Chapter I

Waves and particles. Introduction to the fundamental ideas of quantum mechanics

In the present state of scientific knowledge, quantum mechanics plays a fundamental role in the description and understanding of natural phenomena. In fact, phenomena that occur on a very small (atomic or subatomic) scale cannot be explained outside the framework of quantum physics. For example, the existence and the properties of atoms, the chemical bond and the propagation of an electron in a crystal cannot be understood

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in terms of classical mechanics. Even when we are concerned only with macroscopic physical objects (that is, whose dimensions are comparable to those encountered in everyday life), it is necessary, in principle, to begin by studying the behavior of their various constituent atoms, ions, electrons, in order to arrive at a complete scientific description. Actually, there are many phenomena that reveal, on a macroscopic scale, the quantum behaviour of nature. It is in this sense that it can be said that quantum mechanics is the basis of our present understanding of all natural phenomena, including those traditionally treated in chemistry, biology, etc...

From a historical point of view, quantum ideas contributed to a remarkable unification of the concepts of fundamental physics by treating material particles and radiation on the same footing. At the end of the nineteenth century, people distinguished between two entities in physical phenomena: matter and radiation. Completely different laws were used for each one. To predict the motion of material bodies, the laws of *Newtonian mechanics* (*cf.* Appendix III) were utilized. Their success, though of long standing, was none the less impressive. With regard to radiation, the *theory of electromagnetism*, thanks to the introduction of Maxwell's equations, had produced a unified interpretation of a set of phenomena which had previously been considered as belonging to different domains: electricity, magnetism and optics. In particular, the electromagnetic theory of radiation had been spectacularly confirmed experimentally by the discovery of Hertzian waves. Finally, *interactions between radiation and matter* were well explained by the Lorentz force. This set of laws had brought physics to a point which could be considered satisfactory, in view of the experimental data at the time.

However, at the beginning of the twentieth century, physics was to be marked by the profound upheaval that led to the introduction of relativistic mechanics and quantum mechanics. The relativistic "revolution" and the quantum "revolution" were, to a large extent, independent, since they challenged classical physics on different points. Classical laws cease to be valid for material bodies travelling at very high speeds, comparable to that of light (relativistic domain). In addition, they are also found to be wanting on an atomic or subatomic scale (quantum domain). However, it is important to note that classical physics, in both cases, can be seen as an approximation of the new theories, an approximation which is valid for most phenomena on an everyday scale. For example, Newtonian mechanics enables us to predict correctly the motion of a solid body, providing it is non-relativistic (speeds much smaller than that of light) and macroscopic (dimensions much greater than atomic ones). Nevertheless, from a fundamental point of view, quantum theory remains indispensable. It is the only theory which enables us to understand the very existence of a solid body and the values of the macroscopic parameters (density, specific heat, elasticity, etc...) associated with it. It is possible to develop a theory that is at the same time quantum and relativistic, but such a theory is relatively complex. However, most atomic and molecular phenomena are well explained by the *non-relativistic quantum mechanics* that we intend to examine here.

This chapter is an introduction to quantum ideas and "vocabulary". *No attempt is made here to be rigorous or complete.* The essential goal is to awaken the curiosity of the reader. Phenomena will be described which unsettle ideas as firmly anchored in our intuition as the concept of a trajectory. We want to render the quantum theory "plausible" for the reader by showing simply and qualitatively how it enables us to solve the problems which are encountered on an atomic scale. We shall later return to the various ideas introduced in this chapter and go into further detail, either from the point

of view of the mathematical formalism (Chap. II) or from the physical point of view (Chap. III).

In the first section (§ A), we introduce the basic quantum ideas (wave-particle duality, the measurement process), relying on well-known optical experiments. Then we show (§ B) how these ideas can be extended to material particles (wave function, Schrödinger equation). We next study in more detail the characteristics of the "wave packet" associated with a particle, and we introduce the Heisenberg relations (§ C). Finally, we discuss some simple examples of typical quantum effects (§ D).

A. Electromagnetic waves and photons

A-1. Light quanta and the Planck-Einstein relations

Newton considered light to be a beam of particles, able, for example, to bounce back upon reflection from a mirror. During the first half of the nineteenth century, the wavelike nature of light was demonstrated (interference, diffraction). This later enabled optics to be integrated into electromagnetic theory. In this framework, the speed of light, c, is related to electric and magnetic constants and light polarization phenomena can be interpreted as manifestations of the vectorial character of the electric field.

However, the study of *blackbody* radiation, which electromagnetic theory could not explain, led Planck to suggest the hypothesis of the *quantization of energy* (1900): for an electromagnetic wave of frequency ν, the only possible energies are integral multiples of the quantum $h\nu$, where h is a new fundamental constant. Generalizing this hypothesis, Einstein proposed a return to the particle theory (1905): light consists of a beam of *photons*, each possessing an energy $h\nu$. Einstein showed how the introduction of photons made it possible to understand, in a very simple way, certain as yet unexplained characteristics of the photoelectric effect. Twenty years had to elapse before the photon was actually shown to exist, as a distinct entity, by the Compton effect (1924).

These results lead to the following conclusion: the interaction of an electromagnetic wave with matter occurs by means of *elementary indivisible processes*, in which the radiation appears to be composed of particles, the photons. Particle parameters (the energy E and the momentum $\mathbf{p}$ of a photon) and wave parameters (the angular frequency $\omega = 2\pi\nu$ and the wave vector $\mathbf{k}$, where $|\mathbf{k}| = 2\pi/\lambda$, with ν the frequency and λ the wavelength) are linked by the fundamental relations:

$$\boxed{\begin{array}{l} E = h\nu = \hbar\omega \\ \mathbf{p} = \hbar\,\mathbf{k} \end{array}} \qquad \text{(Planck-Einstein relations)} \tag{A-1}$$

where $\hbar = h/2\pi$ is defined in terms of the Planck constant h:

$$h \simeq 6.62\ \ 10^{-34}\ \ \text{Joule} \times \text{second} \tag{A-2}$$

During each elementary process, energy and total momentum must be conserved.

A-2. Wave-particle duality

Thus we have returned to a particle conception of light. Does this mean that we must abandon the wave theory? Certainly not. We shall see that typical wave

phenomena such as interference and diffraction could not be explained in a purely particle framework. Analyzing Young's well-known double-slit experiment will lead us to the following conclusion: a complete interpretation of the phenomena can be obtained only by conserving *both* the wave aspect and the particle aspect of light (although they seem *a priori* irreconcilable). We shall then show how this paradox can be resolved by the introduction of the fundamental quantum concepts.

A-2-a. Analysis of Young's double-slit experiment

The device used in this experiment is shown schematically in Figure 1. The monochromatic light emitted by the source $\mathscr{S}$ falls on an opaque screen $\mathscr{P}$ pierced by two narrow slits F_1 and F_2, which illuminate the observation screen $\mathscr{E}$ (a photographic plate, for example). If we block F_2, we obtain on $\mathscr{E}$ a light intensity distribution $I_1(x)$ which is the diffraction pattern of F_1. In the same way, when F_1 is obstructed, the diffraction pattern of F_2 is described by $I_2(x)$. When the two slits F_1 and F_2 are open at the same time, we observe a system of interference fringes on the screen. In particular, we note that the corresponding intensity $I(x)$ is not the sum of the intensities produced by F_1 and F_2 separately:

$$I(x) \neq I_1(x) + I_2(x) \tag{A-3}$$

How could one conceive of explaining, in terms of a particle theory (seen, in the preceding section, to be necessary), the experimental results just described? The existence of a diffraction pattern when only one of the two slits is open could, for example, be explained as being due to photon collisions with the edges of the slit. Such an explanation would, of course, have to be developed more precisely, and a more detailed study would show it to be insufficient. Instead, let us concentrate on the interference phenomenon. We could attempt to explain it by an interaction between the photons which pass through the slit F_1 and those which pass through the slit F_2. Such an explanation would lead to the following prediction: if the intensity of the source $\mathscr{S}$ (the number of photons emitted per second) is diminished until the photons strike the screen practically one by one, the interaction between the photons must diminish and, eventually, vanish. The interference fringes should therefore disappear.

Before we indicate the answer given by experiment, recall that the wave theory provides a completely natural interpretation of the fringes. The light intensity at a point of the screen $\mathscr{E}$ is proportional to the square of the amplitude of the electric field at this point. If $E_1(x)$ and $E_2(x)$ represent, in complex notation, the electric fields produced at x by slits F_1 and F_2 respectively (the slits behave like secondary sources), the total resultant field at this point when F_1 and F_2 are both open is[1]:

$$E(x) = E_1(x) + E_2(x) \tag{A-4}$$

Using complex notation, we then have:

$$I(x) \propto |E(x)|^2 = |E_1(x) + E_2(x)|^2 \tag{A-5}$$

Since the intensities $I_1(x)$ and $I_2(x)$ are proportional, respectively, to $|E_1(x)|^2$ and $|E_2(x)|^2$, formula (A-5) shows that $I(x)$ differs from $I_1(x) + I_2(x)$ by an interference

[1] Since the experiment studied here is performed with unpolarized light, the vectorial character of the electric field does not play an essential role. For the sake of simplicity, we ignore it in this paragraph.

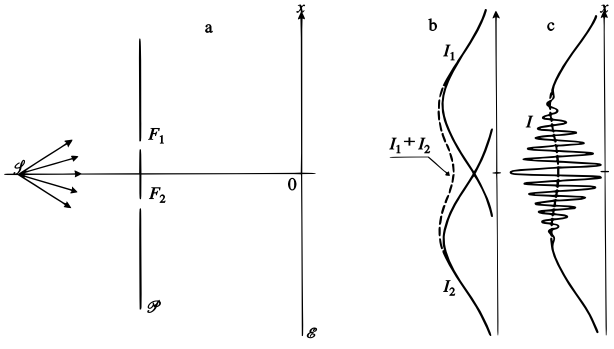

Figure 1: Diagram of Young's double-slit light interference experiment (fig. a). Each of the slits F_1 and F_2 produces a diffraction pattern on the screen $\mathcal{E}$. The corresponding intensities are $I_1(x)$ and $I_2(x)$ (solid lines in figure b). When the two slits F_1 and F_2 are open simultaneously, the intensity $I(x)$ observed on the screen is not the sum $I_1(x) + I_2(x)$ (dashed lines in figure b), but shows oscillations due to the interference between the electric fields radiated by F_1 and F_2 (solid line in figure c).

term which depends on the phase difference between E_1 and E_2 and whose presence explains the fringes. The wave theory thus predicts that diminishing the intensity of the source $\mathscr{S}$ will simply cause the fringes to diminish in intensity but not vanish.

What actually happens when $\mathscr{S}$ emits photons practically one by one? *Neither the predictions of the wave theory nor those of the particle theory are verified.* In fact:

(*i*) If we cover the screen $\mathscr{E}$ with a photographic plate and increase the exposure time so as to capture a large number of photons on each photograph, we observe when we develop them that the *fringes have not disappeared. Therefore, the purely corpuscular interpretation*, according to which the fringes are due to an interaction between photons, *must be rejected.*

(*ii*) On the other hand, we can expose the photographic plate during a time so short that it can only receive a few photons. We then observe that each photon produces a *localized impact* on $\mathscr{E}$ and not a very weak interference pattern. *Therefore, the purely wave interpretation must also be rejected.*

In reality, as more and more photons strike the photographic plate, the following phenomenon occurs. Their individual impacts seem to be distributed in a *random manner*, and only when a great number of them have reached $\mathscr{E}$ does the distribution of the impacts begin to have a continuous aspect. The density of the impacts at each point of $\mathscr{E}$ corresponds to the interference fringes: maximum on a bright fringe and zero on a dark fringe. It can thus be said that the photons, as they arrive, build up the interference pattern.

The result of this experiment therefore leads, apparently, to a paradox. Within the framework of the particle theory, for example, it can be expressed in the following way. Since photon-photon interactions are excluded, each photon must be considered separately. But then it is not clear why the phenomena should change drastically according to whether only one slit or both slits are open. For a photon passing through one of the slits, why should the fact that the other is open or closed have such a critical

importance?

Before we discuss this problem, note that in the preceding experiment we did not seek to determine through which slit each photon passed before it reached the screen. In order to obtain this information, we can imagine placing detectors (photomultipliers) behind F_1 and F_2. It will then be observed that, if the photons arrive one by one, each one passes through a well-determined slit (a signal is recorded either by the detector placed behind F_1 or by the one covering F_2 but not by both at once). But, obviously, the photons detected in this way are absorbed and do not reach the screen. Remove the photomultiplier which blocks F_1, for example. The one which remains behind F_2 tells us that, out of a large number of photons, about half pass through F_2. We conclude that the others (which can continue as far as the screen) pass through F_1. But the pattern that they gradually construct on the screen is not an interference pattern, since F_2 is blocked. It is only the diffraction pattern of F_1.

A-2-b. Quantum unification of the two aspects of light

The preceding analysis shows that it is impossible to explain all the phenomena observed if only one of the two aspects of light, wave or particle, is considered. Now these two aspects seem to be mutually exclusive. To overcome this difficulty, it thus becomes indispensable to reconsider in a critical way the concepts of classical physics. We must accept the possibility that these concepts, although our everyday experience leads us to consider them well-founded, may not be valid in the new ("microscopic") domain which we are entering. For example, an essential characteristic of this new domain appeared when we placed counters behind Young's slits: *when one performs a measurement on a microscopic system, one disturbs it in a fundamental fashion.* This is a new property since, in the macroscopic domain, we always have the possibility of conceiving measurement devices whose influence on the system is practically as weak as one might wish. This critical revision of classical physics is imposed by experiment and must of course be guided by experiment.

Let us reconsider the "paradox" stated above concerning the photon which passes through one slit but behaves differently depending on whether the other slit is open or closed. We saw that if we try to detect the photons when they cross the slits, we prevent them from reaching the screen. More generally, a detailed experimental analysis shows that *it is impossible to observe the interference pattern and to know at the same time through which slit each photon has passed* (*cf.* Complement $\mathrm{D_I}$). Thus it is necessary, in order to resolve the paradox, to give up the idea that a photon inevitably passes through a particular slit. We are then led to question the concept, which is a fundamental one of classical physics, of a particle's trajectory.

Moreover, as the photons arrive one by one, their impacts on the screen gradually build up the interference pattern. This implies that, for a particular photon, we are not certain in advance where it will strike the screen. Now these photons are all emitted under the same conditions. Thus another classical idea has been destroyed: that the initial conditions completely determine the subsequent motion of a particle. We can only say, when a photon is emitted, that the probability of its striking the screen at x is proportional to the intensity $I(x)$ calculated using wave theory, that is, to $|E(x)|^2$.

After many tentative efforts that we shall not describe here, the concept of *wave-particle duality* was formulated. We can summarize it schematically as follows[2]:

[2]It is worth noting that this interpretation of physical phenomena, generally considered to be "ortho-

(i) The particle and wave aspects of light are inseparable. *Light behaves simultaneously like a wave and like a flux of particles, the wave enabling us to calculate the probability of the manifestation of a particle.*

(ii) Predictions about the behavior of a photon can only be probabilistic.

(iii) The information about a photon at time t is given by the wave $E(\mathbf{r}, t)$, which is a solution of Maxwell's equations. We say that this wave characterizes the state of the photons at time t; $E(\mathbf{r}, t)$ is interpreted as the *probability amplitude* of a photon appearing, at time t, at the point $\mathbf{r}$. This means that the corresponding probability is proportional to $|E(\mathbf{r}, t)|^2$.

Comments:

(i) Since Maxwell's equations are linear and homogeneous, we can use a *superposition principle*: if E_1 and E_2 are two solutions of these equations, then $E = \lambda_1 E_1 + \lambda_2 E_2$, where λ_1 and λ_2 are constants, is also a solution. It is this superposition principle which explains wave phenomena in classical optics (interference, diffraction). In quantum physics, the interpretation of $E(\mathbf{r}, t)$ as a probability amplitude is thus essential to the persistence of such phenomena.

(ii) The theory merely allows one to calculate the probability of the occurence of a given event. Experimental verifications must thus be founded on the repetition of a large number of identical experiments. In the above experiment, a large number of photons, all produced in the same way, are emitted successively and build up the interference pattern, according to the calculated probabilities.

(iii) We are talking here about "the photon state" so as to be able to develop in § B an analogy between $E(\mathbf{r}, t)$ and the wave function $\psi(\mathbf{r}, t)$ that characterizes the quantum state of a material particle. This "optical analogy" is very fruitful. In particular, as we shall see in § D, it allows us to understand, simply and without recourse to calculation, various quantum properties of material particles. However, we should not push it too far and let it lead us to believe that it is rigorously correct to consider $E(\mathbf{r}, t)$ as characterizing the quantum state of a photon.

Furthermore, we shall see that the fact that $\psi(\mathbf{r}, t)$ is complex is essential in quantum mechanics, while the complex notation $E(\mathbf{r}, t)$ is used in optics purely for convenience (only its real part has a physical meaning). The precise definition of the (complex) quantum state of radiation can only be given in the framework of quantum electrodynamics, a theory which is simultaneously quantum mechanical and relativistic. We shall not consider these problems here (they will briefly be discussed in Complement $\mathrm{K_V}$).

A-3. The principle of spectral decomposition

Armed with the ideas introduced in § A-2, we are now going to discuss another simple optical experiment, whose subject is the polarization of light. This will permit us to introduce the fundamental concepts which concern the measurement of physical quantities.

dox", is not unique; other interpretations have been proposed, which are still discussed among physicists.

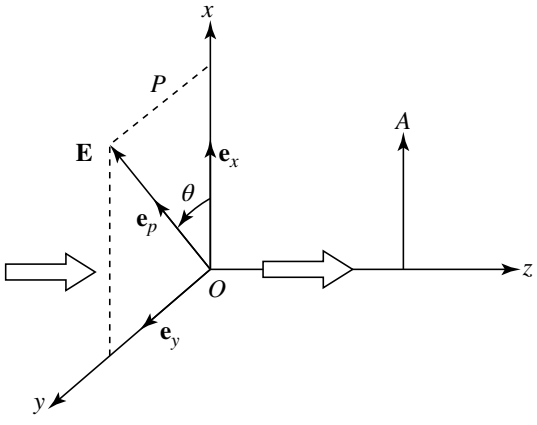

Figure 2: A simple measurement experiment relating to the polarization of a light wave. A beam of light propagates along the direction Oz and crosses successively the polarizer P and the analyzer A; θ is the angle between Ox and the electric field of the wave transmitted by P. The vibrations transmitted by A are parallel to Ox.

The experiment consists of directing a polarized monochromatic plane light wave onto an analyzer A. Oz designates the direction of propagation of this wave and $\mathbf{e}_p$, the unit vector describing its polarization (*cf.* Fig. 2). The analyzer A transmits light polarized parallel to Ox and absorbs light polarized parallel to Oy.

The classical description of this experiment (a description which is valid for a sufficiently intense light beam) is the following. The polarized plane wave is characterized by an electric field of the form:

$$\mathbf{E}(\mathbf{r},t) = E_0\ \mathbf{e}_p\ \mathrm{e}^{i(kz-\omega t)} \tag{A-6}$$

where E_0 is a constant. The light intensity I is proportional to $|E_0|^2$. After its passage through the analyzer A, the plane wave is polarized along Ox:

$$\mathbf{E}'(\mathbf{r},t) = E'_0\ \mathbf{e}_x\ \mathrm{e}^{i(kz-\omega t)} \tag{A-7}$$

and its intensity I', proportional to $|E'_0|^2$, is given by *Malus' law*:

$$I' = I\ \cos^2\ \theta \tag{A-8}$$

[$\mathbf{e}_x$ is the unit vector of the Ox axis and θ is the angle between $\mathbf{e}_x$ and $\mathbf{e}_p$].

What will happen on the quantum level, that is, when I is weak enough for the photons to reach the analyzer one by one? (We then place a photon detector behind this analyser.) First of all, the detector never registers a "fraction of a photon". Either the photon crosses the analyzer or it is entirely absorbed by it. Next (except in special cases that we shall examine in a moment), we cannot predict with certainty whether a given incident photon will pass or be absorbed. We can only know the corresponding

probabilities. Finally, if we send out a large number N of photons one after the other, the result will correspond to the classical law, in the sense that about $N \cos^2 \theta$ photons will be detected after the analyzer.

We shall retain the following ideas from this description:

(*i*) The measurement device (the analyzer, in this case) can give only certain privileged results, which we shall call *eigen* (or proper) *results*[3]. In the above experiment, there are only two possible results: the photon crosses the analyzer or it is stopped. One says that there is quantization of the result of the measurement, in contrast to the classical case [*cf.* formula (A-8)] where the transmitted intensity I' can vary continuously, according to the value of θ, between 0 and I.

(*ii*) To each of these eigen results corresponds an *eigenstate*. Here, the two eigenstates are characterized by:

$$\begin{array}{ll} & \mathbf{e}_p = \mathbf{e}_x \\ \text{or} & \mathbf{e}_p = \mathbf{e}_y \end{array} \tag{A-9}$$

($\mathbf{e}_y$ is the unit vector of the Oy axis). If $\mathbf{e}_p = \mathbf{e}_x$, we know with certainty that the photon will traverse the analyzer; if $\mathbf{e}_p = \mathbf{e}_y$, it will, on the contrary, definitely be stopped. The correspondence between eigen results and eigenstates is therefore the following. If the particle is, before the measurement, in one of the eigenstates, the result of this measurement is certain: it can only be the associated eigen result.

(*iii*) When the state before the measurement is arbitrary, only the probabilities of obtaining the different eigen results can be predicted. To find these probabilities, one decomposes the state of the particles into a linear combination of the various eigenstates. Here, for an arbitrary $\mathbf{e}_p$, we write:

$$\mathbf{e}_p = \mathbf{e}_x \cos \theta + \mathbf{e}_y \sin \theta \tag{A-10}$$

The probability of obtaining a given eigen result is then proportional to the square of the absolute value of the coefficient of the corresponding eigenstate.

The proportionality factor is determined by the condition that the sum of all these probabilities must be equal to 1. We thus deduce from (A-10) that each photon has a probability $\cos^2 \theta$ of traversing the analyzer and a probability $\sin^2 \theta$ of being absorbed by it (we know that $\cos^2 \theta + \sin^2 \theta = 1$). This is indeed what was stated above. This rule is called in quantum mechanics the *principle of spectral decomposition*. Note that the decomposition to be performed depends on the type of measurement device being considered, since one must use the eigenstates which correspond to it: in formula (A-10), the choice of the axes Ox and Oy is fixed by the analyzer.

(*iv*) After passing through the analyzer, the light is completely polarized along $\mathbf{e}_x$. If we place, after the first analyzer A, a second analyzer A', having the same axis, all the photons which traversed A will also traverse A'. According to what we have just seen in point (*ii*), this means that, after they have crossed A, the state of the photons is the eigenstate characterized by $\mathbf{e}_x$. There has therefore been an abrupt change in the state of the particles. Before the measurement, this state was defined by a vector $\mathbf{E}(\mathbf{r}, t)$ which was collinear with $\mathbf{e}_p$. After the measurement, we possess an additional piece of information (the photon has passed) which is incorporated by describing the state by a different vector, which is now collinear with $\mathbf{e}_x$. This expresses the fact, already pointed

[3]The reason for this name will appear in Chapter III.

out in § A-2, that *the measurement disturbs the microscopic system* (here, the photon) in *a fundamental fashion.*

Comment:

The certain prediction of the result when $\mathbf{e}_p = \mathbf{e}_x$ or $\mathbf{e}_p = \mathbf{e}_y$ is only a special case. The probability of one of the possible events is then indeed equal to 1. But, in order to verify this prediction, one must perform a large number of experiments. One must be sure that *all* the photons pass (or are stopped), since the fact that a particular photon crosses the analyzer (or is absorbed) is not characteristic of $\mathbf{e}_p = \mathbf{e}_x$ (or $\mathbf{e}_p = \mathbf{e}_y$).

B. Material particles and matter waves

B-1. The de Broglie relations

Parallel to the discovery of photons, the study of atomic emission and absorption spectra uncovered a fundamental fact, which classical physics was unable to explain: these spectra are composed of *narrow lines.* In other words, a given atom emits or absorbs only photons having well-determined frequencies (that is, energies). This fact can be interpreted very easily if one accepts that *the energy of the atom is quantized*, that is, it can take on only certain discrete values E_i ($i = 1, 2, ..., n, ...$): the emission or absorption of a photon is then accompanied by a "jump" in the energy of the atom from one permitted value E_i to another E_j. Conservation of energy implies that the photon has a frequency ν_{ij} such that:

$$h\,\nu_{ij} = |E_i - E_j| \tag{B-1}$$

Only frequencies which obey (B-1) can therefore be emitted or absorbed by the atom.

The existence of such discrete energy levels was confirmed independently by the Franck-Hertz experiment. Bohr interpreted this in terms of privileged electronic orbits and stated, with Sommerfeld, an empirical rule which permitted the calculation of these orbits for the case of the hydrogen atom. But the fundamental origin of these quantization rules remained mysterious.

In 1923, however, de Broglie put forth the following hypothesis: *material particles, just like photons, can have a wavelike aspect.* He then derived the Bohr-Sommerfeld quantization rules as a consequence of this hypothesis, the various permitted energy levels appearing as analogues of the normal modes of a vibrating string. Electron diffraction experiments (Davisson and Germer, 1927) strikingly confirmed the existence of a wavelike aspect of matter by showing that *interference patterns could be obtained with material particles such as electrons.*

One therefore associates with a material particle of energy E and momentum $\mathbf{p}$, a wave whose angular frequency $\omega = 2\pi\nu$ and wave vector $\mathbf{k}$ are given by the same relations as for photons (*cf.* § A-1):

$$\begin{cases} E = h\nu = \hbar\omega \\ \mathbf{p} = \hbar\mathbf{k} \end{cases} \tag{B-2}$$

In other words, the corresponding wavelength is:

$$\lambda = \frac{2\pi}{|\mathbf{k}|} = \frac{h}{|\mathbf{p}|} \qquad \text{(de Broglie relation)} \tag{B-3}$$

Comment:

The very small value of the Planck constant h explains why the wavelike nature of matter is very difficult to demonstrate on a macroscopic scale. Complement A_I of this chapter discusses the orders of magnitude of the de Broglie wavelengths associated with various material particles.

B-2. Wave functions. Schrödinger equation

In accordance with de Broglie's hypothesis, we shall apply the ideas introduced in § A for the case of the photon to all material particles. Recalling the conclusions of this paragraph, we are led to the following formulation:

(*i*) For the classical concept of a position and momentum, we must substitute the concept of a time-varying *state*. The quantum state of a particle such as the electron[4] is characterized by a *wave function* $\psi(\mathbf{r}, t)$, which contains all the information it is possible to obtain about the particle.

(*ii*) $\psi(\mathbf{r}, t)$ is interpreted as a *probability amplitude of the particle's presence*. Since the possible positions of the particle form a continuum, the probability $\mathrm{d}\mathscr{P}(\mathbf{r}, t)$ of the particle being, at time t, in a volume element $\mathrm{d}^3r = \mathrm{d}x\ \mathrm{d}y\ \mathrm{d}z$ situated at the point $\mathbf{r}$ must be proportional to d^3r. It is therefore infinitesimal, and $|\psi(\mathbf{r}, t)|^2$ is interpreted as the corresponding *probability density*, with:

$$\mathrm{d}\mathscr{P}(\mathbf{r}, t) = C\ |\psi(\mathbf{r}, t)|^2\ \mathrm{d}^3r \tag{B-4}$$

where C is a normalization constant [see comment (*i*) at the end of § B-2].

(*iii*) *The principle of spectral decomposition* applies to the measurement of an arbitrary physical quantity:

– The result found must belong to a set of eigen results $\{a\}$.

– With each eigenvalue a is associated an eigenstate, that is, an eigenfunction $\psi_a(\mathbf{r})$. This function is such that, if $\psi(\mathbf{r}, t_0) = \psi_a(\mathbf{r})$ (where t_0 is the time at which the measurement is performed), the measurement will always yield a.

– For any $\psi(\mathbf{r}, t)$, the probability $\mathscr{P}_a$ of finding the eigenvalue a for a measurement at time t_0 is found by decomposing $\psi(\mathbf{r}, t_0)$ in terms of the functions $\psi_a(\mathbf{r})$:

$$\psi(\mathbf{r}, t_0) = \sum_a c_a\ \psi_a(\mathbf{r}) \tag{B-5}$$

Then:

$$\mathscr{P}_a = \frac{|c_a|^2}{\sum_a |c_a|^2} \tag{B-6}$$

[4] We shall not take into account here the existence of electron spin (*cf.* Chap. IX).

$\Big($the presence of the denominator ensures that the total probability is equal to unity: $\sum_a \mathscr{P}_a = 1\Big)$.

– If the measurement indeed yields a, the wave function of the particle immediately after the measurement is:

$$\psi'(\mathbf{r}, t_0) = \psi_a(\mathbf{r}) \tag{B-7}$$

(*iv*) The equation describing the evolution of the function $\psi(\mathbf{r}, t)$ remains to be written. It is possible to introduce it in a very natural way, using the Planck and de Broglie relations. Nevertheless, we have no intention of proving this fundamental equation, which is called the *Schrödinger equation*. We shall simply assume it. Later, we shall discuss some of its consequences (whose experimental verification will prove its validity). Besides, we shall consider this equation in much more detail in Chapter III.

When the particle (of mass m) is subjected to the influence of a potential[5] $V(\mathbf{r}, t)$, the Schrödinger equation takes on the form:

$$\boxed{i\hbar \frac{\partial}{\partial t}\, \psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\, \Delta\psi(\mathbf{r}, t) + V(\mathbf{r}, t)\, \psi(\mathbf{r}, t)} \tag{B-8}$$

where Δ is the Laplacian operator $\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$.
We notice immediately that this equation is linear and homogeneous in ψ. Consequently, for material particles, there exists a superposition principle which, combined with the interpretation of ψ as a probability amplitude, is the source of wavelike effects. Note, moreover, that the differential equation (B-8) is first-order with respect to time. This condition is necessary if the state of the particle at a time t_0, characterized by $\psi(\mathbf{r}, t_0)$, is to determine its subsequent state.

Thus there exists a fundamental analogy between matter and radiation: in both cases, a correct description of the phenomena necessitates the introduction of quantum concepts, and, in particular, the idea of wave-particle duality.

Comments:

(*i*) For a system composed of only one particle, the total probability of finding the particle anywhere in space, at time t, is equal to 1:

$$\int \mathrm{d}\mathscr{P}(\mathbf{r}, t) = 1 \tag{B-9}$$

Since $\mathrm{d}\mathscr{P}(\mathbf{r}, t)$ is given by formula (B-4), we conclude that the *wave function* $\psi(\mathbf{r}, t)$ *must be square-integrable*:

$$\int |\psi(\mathbf{r}, t)|^2\, \mathrm{d}^3 r \quad \text{is finite} \tag{B-10}$$

[5] $V(\mathbf{r}, t)$ designates a potential energy here. For example, it may be the product of an electric potential and the particle's charge. In quantum mechanics, $V(\mathbf{r}, t)$ is commonly called a potential.

The normalization constant C that appears in (B-4) is then given by the relation:

$$\frac{1}{C} = \int |\psi(\mathbf{r}, t)|^2 \, \mathrm{d}^3 r \tag{B-11}$$

(we shall later see that the form of the Schrödinger equation implies that C is time-independent). One often uses wave functions which are normalized, such that:

$$\int |\psi(\mathbf{r}, t)|^2 \, \mathrm{d}^3 r = 1 \tag{B-12}$$

The constant C is then equal to 1.

(*ii*) Note the important difference between the concepts of classical states and quantum states. The classical state of a particle is determined at time t by the specification of six parameters characterizing its position and its velocity at time t: x, y, z; v_x, v_y, v_z. The quantum state of a particle is determined by an *infinite number* of parameters: the values at the various points in space of the wave function $\psi(\mathbf{r}, t)$ which is associated with it. For the classical idea of a trajectory (the succession in time of the various states of the classical particle), we must substitute the idea of the propagation of the wave associated with the particle. Consider, for example, Young's double-slit experiment, previously described for the case of photons, but which in principle can also be performed with material particles such as electrons. When the interference pattern is observed, it makes no sense to ask through which slit each particle has passed, since the wave associated with it passed through both.

(*iii*) It is worth noting that, unlike photons, which can be emitted or absorbed during an experiment, material particles can neither be created nor destroyed. The electrons emitted by a heated filament for example already existed in the filament. In the same way, an electron absorbed by a counter does not disappear; it becomes part of an atom or an electric current. Actually, the theory of relativity shows that it is possible to create and annihilate material particles: for example, a photon having sufficient energy, passing near an atom, can materialize into an electron-positron pair. Inversely, the positron, when it collides with an electron, annihilates with it, emitting photons. However, we pointed out in the beginning of this chapter that we would limit ourselves here to the non-relativistic quantum domain, and we have indeed treated time and space coordinates asymmetrically. In the framework of non-relativistic quantum mechanics, material particles can neither be created nor annihilated. This conservation law, as we shall see, plays a role of primary importance. The need to abandon it is one of the important difficulties encountered when one tries to construct a relativistic quantum mechanics.

C. Quantum description of a particle. Wave packets

In the preceding paragraph, we introduced the fundamental concepts necessary for the quantum description of a particle. In this paragraph, we are going to familiarize ourselves with these concepts and deduce from them several very important properties. We start with the very simple case of a free particle.

C-1. Free particle

Consider a particle whose potential energy is zero (or has a constant value) at every point in space. The particle is thus not subjected to any force; it is said to be free.

When $V(\mathbf{r}, t) = 0$, the Schrödinger equation becomes:

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{r}, t) \tag{C-1}$$

This differential equation is obviously satisfied by solutions of the form:

$$\psi(\mathbf{r}, t) = A\, \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \tag{C-2}$$

(where A is a constant), on the condition that $\mathbf{k}$ and ω satisfy the relation:

$$\omega = \frac{\hbar\mathbf{k}^2}{2m} \tag{C-3}$$

Observe that, according to the de Broglie relations [see (B-2)], condition (C-3) expresses the fact that the energy E and the momentum $\mathbf{p}$ of a free particle satisfy the equation, which is well-known in classical mechanics:

$$E = \frac{\mathbf{p}^2}{2m} \tag{C-4}$$

We shall come back later (§ C-3) to the physical interpretation of a state of the form (C-2). We already see that, since

$$|\psi(\mathbf{r}, t)|^2 = |A|^2 \tag{C-5}$$

a plane wave of this type represents a particle whose probability of presence is uniform throughout all space (see comment below).

The principle of superposition tells us that every linear combination of plane waves satisfying (C-3) will also be a solution of equation (C-1). Such a superposition can be written:

$$\psi(\mathbf{r}, t) = \frac{1}{(2\pi)^{3/2}}\int g(\mathbf{k})\, \mathrm{e}^{i[\mathbf{k}\cdot\mathbf{r}-\omega(k)t]}\, \mathrm{d}^3k \tag{C-6}$$

(d^3k represents, by definition, the infinitesimal volume element in $\mathbf{k}$-space: $\mathrm{d}k_x\, \mathrm{d}k_y\, \mathrm{d}k_z$). $g(\mathbf{k})$, which can be complex, must be sufficiently regular to allow differentiation inside the integral. It can be shown, moreover, that any square-integrable solution can be written in the form (C-6).

A wave function such as (C-6), a superposition of plane waves, is called a three-dimensional "wave packet". For the sake of simplicity, we shall often be led to study the case of a one-dimensional wave packet[6] of plane waves all propagating parallel to Ox. The wave function then depends only on x and t:

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} g(k)\, \mathrm{e}^{i[kx-\omega(k)t]}\, \mathrm{d}k \tag{C-7}$$

[6] A simple model of a two-dimensional wave packet is presented in Complement $\mathrm{E_I}$. Some general properties of three-dimensional wave packets are studied in Complement $\mathrm{F_I}$, which also shows how, in certain cases, a three-dimensional problem can be reduced to several one-dimensional problems.

In the following paragraph, we shall be interested in the form of the wave packet at a given instant. If we choose this instant as the time origin, the wave function is written:

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int g(k)\, \mathrm{e}^{ikx}\, \mathrm{d}k \tag{C-8}$$

We see that $g(k)$ is simply the Fourier transform (*cf.* Appendix I) of $\psi(x,0)$:

$$g(k) = \frac{1}{\sqrt{2\pi}} \int \psi(x,0)\, \mathrm{e}^{-ikx}\, \mathrm{d}x \tag{C-9}$$

Consequently, the validity of formula (C-8) is not limited to the case of the free particle: whatever the potential, $\psi(x,0)$ can always be written in this form. The consequences that we shall derive from this in §§ C-2 and C-3 below are thus perfectly general. It is not until § C-4 that we shall return explicitly to the free particle.

Comment:

A plane wave of type (C-2), whose modulus is constant throughout all space [*cf.* (C-5)], is not square-integrable. Therefore, rigorously, it cannot represent a physical state of the particle (in the same way as, in optics, a monochromatic plane wave is not physically realizable). On the other hand, a superposition of plane waves like (C-7) can be square-integrable.

C-2. Form of the wave packet at a given time

The form of the wave packet is given by the x-dependence of $\psi(x,0)$ defined by equation (C-8). Imagine that $|g(k)|$ has the shape depicted in Figure 3, with a pronounced peak situated at $k = k_0$ and a width (defined, for example, at half its maximum value) of Δk.

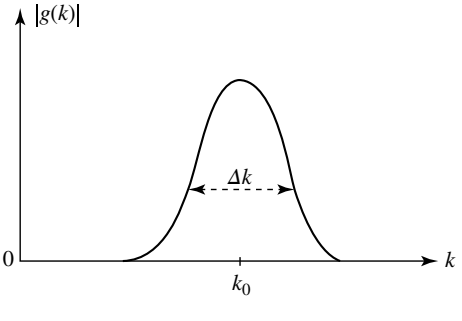

Figure 3: Shape of the function $|g(k)|$, modulus of the Fourier transform of $\psi(x,0)$: we assume that it is centered at $k = k_0$, where it reaches a maximum, and has a width of Δk.

Let us begin by trying to understand qualitatively the behavior of $\psi(x,0)$ through the study of a very simple special case. Let $\psi(x,0)$, instead of being the superposition of an infinite number of plane waves e^{ikx} as in formula (C-8), be the sum of only three plane waves. The wave vectors of these plane waves are k_0, $k_0 - \dfrac{\Delta k}{2}$, $k_0 + \dfrac{\Delta k}{2}$, and their

amplitudes are proportional, respectively, to 1, 1/2 and 1/2. We then have:

$$\psi(x) = \frac{g(k_0)}{\sqrt{2\pi}} \left[\mathrm{e}^{ik_0 x} + \frac{1}{2}\,\mathrm{e}^{i\left(k_0 - \frac{\Delta k}{2}\right)x} + \frac{1}{2}\,\mathrm{e}^{i\left(k_0 + \frac{\Delta k}{2}\right)x} \right]$$
$$= \frac{g(k_0)}{\sqrt{2\pi}}\ \mathrm{e}^{ik_0 x} \left[1 + \cos\left(\frac{\Delta k}{2} x \right) \right] \qquad \text{(C-10)}$$

We see that $|\psi(x)|$ is maximum when $x = 0$. This result is due to the fact that, when x takes on this value, the three waves are in phase and interfere constructively, as shown in Figure 4. As one moves away from the value $x = 0$, the waves become more and more out of phase, and $|\psi(x)|$ decreases. The interference becomes completely destructive when the phase shift between $\mathrm{e}^{ik_0 x}$ and $\mathrm{e}^{i(k_0 \mp \Delta k/2)x}$ is equal to $\pm\,\pi$: $\psi(x)$ goes to zero when $x = \pm\,\Delta x/2$, Δx being given by:

$$\Delta x\ \Delta k = 4\pi \qquad \text{(C-11)}$$

This formula shows that the smaller the width Δk of the function $|g(k)|$, the larger the width Δx of the function $|\psi(x)|$ (the distance between two zeros of $|\psi(x)|$).

Comment:

Formula (C-10) shows that $|\psi(x)|$ is periodic in x and therefore has a series of maxima and minima. This arises from the fact that $\psi(x)$ is the superposition of a finite number of waves (here, three). For a continuous superposition of an infinite number of waves, as in formula (C-8), such a phenomenon does not occur, and $|\psi(x, 0)|$ can have only one maximum.

Let us now return to the general wave packet of formula (C-8). Its form also results from an interference phenomenon: $|\psi(x, 0)|$ is maximum when the different plane waves interfere constructively.

Let $\alpha(k)$ be the argument of the function $g(k)$:

$$g(k) = \ |g(k)|\,\mathrm{e}^{i\alpha(k)} \qquad \text{(C-12)}$$

Assume that $\alpha(k)$ varies sufficiently smoothly within the interval $\left[k_0 - \dfrac{\Delta k}{2},\ k_0 + \dfrac{\Delta k}{2} \right]$ where $|g(k)|$ is appreciable; then, when Δk is sufficiently small, one can expand $\alpha(k)$ in the neighborhood of $k = k_0$:

$$\alpha(k) \simeq \alpha\,(k_0) + (k - k_0) \left[\frac{\mathrm{d}\alpha}{\mathrm{d}k} \right]_{k=k_0} \qquad \text{(C-13)}$$

which enables us to rewrite (C-8) in the form:

$$\psi(x, 0) \simeq \frac{\mathrm{e}^{i[k_0 x + \alpha(k_0)]}}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} |g(k)|\,\mathrm{e}^{i(k - k_0)(x - x_0)}\,\mathrm{d}k \qquad \text{(C-14)}$$

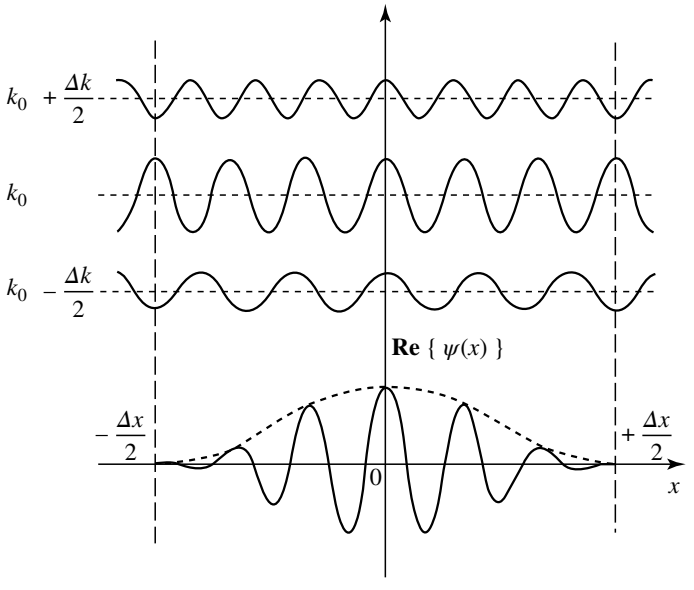

Figure 4: The real parts of the three waves whose sum gives the function $\psi(x)$ of (C-10). At $x = 0$, the three waves are in phase and interfere constructively. As one moves away from $x = 0$, they go out of phase and interfere destructively for $x = \pm\Delta x/2$.
In the lower part of the figure, $Re\{\psi(x)\}$ is shown. The dashed-line curve corresponds to the function $\left[1 + \cos\left(\frac{\Delta k}{2}x\right)\right]$, which, according to (C-10), gives $|\psi(x)|$ (and therefore, the form of the wave packet).

with:

$$x_0 = -\left[\frac{\mathrm{d}\alpha}{\mathrm{d}k}\right]_{k=k_0} \tag{C-15}$$

The form (C-14) is useful for studying the variations of $|\psi(x,0)|$ in terms of x. When $|x - x_0|$ is large, the function of k which is to be integrated oscillates a very large number of times within the interval Δk. We then see (*cf.* Fig. 5-a, in which the real part of this function is depicted) that the contributions of the successive oscillations cancel each other out, and the integral over k becomes negligible. In other words, when x is fixed at a value far from x_0, the phases of the various waves which make up $\psi(x,0)$ vary very rapidly in the domain Δk, and these waves destroy each other by interference. On the other hand, if $x \simeq x_0$, the function to be integrated over k oscillates hardly at all (*cf.* Fig. 5-b), and $|\psi(x,0)|$ is maximum.

The position $x_M(0)$ of the center of the wave packet is therefore:

$$x_M(0) = x_0 = -\left[\frac{\mathrm{d}\alpha}{\mathrm{d}k}\right]_{k=k_0} \tag{C-16}$$

Actually the result (C-16) can be obtained very easily. An integral such as the one appearing in (C-8) will be maximum (in absolute value) when the waves having the

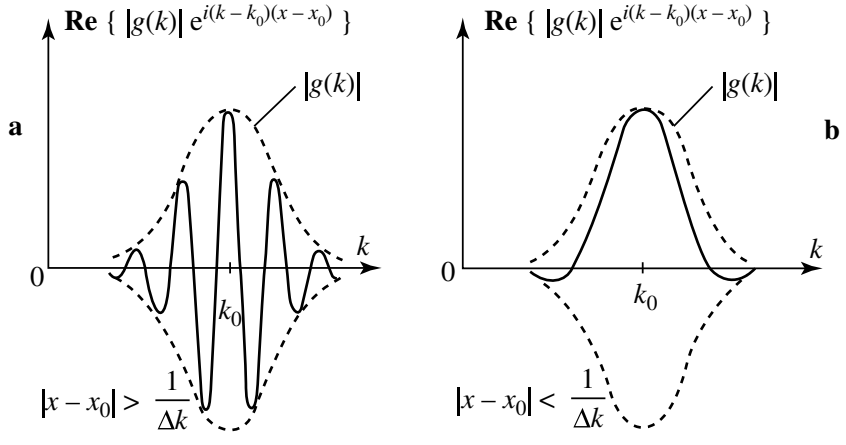

Figure 5: Variations with respect to k of the function to be integrated over k in order to obtain $\psi(x,0)$. In figure (a), x is fixed at a value such that $|x-x_0| > 1/\Delta k$, and the function to be integrated oscillates several times within the interval Δk. In figure (b), x is fixed such that $|x-x_0| < 1/\Delta k$, and the function to be integrated hardly oscillates, so that its integral over k takes on a relatively large value. Consequently, the center of the wave packet [point where $|\psi(x,0)|$ is maximum] is situated at $x = x_0$.

largest amplitude (those with k close to k_0) interfere constructively. This occurs when the k-dependent phases of these waves vary only slightly around $k = k_0$. To obtain the center of the wave packet, one then imposes (*stationary phase* condition) that the derivative with respect to k of the phase is zero for $k = k_0$. In the particular case which we are studying, the phase of the wave corresponding to k is $kx+\alpha(k)$. Therefore, $x_M(0)$ is that value of x for which the derivative $x + \mathrm{d}\alpha/\mathrm{d}k$ is zero at $k = k_0$.

When x moves away from the value x_0, $|\psi(x,0)|$ decreases. This decrease becomes appreciable if $\mathrm{e}^{i(k-k_0)(x-x_0)}$ oscillates approximately once when k traverses the domain Δk, that is, when:

$$\Delta k \;.\; (x - x_0) \simeq 1 \tag{C-17}$$

If Δx is the approximate width of the wave packet, we therefore have:

$$\Delta k \;.\; \Delta x \gtrsim 1 \tag{C-18}$$

We are thus brought back to a classical relation between the widths of two functions which are Fourier transforms of each other. The important fact is that the product $\Delta x \;.\; \Delta k$ has a lower bound; the exact value of this bound clearly depends on the precise definition of the widths Δx and Δk.

A wave packet such as (C-7) thus represents the state of a particle whose probability of presence, at the time $t = 0$, is practically zero outside an interval of approximate width Δx centered at the value x_0.

Comment:

The preceding argument could lead one to believe that the product $\Delta x \,.\, \Delta k$ is always of the order of 1 [*cf.* (C-17)]. Let us stress the fact that this is a lower limit. Although it is impossible to construct wave packets for which the product $\Delta x \,.\, \Delta k$ is negligible compared to 1, it is perfectly possible to construct packets for which this product is as large as desired [see, for example, Complement G_I, especially comment (*ii*) of § 3-c]. This is why (C-18) is written in the form of an inequality.

C-3. Heisenberg relations

In quantum mechanics, inequality (C-18) has extremely important physical consequences. We intend to discuss these now (we shall stay, for simplicity, within the framework of a one-dimensional model).

We have seen that a plane wave $e^{i(k_0 x - \omega_0 t)}$ corresponds to a constant probability density for the particle's presence along the Ox axis, for all values of t. This result can be roughly expressed by saying that the corresponding value of Δx is infinite. On the other hand, only one angular frequency ω_0 and one wave vector k_0 are involved. According to the de Broglie relations, this means that the energy and momentum of the particle are well-defined: $E = \hbar\omega_0$ and $p = \hbar k_0$. Such a plane wave can, moreover, be considered to be a special case of (C-7), for which $g(k)$ is a "delta function" (*cf.* Appendix II):

$$g(k) = \delta(k - k_0) \tag{C-19}$$

The corresponding value of Δk is then zero.

This property can also be interpreted in the following manner, using the principle of spectral decomposition (*cf.* §§ A-3 and B-1). To say that a particle, described at $t = 0$ by the wave function $\psi(x, 0) = A\, e^{ikx}$, has a well-determined momentum, is to say that a measurement of the momentum at this time will definitely yield $p = \hbar k$. From this we deduce that e^{ikx} *characterizes the eigenstate corresponding to* $p = \hbar k$. Since there exists a plane wave for every real value of k, the eigenvalues which one can expect to find in a measurement of the momentum on an arbitrary state include all real values. In this case, there is no quantization of the possible results: as in classical mechanics, all values of the momentum are allowed.

Now consider formula (C-8). In this formula, $\psi(x, 0)$ appears as a linear superposition of the momentum eigenfunctions in which the coefficient of e^{ikx} is $g(k)$. We are thus led to interpret $|g(k)|^2$ (to within a constant factor) as the probability of finding $p = \hbar k$ if one measures, at $t = 0$, the momentum of a particle whose state is described by $\psi(x, t)$. In reality, the possible values of p, like those of x, form a continuous set, and $|g(k)|^2$ is proportional to a *probability density*: the probability $\overline{\mathrm{d}\mathscr{P}}(k)$ of obtaining a value between $\hbar k$ and $\hbar(k + \mathrm{d}k)$ is, to within a constant factor, $|g(k)|^2\, \mathrm{d}k$. More precisely, if we rewrite formula (C-8) in the form:

$$\psi(x, 0) = \frac{1}{\sqrt{2\pi\hbar}} \int \overline{\psi}(p)\, e^{ipx/\hbar}\, \mathrm{d}p \tag{C-20}$$

we know that $\overline{\psi}(p)$ and $\psi(x, 0)$ satisfy the Parseval-Plancherel relation (*cf.* Appendix I):

$$\int_{-\infty}^{+\infty} |\psi(x,0)|^2 \, \mathrm{d}x = \int_{-\infty}^{+\infty} |\overline{\psi}(p)|^2 \, \mathrm{d}p \tag{C-21}$$

If the common value of these integrals is C, $\mathrm{d}\mathscr{P}(x) = \dfrac{1}{C} |\psi(x,0)|^2 \, \mathrm{d}x$ is the probability of the particle being found, at $t = 0$, between x and $x + \mathrm{d}x$. In the same way:

$$\overline{\mathrm{d}\mathscr{P}}(p) = \frac{1}{C} |\overline{\psi}(p)|^2 \, \mathrm{d}p \tag{C-22}$$

is the probability that the measurement of the momentum will yield a result included between p and $p + \mathrm{d}p$ [relation (C-21) then insures that the total probability of finding any value is indeed equal to 1].

Now let us go back to the inequality (C-18). We can write it as:

$$\Delta x \, . \, \Delta p \gtrsim \hbar \tag{C-23}$$

($\Delta p = \hbar \Delta k$ is the width of the curve representing $|\overline{\psi}(p)|$). Consider a particle whose state is defined by the wave packet (C-20). We know that its position probability at $t = 0$, is appreciable only within a region of width Δx about x_0: its position is known within an uncertainty Δx. If one measures the momentum of this particle at the same time, one will find a value between $p_0 + \dfrac{\Delta p}{2}$ and $p_0 - \dfrac{\Delta p}{2}$, since $|\overline{\psi}(p)|^2$ is practically zero outside this interval: the uncertainty in the momentum is therefore Δp. The interpretation of relation (C-23) is then as follows: it is impossible to define at a given time both the position of the particle and its momentum to an arbitrary degree of accuracy. When the lower limit imposed by (C-23) is reached, increasing the accuracy in the position (decreasing Δx) implies that the accuracy in the momentum diminishes (Δp increases), and vice versa. This relation is called the *Heisenberg relation* (or sometimes *uncertainty relation*, for historical reasons).

We know of nothing like this in classical mechanics. The limitation expressed by (C-23) arises from the fact that h is not zero. It is the very small value of h on the macroscopic scale which renders this limitation totally negligible in classical mechanics (an example is discussed in detail in Complement $\mathrm{B_I}$).

Comment:

The inequality (C-18) with which we started is not an inherently quantum mechanical principle. It merely expresses a general property of Fourier transforms, numerous applications of which can be found in classical physics. For example, it is well known from electromagnetic theory that there exists no packet of electromagnetic waves for which one can define the position and the wavelength with infinite accuracy at the same time. Quantum mechanics enters when one associates a wave with a material particle and requires that the wavelength and the momentum satisfy de Broglie's relation.

C-4. Time evolution of a free wave packet

Until now, we have been concerned only with the form of a wave packet at a given instant; in this paragraph, we are going to study its time evolution. Let us return,

therefore, to the case of a free particle whose state is described by the one-dimensional wave packet (C-7).

A given plane wave $e^{i(kx-\omega t)}$ propagates along the Ox axis with the velocity:

$$V_\varphi(k) = \frac{\omega}{k} \tag{C-24}$$

since it depends on x and t only through $\left(x - \frac{\omega}{k}\,t\right)$; $V_\varphi(k)$ is called the *phase velocity* of the plane wave.

We know that in the case of an electromagnetic wave propagating in a vacuum, V_φ is independent of k and equal to the speed of light c. All the waves making up a wave packet move at the same velocity, so that the packet as a whole also moves with the same velocity, without changing its shape. On the other hand, we know that this is not true in a dispersive medium, where the phase velocity is given by:

$$V_\varphi(k) = \frac{c}{n(k)} \tag{C-25}$$

$n(k)$ being the index of the medium, which varies with the wavelength.

The case that we are considering here corresponds to a dispersive medium, since the phase velocity is equal to [*cf.* equation (C-3)]:

$$V_\varphi(k) = \frac{\hbar k}{2m} \tag{C-26}$$

We shall see that when the different waves have unequal phase velocities, the velocity of the maximum x_M of the wave packet is not the average phase velocity $\frac{\omega_0}{k_0} = \frac{\hbar k_0}{2m}$, contrary to what one might expect.

As we did before, we shall begin by trying to understand qualitatively what happens, before taking a more general point of view. Therefore, let us return to the superposition of three waves considered in § C-2. For arbitrary t, $\psi(x,t)$ is given by:

$$\begin{aligned}\psi(x,t) &= \frac{g(k_0)}{\sqrt{2\pi}}\left\{e^{i[k_0x-\omega_0t]} + \frac{1}{2}\,e^{i\left[\left(k_0-\frac{\Delta k}{2}\right)x-\left(\omega_0-\frac{\Delta\omega}{2}\right)t\right]}\right.\\ &\qquad\left. + \frac{1}{2}\,e^{i\left[\left(k_0+\frac{\Delta k}{2}\right)x-\left(\omega_0+\frac{\Delta\omega}{2}\right)t\right]}\right\}\\ &= \frac{g(k_0)}{\sqrt{2\pi}}\,e^{i[k_0x-\omega_0t]}\left[1+\cos\left(\frac{\Delta k}{2}\,x - \frac{\Delta\omega}{2}\,t\right)\right]\end{aligned} \tag{C-27}$$

We see that the maximum of $|\psi(x,t)|$, which was at $x=0$ at $t=0$, is now at point:

$$x_M(t) = \frac{\Delta\omega}{\Delta k}\,t \tag{C-28}$$

and not at point $x = \frac{\omega_0}{k_0}\,t$. The physical origin of this result appears in Figure 6.

Part *a*) of this figure represents the position at time $t=0$ of three adjacent maxima (1), (2), (3), for the real parts of each of the three waves. Since the maxima denoted by the index (2) coincide at $x=0$, there is constructive interference at this point,

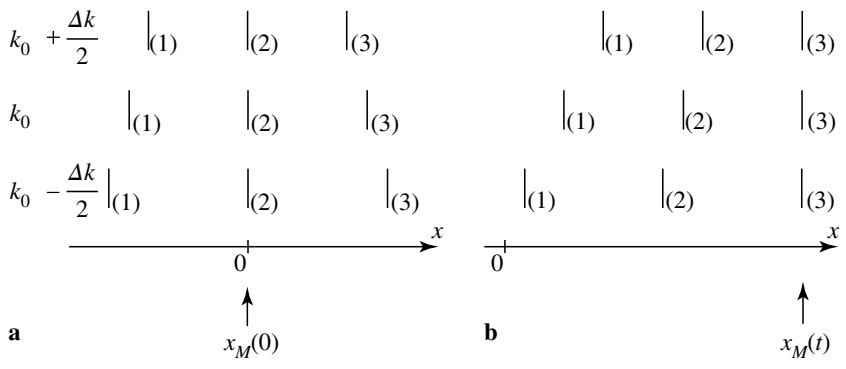

Figure 6: Positions of the maxima of the three waves of Figure 4 at time $t = 0$ (fig. a) and at a subsequent time t (fig. b). At time $t = 0$, it is the maxima (2), situated at $x = 0$, which interfere constructively: the position of the center of the wave packet is $x_M(0) = 0$. At time t, the three waves have advanced with different phase velocities V_φ. It is then the maxima (3) which interfere constructively and the center of the wave packet is situated at $x = x_M(t)$. We thus see that the velocity of the center of the wave packet (group velocity) is different from the phase velocities of the three waves.

which thus corresponds to the position of the maximum of $|\psi(x,0)|$. Since the phase velocity increases with k [formula (C-26)], the maximum (3) of the wave $\left(k_0 + \frac{\Delta k}{2}\right)$ will gradually catch up with that of the wave (k_0), which will in turn catch up with that of the wave $\left(k_0 - \frac{\Delta k}{2}\right)$. After a certain time, we shall thus have the situation shown in Figure 6-*b*: it will be the maxima (3) which coincide and thus determine the position of the maximum $x_M(t)$ of $|\psi(x,t)|$. We clearly see in the figure that $x_M(t)$ is not equal to $\frac{\omega_0}{k_0}\,t$, and a simple calculation again yields (C-28).

The shift of the center of the wave packet (C-7) can be found in an analogous fashion, by applying the "stationary phase" method. It can be seen from the form (C-7) of the free wave packet that, in order to go from $\psi(x,0)$ to $\psi(x,t)$, all we need to do is change $g(k)$ to $g(k)\,\mathrm{e}^{-i\omega(k)t}$. The reasoning of § C-2 thus remains valid, on the condition that we replace the argument $\alpha(k)$ of $g(k)$ by:

$$\alpha(k) - \omega(k)t \tag{C-29}$$

The condition (C-16) then gives:

$$x_M(t) = \left[\frac{\mathrm{d}\omega}{\mathrm{d}k}\right]_{k=k_0} t \;-\; \left[\frac{\mathrm{d}\alpha}{\mathrm{d}k}\right]_{k=k_0} \tag{C-30}$$

We are thus brought back to result (C-28): the velocity of the maximum of the wave packet is:

$$V_G(k_0) = \left[\frac{\mathrm{d}\omega}{\mathrm{d}k}\right]_{k=k_0} \tag{C-31}$$

$V_G(k_0)$ is called the *group velocity*indexGroup velocity of the wave packet. With the dispersion relation given in (C-3), we obtain:

$$V_G(k_0) = \frac{\hbar k_0}{m} = 2V_\varphi(k_0) \tag{C-32}$$

This result is important, for it enables us to retrieve the classical description of the free particle, for the cases where this description is valid. For example, when one is dealing with a macroscopic particle (and the example of the dust particle discussed in Complement B_I shows how small it can be), the uncertainty relation does not introduce an observable limit on the accuracy with which its position and momentum are known. This means that we can construct, in order to describe such a particle in a quantum mechanical way, a wave packet whose characteristic widths Δx and Δp are negligible. We would then speak, in classical terms, of the position $x_M(t)$ and the momentum p_0 of the particle. But then its velocity must be $v = \frac{p_0}{m}$. This is indeed what is implied by formula (C-32), obtained in the quantum description: in the cases where Δx and Δp can both be made negligible, the maximum of the wave packet moves like a particle that obeys the laws of classical mechanics.

Comment:

We have stressed here the motion of the center of the free wave packet. It is also possible to study the way in which its form evolves in time. It is then easy to show that, if the width Δp is a constant of the motion, Δx varies over time and, for sufficiently long times, increases without limit (spreading of the wave packet). The discussion of this phenomenon is given in Complement G_I, where the special case of a Gaussian wave packet is treated.

D. Particle in a time-independent scalar potential

We have seen, in § C, how the quantum mechanical description of a particle reduces to the classical description when Planck's constant h can be considered to be negligible. In the classical approximation, the wavelike character does not appear because the wavelength $\lambda = \frac{h}{p}$ associated with the particle is much smaller than the characteristic lengths of its motion. This situation is analogous to the one encountered in optics. Geometrical optics, which ignores the wavelike properties of light, constitutes a good approximation when the corresponding wavelength can be neglected compared to the lengths with which one is concerned. Classical mechanics thus plays, with respect to quantum mechanics, the same role played by geometrical optics with respect to wave optics.

In this paragraph, we are going to be concerned with a particle in a time-independent potential. What we have just said implies that typically quantum effects (that is, those of wave origin) should arise when the potential varies appreciably over distances shorter than the wavelength, which cannot then be neglected. This is why we are going to study the behavior of a quantum particle placed in various "square potentials", that is, "step potentials", as shown in Figure 7-a. Such a potential, which is discontinuous, clearly varies considerably over intervals of the order of the wavelength, however small it is: quantum effects must therefore always appear. Before beginning this investigation, we

shall discuss some important properties of the Schrödinger equation when the potential is not time-dependent.

D-1. Separation of variables. Stationary states

The wave function of a particle whose polential energy $V(\mathbf{r})$ is not time-dependent must satisfy the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\,\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\,\Delta\psi(\mathbf{r},t) + V(\mathbf{r})\,\psi(\mathbf{r},t) \tag{D-1}$$

D-1-a. Existence of stationary states

Let us see if there exist solutions of this equation of the form:

$$\psi(\mathbf{r},t) = \varphi(\mathbf{r})\,\chi(t) \tag{D-2}$$

Substituting (D-2) into (D-1), we obtain:

$$i\hbar\,\varphi(\mathbf{r})\frac{\mathrm{d}\chi(t)}{\mathrm{d}t} = \chi(t)\left[-\frac{\hbar^2}{2m}\,\Delta\varphi(\mathbf{r})\right] + \chi(t)\,V(\mathbf{r})\,\varphi(\mathbf{r}) \tag{D-3}$$

If we divide both sides by the product $\varphi(\mathbf{r})\,\chi(t)$, we find:

$$\frac{i\hbar}{\chi(t)}\,\frac{\mathrm{d}\chi(t)}{\mathrm{d}t} = \frac{1}{\varphi(\mathbf{r})}\left[-\frac{\hbar^2}{2m}\,\Delta\varphi(\mathbf{r})\right] + V(\mathbf{r}) \tag{D-4}$$

This equation equates a function of t only (left-hand side) and a function of $\mathbf{r}$ only (right-hand side). This equality is only possible if each of these functions is in fact a constant, which we shall set equal to $\hbar\omega$, where ω has the dimensions of an angular frequency.

Setting the left-hand side equal to $\hbar\omega$, we obtain for $\chi(t)$ a differential equation which can easily be integrated to give:

$$\chi(t) = A\,\mathrm{e}^{-i\omega t} \tag{D-5}$$

In the same way, $\varphi(\mathbf{r})$ must satisfy the equation:

$$-\frac{\hbar^2}{2m}\,\Delta\varphi(\mathbf{r}) + V(\mathbf{r})\,\varphi(\mathbf{r}) = \hbar\omega\,\varphi(\mathbf{r}) \tag{D-6}$$

If we set $A = 1$ in equation (D-5) [which is possible if we incorporate, for example, the constant A in $\varphi(\mathbf{r})$], we achieve the following result: the function

$$\psi(\mathbf{r},t) = \varphi(\mathbf{r})\,\mathrm{e}^{-i\omega t} \tag{D-7}$$

is a solution of the Schrödinger equation, on the condition that $\varphi(\mathbf{r})$ is a solution of (D-6). The time and space variables are said to have been separated.

A wave function of the form (D-7) is called a *stationary solution of the Schrödinger equation*: it leads to a time-independent probability density $|\psi(\mathbf{r},t)|^2 = |\varphi(\mathbf{r})|^2$. In a stationary function, only one angular frequency ω appears; according to the Planck-Einstein relations, *a stationary state is a state with a well-defined energy* $E = \hbar\omega$ (energy eigenstate). In classical mechanics, when the potential energy is time-independent, the total

energy is a constant of the motion; in quantum mechanics, there exist well-determined energy states.

Equation (D-6) can therefore be written:

$$\left[-\frac{\hbar^2}{2m}\,\Delta + V(\mathbf{r})\right]\varphi(\mathbf{r}) = E\,\varphi(\mathbf{r}) \tag{D-8}$$

or:

$$\boxed{H\,\varphi(\mathbf{r}) = E\,\varphi(\mathbf{r})} \tag{D-9}$$

where H is the differential operator:

$$\boxed{H = -\frac{\hbar^2}{2m}\,\Delta + V(\mathbf{r})} \tag{D-10}$$

H is a linear operator since, if λ_1 and λ_2 are constants, we have:

$$H\left[\lambda_1\varphi_1(\mathbf{r}) + \lambda_2\,\varphi_2(\mathbf{r})\right] = \lambda_1 H\varphi_1(\mathbf{r}) + \lambda_2 H\varphi_2(\mathbf{r}) \tag{D-11}$$

Equation (D-9) is thus the *eigenvalue equation* of the linear operator H: the application of H to the "eigenfunction" $\varphi(\mathbf{r})$ yields the same function, multiplied by the corresponding "eigenvalue" E. *The allowed energies are therefore the eigenvalues of the operator H*. We shall see later that equation (D-9) has square-integrable solutions $\varphi(\mathbf{r})$ only for certain values of E (*cf.* § D-2-c and § 2-c of Complement $\mathrm{H_I}$): this is the origin of *energy quantization*.

Comment:

Equation (D-8) [or (D-9)] is sometimes called the "time-independent Schrödinger equation", as opposed to the "time-dependent Schrödinger equation" (D-1). We stress their essential difference: equation (D-1) is a general equation which gives the evolution of the wave function, whatever the state of the particle; on the other hand, the eigenvalue equation (D-9) enables us to find, amongst all the possible states of the particle, those which are stationary.

D-1-b. Superposition of stationary states

In order to distinguish between the various possible values of the energy E (and the corresponding eigenfunctions $\varphi(\mathbf{r})$), we label them with an index n. Thus we have:

$$H\,\varphi_n(\mathbf{r}) = E_n\,\varphi_n(\mathbf{r}) \tag{D-12}$$

and the stationary states of the particle have as wave functions:

$$\psi_n(\mathbf{r}, t) = \varphi_n(\mathbf{r})\,\mathrm{e}^{-iE_n t/\hbar} \tag{D-13}$$

$\psi_n(\mathbf{r}, t)$ is a solution of the Schrödinger equation (D-1). Since this equation is linear, it has a whole series of other solutions of the form:

$$\psi(\mathbf{r}, t) = \sum_n c_n \varphi_n(\mathbf{r})\,\mathrm{e}^{-iE_n t/\hbar} \tag{D-14}$$

where the coefficients c_n are arbitrary complex constants. In particular, we have:

$$\psi(\mathbf{r},0) = \sum_n c_n \varphi_n(\mathbf{r}) \tag{D-15}$$

Inversely, assume that we know $\psi(\mathbf{r},0)$, the state of the particle at $t=0$. We shall see later that any function $\psi(\mathbf{r},0)$ can always be decomposed in terms of eigenfunctions of H, as in (D-15). The coefficients c_n are therefore determined by $\psi(\mathbf{r},0)$. The corresponding solution $\psi(\mathbf{r},t)$ of the Schrödinger equation is then given by (D-14). It is simply obtained by multiplying each term of (D-15) by the factor $\mathrm{e}^{-iE_nt/\hbar}$, where E_n is the eigenvalue associated with $\varphi_n(\mathbf{r})$. We stress the fact that these phase factors differ from one term to another. It is only in the case of stationary states that the t-dependence involves only one exponential [formula (D-13)].

D-2. One-dimensional "square" potentials. Qualitative study

We said at the beginning of § D that in order to display quantum effects we were going to consider potentials that varied considerably over small distances. We shall limit ourselves here to a qualitative study, so as to concentrate on the simple physical ideas. A more detailed study is presented in the complements of this chapter (Complement $\mathrm{H_I}$). To simplify the problem, we shall consider a one-dimensional model, in which the potential energy depends only on x (the justification for such a model is given in Complement $\mathrm{F_I}$).

D-2-a. Physical meaning of a square potential

We consider a one-dimensional problem with a potential of the type shown in Figure 7-a. The Ox axis is divided into a certain number of constant-potential regions. At the border of two adjacent regions the potential makes an abrupt jump (discontinuity). Actually, such a function cannot really represent a physical potential, which must be continuous. We use it to represent schematically a potential energy $V(x)$ which actually has the shape shown in Figure 7-b: there are no discontinuities, but $V(x)$ varies very rapidly in the neighborhood of certain values of x. When the intervals over which these variations occur are much smaller than all other distances involved in the problem (in particular, the wavelength associated with the particle), we can replace the true potential by the square potential of Figure 7-a. This is an approximation, which would cease to be valid, for example, for a particle having too high an energy, whose wavelength would be very short.

The predictions of classical mechanics concerning the behavior of a particle in a potential such as that of Figure 7 are easy to determine. For example, imagine that $V(x)$ is the gravitational potential energy. Figure 7-b then represents the real profile of the terrain on which the particle moves: the corresponding discontinuities are sharp slopes, separated by horizontal plateaus. Notice that, if we fix the total energy E of the particle, the domains of the Ox axis where $V > E$ are forbidden to it (its kinetic energy $E_c = E - V$ must be positive).

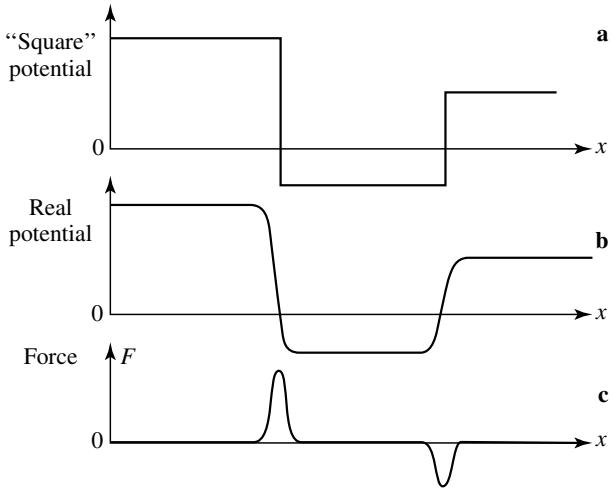

Figure 7: Square potential (fig. a) which schematically represents a real potential (fig. b) for which the force has the shape shown in figure c.

Comment:

The force exerted on the particle is $F(x) = -\dfrac{\mathrm{d}V(x)}{\mathrm{d}x}$. In Figure 7-c, we have depicted this force, obtained from the potential $V(x)$ of Figure 7-b. It can be seen that this particle, in all the regions where the potential is constant, is not subjected to any force. Its velocity is then constant. It is only in the frontier zones between these plateaus that a force acts on the particle and, depending on the case, accelerates it or slows it down.

D-2-b. Optical analogy

We are going to consider the stationary states (§ D-1) of a particle in a one-dimensional "square" potential.

In a region where the potential has a constant value V, the eigenvalue equation (D-9) is written:

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V\right]\varphi(x) = E\varphi(x) \tag{D-16}$$

or:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - V)\right]\varphi(x) = 0 \tag{D-17}$$

Now, in optics, there exists a completely analogous equation. Consider a transparent medium whose index n depends neither on $\mathbf{r}$ nor on time. In this medium, there can be electromagnetic waves whose electric field $\mathbf{E}(\mathbf{r}, t)$ is independent of y and z and has the form:

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{e}\, E(x)\, \mathrm{e}^{-i\Omega t} \tag{D-18}$$

where **e** is a unit vector perpendicular to Ox; $E(x)$ must then satisfy:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{n^2\Omega^2}{c^2}\right] E(x) = 0 \tag{D-19}$$

We see that equations (D-17) and (D-19) become identical if we set:

$$\frac{2m}{\hbar^2}(E - V) = \frac{n^2\Omega^2}{c^2} \tag{D-20}$$

Moreover, at a point x where the potential energy V [and, consequently, the index n given by (D-20)] is discontinuous, the boundary conditions for $\varphi(x)$ and $E(x)$ are the same: these two functions, as well as their first derivatives, must remain continuous (*cf.* Complement $\mathrm{H_I}$, § 1-b). The structural analogy between the two equations (D-17) and (D-19) thus enables us to associate with a quantum mechanical problem, corresponding to the potential of Figure 7-a, an optical problem: the propagation of an electromagnetic wave of angular frequency Ω in a medium whose index n has discontinuities of the same type. According to (D-20), the relation between the optical and mechanical parameters is:

$$n(\Omega) = \frac{1}{\hbar\Omega}\sqrt{2mc^2(E - V)} \tag{D-21}$$

For the light wave, a region where $E > V$ corresponds to a transparent medium whose index is real. The wave is then of the form e^{ikx}.

What happens when $V > E$? Formula (D-20) gives a pure imaginary index. In relation (D-19), n^2 is negative and the solution is of the form $\mathrm{e}^{-\rho x}$: it is the analogue of an "evanescent wave". Certain aspects of the situation recall the propagation of an electromagnetic wave in a metallic medium[7].

Thus we can transpose the well-known results of wave optics to the problems which we are studying here. It is important, however, to realize that this is merely an analogy. The interpretation that we give for the wave function is fundamentally different from that which classical wave optics attributes to the electromagnetic wave.

D-2-c. Examples

α. Potential step and barrier

Consider a particle of energy E which, coming from the region of negative x, arrives at the potential "step" of height V_0 shown in Figure 8.

If $E > V_0$ (the case in which the classical particle clears the potential step and continues towards the right with a smaller velocity), the optical analogy is the following: a light wave propagates from left to right in a medium of index n_1:

$$n_1 = \frac{c}{\hbar\Omega}\sqrt{2mE} \tag{D-22}$$

at $x = x_1$, there is a discontinuity, and the index, for $x > x_1$, is:

$$n_2 = \frac{c}{\hbar\Omega}\sqrt{2m(E - V_0)} \tag{D-23}$$

[7] This analogy should not be pushed too far, since the index n of a metallic medium has both a real and a complex part (in a metal, an optical wave continues to oscillate as it damps out).

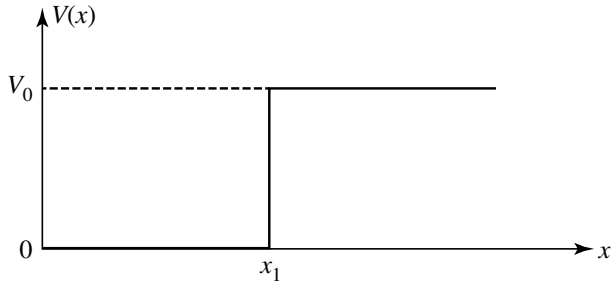

Figure 8: Potential step.

We know that the incident wave coming from the left splits into a reflected wave and a transmitted wave. Let us transpose this result to quantum mechanics: *the particle has a certain probability $\mathscr{P}$ of being reflected*, and only the probability $1 - \mathscr{P}$ of pursuing its course towards the right. This result is contrary to what is predicted by classical mechanics.

When $E < V_0$, the index n_2, which corresponds to the region $x > x_1$, becomes pure imaginary, and the incident light wave is totally reflected. The quantum prediction therefore coincides at this point with that of classical mechanics. Nevertheless, the existence, for $x > x_1$, of an evanescent wave, shows that the quantum particle has a non-zero probability of being found in this region.

The role of this evanescent wave is more striking in the case of a potential barrier (Fig. 9). For $E < V_0$, a classical particle would always turn back. But, in the corresponding optical problem, we would have a layer of finite thickness, with an imaginary index, surrounded by a transparent medium. If this thickness is not much greater than the range $1/\rho$ of the evanescent wave, part of the incident wave is transmitted into the region $x > x_2$. Therefore, even for $E < V_0$, we find a *nonzero probability of the particle crossing the barrier*. This is called the "tunnel effect".

β. *Potential well*

The function $V(x)$ now has the form shown in Figure 10. The predictions of classical mechanics are the following: when the particle has a negative energy E (but greater than $-V_0$), it can only oscillate between x_1 and x_2, with kinetic energy $E_c = E + V_0$; when the particle has a positive energy and arrives from the left, it undergoes an

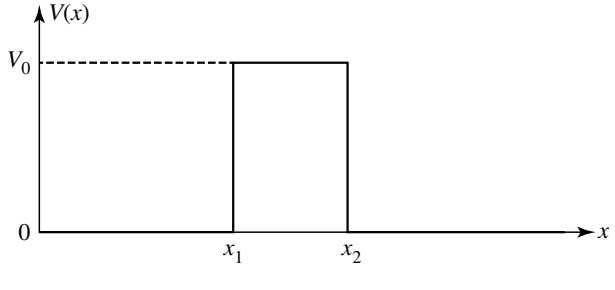

Figure 9: Potential barrier.

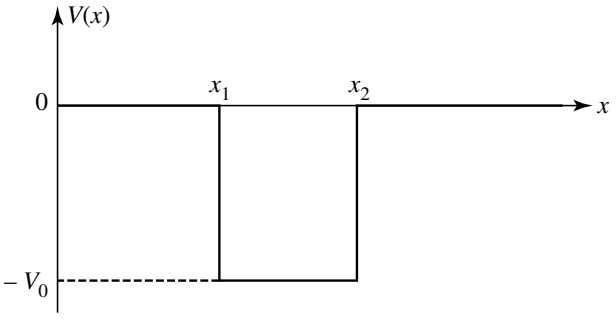

Figure 10: Potential well.

abrupt acceleration at x_1, then an equal deceleration at x_2, and then continues towards the right.

In the optical analogue of the case $-V_0 < E < 0$, the indices n_1 and n_3, which correspond to the regions $x < x_1$ and $x > x_2$, are imaginary, while the index n_2, which characterizes the interval $[x_1, x_2]$, is real. Thus we have the equivalent of a layer of air, for example, between two reflecting media. The different waves reflected successively at x_1 and x_2 destroy each other through interference, except for certain well-determined frequencies ("normal modes") that allow stable stationary waves to be established. From the quantum point of view, this implies that *the negative energies are quantized*[8], while, classically, all values included between $-V_0$ and 0 are possible.

For $E > 0$, the indices n_1, n_2 and n_3 are real:

$$n_1 = n_3 = \frac{c}{\Omega}\frac{1}{\hbar}\sqrt{2mE} \tag{D-24}$$

$$n_2 = \frac{c}{\Omega}\frac{1}{\hbar}\sqrt{2m(E+V_0)} \tag{D-25}$$

Since n_2 is greater than n_1 and n_3, the situation is analogous to that of a layer of glass in air. In order to obtain the reflected wave for $x < x_1$, or the transmitted wave in the region $x > x_2$, it is necessary to superpose an infinite number of waves that arise from successive reflections at x_1 and x_2 (multiple wave interferometer analogous to a Fabry-Perot). We then find that, for certain incident frequencies, the wave is entirely transmitted. From the quantum point of view, the particle thus has, in general, a certain probability of being reflected. However, there exist energy values, called *resonance energies*, for which the probability of transmission is 1 and, consequently, the probability of reflection is 0.

These few examples show how much the predictions of quantum mechanics can differ from those of classical mechanics. They also clearly stress the primordial role of potential discontinuities (which represent, schematically, rapid variations).

CONCLUSION

In this chapter we have introduced and discussed, in a qualitative and intuitive manner, certain fundamental ideas of quantum mechanics. We shall later return to

[8]The allowed energy values are not given by the well-known condition: $x_2 - x_1 = k\lambda_2/2$, for it is necessary to take into account the existence of evanescent waves, which introduce a phase shift upon reflection at $x = x_1$ and $x = x_2$ (*cf.* Complement H_I, § 2-c).

these ideas (Chap. III) so as to present them in a more precise and systematic way. Nevertheless, it is already clear that the quantum description of physical systems differs radically from the one given by classical mechanics (although the latter constitutes, in numerous cases, an excellent approximation). We have limited ourselves in this chapter to the case of physical systems composed of only one particle. The description of these systems at a given time is, in classical mechanics, founded on the specification of six parameters, which are the components of the position $\mathbf{r}(t)$ and the velocity $\mathbf{v}(t)$ of the particle. All the dynamical variables (energy, linear momentum, angular momentum) are determined by the specification of $\mathbf{r}(t)$ and $\mathbf{v}(t)$. Newton's laws enable us to calculate $\mathbf{r}(t)$ through the solution of second-order differential equations with respect to time. Consequently, they fix the values of $\mathbf{r}(t)$ and $\mathbf{v}(t)$ for any time t when they are known for the initial time.

Quantum mechanics uses a more complicated description of phenomena. The dynamic state of a particle, at a given time, is characterized by a wave function. It no longer depends on only six parameters, but on an infinite number [the values of $\psi(\mathbf{r}, t)$ at all points $\mathbf{r}$ of space]. Moreover, the predictions of the measurement results are now only probabilistic (they yield only the probability of obtaining a given result in the measurement of a dynamical variable). The wave function is a solution of the Schrödinger equation, which enables us to calculate $\psi(\mathbf{r}, t)$ from $\psi(\mathbf{r}, 0)$. This equation implies a principle of superposition which leads to wave effects.

This upheaval in our conception of mechanics was imposed by experiment. The structure and behavior of matter on an atomic level are incomprehensible in the framework of classical mechanics. The theory has thereby lost some of its simplicity, but it has gained a great deal of unity, since matter and radiation are described in terms of the same general scheme (wave-particle duality). We stress the fact that this general scheme, although it runs counter to our ideas and habits drawn from the study of the macroscopic domain, is perfectly consistent. No one has ever succeeded in imagining an experiment that could violate the uncertainty principle (*cf.* Complement D_I of this chapter). In general, no observation has, to date, contradicted the fundamental principles of quantum mechanics. Nevertheless, at present, there is no global theory including quantum phenomena within general relativity (gravity) and, of course, nothing prevents the possibility of a new upheaval.

References and suggestions for further reading:

Description of physical phenomena which demonstrate the necessity of introducing quantum mechanical concepts: see the subsection "Introductory work – quantum physics" of section 1 of the bibliography; in particular, Wichmann (1.1) and Feynman III (1.2), Chaps. 1 and 2.

History of the development of quantum mechanical concepts: references of section 4 of the bibliography, in particular, Jammer (4.8); also see references (5.11) and (5.12), which contain numerous references to the original articles.

Fundamental experiments: references to the original articles can be found in section 3 of the bibliography.

The problem of interpretation in quantum mechanics: section 5 of the bibliography; in particular, the "Resource Letter" (5.11), which contains many references.

Analogies and differences between matter waves and electromagnetic waves: Bohm (5.1), Chap. 4; in particular, the table "Summary on Probabilities" at the end of the chapter.

See also the articles by Schrödinger (1.25), Gamow (1.26), Born and Biem (1.28), Scully and Sargent (1.30).