= -\nabla V(x), \\ x(t_0) &= x_0, \\ p(t_0) &= p_0. \end{aligned}$$

We can rewrite again these equations by using the **Hamilton function** (or Hamiltonian), which is a real-valued function on phase space defined by

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

The function

$$T(p) = \frac{1}{2m}p \cdot p$$

is called the **kinetic energy function**. The Hamiltonian  $H(x, p)$  represents the total energy of the particle at position  $x$  with momentum  $p$  (it is the sum of the kinetic energy and the potential energy). Now **Hamilton's equations** take the form

$$\begin{aligned}\dot{x} &= \frac{\partial H}{\partial p}(x, p), \\ \dot{p} &= -\frac{\partial H}{\partial x}(x, p), \\ x(t_0) &= x_0, \\ p(t_0) &= p_0.\end{aligned}$$

If  $V(x) \geq a - b|x|^2$ , where  $a$  and  $b$  are constants with  $b > 0$ , the initial value problem has a unique solution defined for all  $t$ . Thus, if at time  $t_0$  the particle is in the state  $(x_0, p_0)$ , the state  $(x(t), p(t))$  of the particle at time  $t$  is determined by Hamilton's equations. A simple calculation shows that if  $(x(t), p(t))$  is a solution to Hamilton's equations the value of  $H(x(t), p(t))$  is equal to a constant  $E$ , called the **energy** of the particle.

**Introduction to quantum mechanics.** On the atomic length scale, position and momentum are important observables, but they are insufficient to describe the state of a particle. The state of a quantum mechanical particle is represented by a complex-valued function  $\psi$  on configuration space called the **wave function**:

$$\psi : \mathbb{R}^d \rightarrow \mathbb{C}.$$

The function  $x \mapsto |\psi(x)|^2$  is interpreted as the probability density for the position of the particle. Thus we require the **normalization condition**

$$\int_{\mathbb{R}^d} |\psi(x)|^2 dx = 1.$$

The space of normalizable wave functions is the space of square-summable functions

$$L^2(\mathbb{R}^d) = \left\{ \psi : \mathbb{R}^d \rightarrow \mathbb{C} \mid \int_{\mathbb{R}^d} |\psi(x)|^2 dx < \infty \right\}.$$

The inner product of two functions in  $L^2(\mathbb{R}^d)$  is defined by

$$\langle \psi, \varphi \rangle = \int_{\mathbb{R}^d} \overline{\psi(x)} \varphi(x) dx.$$

In 1926, Schrödinger postulated an equation that describes the time evolution of the wave function, which is considered the fundamental equation of quantum mechanics. According to Schrödinger, if the particle is in the state  $\psi_0(x)$  at time  $t_0$ , the state  $\psi(x, t)$  of the particle at time  $t$  is determined by the initial value problem

$$\begin{aligned} i\hbar \frac{\partial \psi}{\partial t} &= H\psi, \\ \psi(x, t_0) &= \psi_0(x). \end{aligned}$$

Here, the parameter  $\hbar$  is the reduced Planck constant and  $H$  is a self-adjoint operator on  $L^2(\mathbb{R}^d)$ , called the **Hamilton operator**. We will describe below the operator  $H$ . The above equation is called **Schrödinger's equation**. The fact that  $H$  is a self-adjoint operator implies that the initial value problem has a unique solution defined for all  $t$ .

In quantum mechanics, the classical energy function  $H(x, p)$  is replaced by an **energy functional** of the wave function defined by

$$\mathcal{E}(\psi) = T_\psi + V_\psi,$$

where

$$T_\psi = \frac{\hbar^2}{2m} \int_{\mathbb{R}^d} |\nabla \psi(x)|^2 dx$$

and

$$V_\psi = \int_{\mathbb{R}^d} V(x) |\psi(x)|^2 dx.$$

The derivatives in the gradient can be interpreted in the distributional sense. The functionals  $\mathcal{E}(\psi)$ ,  $T_\psi$  and  $V_\psi$  are called the total, kinetic and potential energy of  $\psi$ , respectively.

A comparison of the kinetic energy function  $T(p)$  and the kinetic energy functional  $T_\psi$  shows that the transition from classical to quantum mechanics is accomplished by replacing the momentum  $p$  by the operator  $-i\hbar\nabla$  applied to  $\psi$  and replacing the dot product on  $\mathbb{R}^d$  by the inner product on  $L^2(\mathbb{R}^d)$ . Hence we define the momentum operator by  $p = -i\hbar\nabla$ . Thus we have

$$T_\psi = \frac{1}{2m} \int_{\mathbb{R}^d} |(p\psi)(x)|^2 dx.$$

Associated to the kinetic energy function  $T(p)$ , we consider the operator

$$T = \frac{1}{2m} p \cdot p = -\frac{\hbar^2}{2m} \Delta,$$

called the kinetic energy operator, which acts on a function by

$$(T\psi)(x) = -\frac{\hbar^2}{2m} \sum_{j=1}^d \frac{\partial^2 \psi}{\partial x_j^2}(x).$$

Associated to the function  $V(x)$ , we consider the operator  $V$ , called the potential operator, which acts on a function by

$$(V\psi)(x) = V(x)\psi(x).$$

Thus, associated to the function  $H(x, p)$  we have the Hamilton operator (or Hamiltonian) defined by

$$H = T + V.$$

If  $\psi$  is a smooth function with bounded support, we can justify the equality

$$\frac{1}{2m}\langle p\psi, p\psi \rangle = -\frac{\hbar^2}{2m}\langle \psi, \Delta\psi \rangle$$

and write

$$\mathcal{E}(\psi) = \langle \psi, H\psi \rangle.$$

Using the functional  $\mathcal{E}(\psi)$ , we may consider the minimization problem

$$E_0 = \inf \left\{ \mathcal{E}(\psi) \mid \psi \in L^2(\mathbb{R}^d) \text{ and } \int_{\mathbb{R}^d} |\psi(x)|^2 dx = 1 \right\}.$$

Suppose that  $V(x)$  is such that the constant  $E_0$  exists. If the infimum is a minimum, that is, if  $E_0 = \mathcal{E}(\psi_0)$  for some  $\psi_0$ , then  $E_0$  is called the **ground state energy** and  $\psi_0$  is called the **ground state**. Suppose that the particle has a ground state. Then a simple variational calculation leads to the equation

$$H\psi_0 = E_0\psi_0.$$

In general,  $E_0$  and  $\psi_0$  are not the only solution to the **time-independent Schrödinger equation**

$$H\psi = E\psi.$$

This equation has usually infinitely many solutions  $E_n$  and  $\psi_n$ , called the eigenvalues and eigenfunctions of  $H$ . The real numbers  $E_n$  represent the possible energies of the particle and  $\psi_n$  the corresponding states, called eigenstates.

We now turn to Schrödinger's equation (and ignore for the moment the initial condition):

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi.$$

A good strategy for investigating a partial differential equation is first to obtain some explicit solution and then, provided that the equation is linear, to construct more complicated solutions using the explicit ones. To obtain explicit solutions, it is often useful to look for solutions of specific form. We will use the method of separation of variables and search for solutions of the form

$$\psi(x, t) = \varphi(x)\chi(t).$$

Substituting this expression into Schrödinger's equation, we obtain

$$\dot{\chi} = -\frac{iE}{\hbar}\chi$$

and

$$H\varphi = E\varphi,$$

where  $E$  is the separation constant. The solutions to the former equation are multiples of

$$\chi(t) = e^{-iEt/\hbar}.$$

The equation for  $\varphi$  is precisely the time-independent Schrödinger equation. Thus, if  $E$  and  $\varphi$  are eigenvalues and eigenfunctions of  $H$ , then

$$\psi(x, t) = \varphi(x)e^{-iEt/\hbar}$$

is a solution to the Schrödinger equation. Solutions of this form are called stationary states because, although  $\psi(x, t)$  depends on time, the probability density

$$|\psi(x, t)|^2 = |\varphi(x)|^2$$

does not depend on time. In addition, if we suppose that the eigenfunctions  $\varphi_n$  form a basis for  $L^2(\mathbb{R}^d)$ , the general solution to the Schrödinger equation is given by

$$\psi(x, t) = \sum_{n=0}^{\infty} c_n \varphi_n(x) e^{-iE_n t/\hbar},$$

where  $c_1, c_2, c_3, \dots$  are constants. When the eigenfunctions  $\varphi_n$  do not form a basis for  $L^2(\mathbb{R}^d)$ , we shall consider a more general theory for the study of the equation  $H\varphi = E\varphi$ , called the spectral theory. In this theory, the spectrum of  $H$  is the set of “generalized eigenvalues” of  $H$ . As these observations suggest, the dynamical properties of the time evolution are closely related to the spectral properties of the Hamiltonian. Therefore, a crucial step in the analysis of quantum systems is investigating the spectrum of  $H$ .

## References

- [1] Lieb E. H., Seiringer R., *The Stability of Matter in Quantum Mechanics*, Cambridge University Press, 2010.