Chapter 2
A Quantum Phenomenon

If, at a party, you ask someone to state a physics formula, the odds are that the answer will be $E = mc^2$. Nevertheless, the formula $E = h\nu$, which was written in the same year 1905 by the same Albert Einstein concerns their daily life considerably more.

In fact, among the three great scientific events of the beginning of the 20th century, 1905 with the special relativity of Einstein, Lorentz, and Poincaré, 1915 with Einstein's general relativity, an extraordinary reflection on gravitation, space, and time, and 1925 with the elaboration of quantum mechanics, it is certainly the last that has had the most profound impact on science and technology.

The first Nobel prize for relativity was awarded in 1993 to Taylor and Hulse for the double pulsar. Nobel prizes for quantum mechanics can hardly be counted (of the order of 120) including Einstein's for the photon in 1921. That reflects discoveries which have had important consequences. About 30 % of the gross internal product of the United States comes from byproducts of quantum mechanics.

Quantum mechanics is inescapable. All physics is quantum physics, from elementary particles to the big bang, semiconductors, and solar energy cells.

It is undoubtedly one of the greatest intellectual achievements of the history of mankind, probably the greatest of those that will remain from the 20th century, before psychoanalysis, computer science, or genome decoding.

This theory exists. It is expressed in a simple set of axioms that we discuss in Chap. 6. Above all, this theory works. For a physicist, it even works too well, in some sense. One cannot determine its limits, except that during 10^{-43} s just after the big bang, we don't know what replaced it. But afterwards, that is, nowadays, it seems unbeatable.

However, this theory is subtle. One can only express it in mathematical language, which is quite frustrating for philosophers. Knowing mathematics is the entrance fee to the group of the happy few who can understand it, even though, as we show, the core of these mathematics is quite simple. It is the physics that is subtle. More important perhaps, we show how and why quantum mechanics is still a subject of debate as to its interpretation and its intellectual content. In some sense, mankind

J.-L. Basdevant, *Lectures on Quantum Mechanics,*
Graduate Texts in Physics, DOI 10.1007/978-3-319-43479-7_2

has made a beautiful and successful intellectual construction that escapes human understanding to some extent. As Richard Feynman put it: "I think I can safely say that nobody understands quantum mechanics".[1]

The discovery of quantum mechanics could have happened by analyzing a variety of physical facts at the end of the 19th century. The notion of quanta was proposed in 1900 by Max Planck. Planck had found semi-empirically a remarkable formula to explain a problem that fascinated people, the spectrum of black-body radiation. The frequency distribution of radiation inside an oven at temperature T depends only on the temperature, not on the nature or shape of the oven. It is a universal law. Planck obtained the good result

$$u(\nu) = \frac{8\pi h}{c^3} \frac{\nu^3}{e^{(h\nu/kT)} - 1}, \tag{2.1}$$

where ν is the frequency, T the temperature, and k Boltzmann's constant, by assuming that radiation of frequency ν can exchange energy with the inner surface of the oven only by discrete quantities that are integer multiples of an elementary energy quantum $h\nu$,

$$\varDelta E = nh\nu. \tag{2.2}$$

Planck understood that the constant h in the above formula, which now bears his name and whose value is

$$h \approx 6,62\, 10^{-34}\,\text{j.s},$$

is a fundamental constant of nature, as the velocity of light c in relativity and Newton's constant G in gravitation. For technical simplicity, we mainly use the reduced Planck constant

$$\hbar \equiv \frac{h}{2\pi} \approx 1,05\, 10^{-34}\text{j.s.}$$

Planck's formula works remarkably well. The direct verification would require us to be inside an oven. We have the great luck to live inside the cosmic background radiation of the big bang, which cooled down as the Universe expanded. The temperature of that radiation is at present 3 K. Its observation and its more and more precise measurement (Fig. 2.1) is perhaps the best observational evidence in favor of the big bang theory, as well as of Planck's formula.

Planck's quanta were somewhat mysterious, and it was Einstein who made a decisive step forward in 1905, the same year as he did for Brownian motion theory and for special relativity. By performing a critique of Planck's ideas, and for reasons due to equilibrium considerations (i.e., entropy) Einstein understood that the quantized aspect is not limited to the energy exchanges between radiation and matter, but that it must be present in the electromagnetic field itself. Light, which was known to be a wave propagation phenomenon since the beginning of the 19th century, must also

---

[1]The Character of Physical Law, MIT Press, Cambridge, MA 1965.

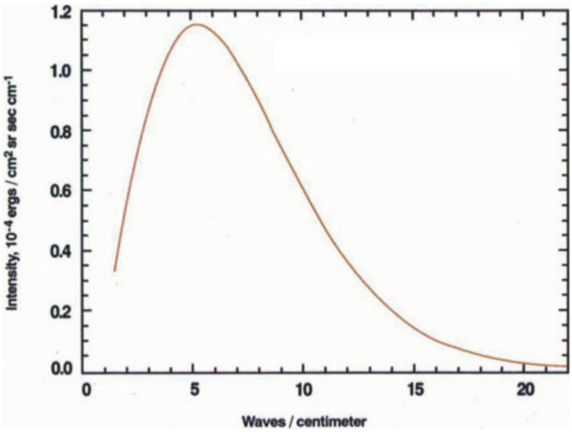

Fig. 2.1 Wave-number distribution of the cosmic background radiation measured in 1992 by the COBE satellite. The agreement between Planck's formula at a temperature $T = 2.728$ K lies within the line (Photo credit: Mather et al., *Astrophys. J.*, **420**, 439, (1994). http://lambda.gsfc.nasa.gov/product/cobe/firas_image.cfm.)

exhibit a particlelike behavior. Light of frequency ν is carried by particles, photons as the chemist Gilbert called them in 1926, of energy

$$E = h\nu, \tag{2.3}$$

and momentum $\boldsymbol{p} = \hbar \boldsymbol{k}$, where $\boldsymbol{k}$ is the wave vector $k = 2\pi/\lambda$, as was proven experimentally by Compton in 1921.

In that respect, Einstein understood an essential feature of quantum theory, the so-called "dual" manifestations of the properties of light, which appear to be both wavelike and particlelike. In the course of his work, Einstein found the explanation of the photoelectric effect, which was one of the first experimental confirmations of his ideas. Such ideas were considered revolutionary or even iconoclastic because they seemed to contradict Maxwell's equations which were a great triumph of the 19th century.

At the same time, atomic spectroscopy was one of the great enigmas of physics. The third breakthrough, which derives in some respect from Einstein's ideas, came in 1913 from Niels Bohr.

There are three parts in Bohr's ideas and results.

- He postulated that matter is also quantized and that there exist discrete energy levels for atoms, which was verified experimentally by Franck and Hertz in 1914.
- He postulated that spectral lines which had been abundantly observed during the 19th century, came from transitions between these energy levels. When atoms absorb or emit radiation, the positions of spectral lines are given by the difference

$$\nu_{nm} = \frac{|E_n - E_m|}{h}. \tag{2.4}$$

- Finally, Bohr constructed an empirical model of the hydrogen atom that works remarkably well and gives the energy levels E_n of this atom as

$$E_n = -\frac{m{q_e}^4}{2(4\pi\varepsilon_0)^2\hbar^2 n^2}, \tag{2.5}$$

where n is a positive integer. With that formula, where all physical constants are known from different experiments, the wavelengths $\lambda = c/\nu_{nm}$ of spectral lines coincide with experiment to one part in a thousand.

Bohr's formula (2.5) expresses the famous "Rydberg constant" of spectroscopists in terms of fundamental constants, which impressed people, in particular, Einstein.[2]

So we are facing three similar formulae, $E = h\nu$. The first (2.2) is an assumption about the interaction of radiation and matter, the second (2.3) has to do with radiation itself, and the third (2.4) is a property of atoms, namely matter.

Bohr's success was fantastic, but it was too easy. Actually one realized later on that it was a piece of luck due to the fact that the hydrogen atom is a simple two-body system. This easy result generated an obscure prequantum era, where people accumulated recipes for more complicated atoms, with fluctuating results deprived of any global coherence.

2.1 Wave Behavior of Particles

The synthetic and coherent formulation of quantum mechanics was performed around 1925. It is due to an incredible collective work of talented people such as Louis de Broglie, Schrödinger, Heisenberg, Max Born, Dirac, Pauli, and Hilbert, among others. Never before, in physics, had one seen such a collective effort to find ideas capable of explaining physical phenomena.

We are now going to discover some of the main features on a simple concrete experiment that shows the wavelike behavior of particles. This is symmetric in some respect to the particlelike behavior of light. We show that the behavior of matter at atomic scales does not follow what we expect from daily "common sense." It is impossible to explain it with our immediate conceptions.

In order to understand quantum mechanics, one must get rid of prejudices and ideas that seem obvious, and one must adopt a critical intellectual attitude in front of experimental facts.

2.1.1 Interferences

Let us recall interference phenomena in wave physics, optics, or acoustics, in the simple case of Young slit fringes.

[2]The $1/n^2$ behavior was known since 1886 and Balmer's empirical discovery.

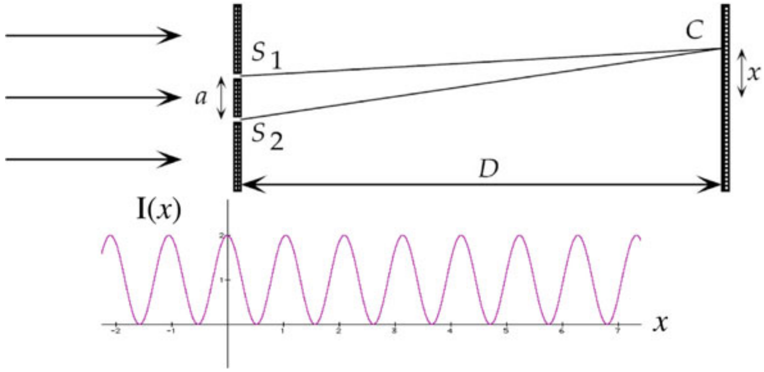

Fig. 2.2 Sketch of a Young two-slit interference experiment

One sends a light beam on a screen pierced with two slits, and one observes the variation of the intensity of light on another screen as a function of the distance x to the center (Fig. 2.2).

The two slits act as secondary sources in phase, and the amplitude of the wave at a point C of the screen is the algebraic sum of the amplitudes issued from each of them.

If the two waves are in phase, the amplitude is twice as large. If they are out of phase by π the amplitude vanishes; there is no luminous energy at that point. And there exist all intermediate cases.

In other words, the amplitude at some point is the sum of amplitudes reaching that point,

$$\text{Amplitude at C} \; : \; A_C = A_1 + A_2 \; , \quad \text{Intensity} \; : \; I(x) = |A_C|^2 . \tag{2.6}$$

The amplitudes emitted by the two slits add up, the intensity is the square of that sum and it presents a periodic variation, the distance of fringes being $x_0 = \lambda D/a$.

2.1.2 Wave Behavior of Matter

We turn to the wave behavior of matter. In 1923, Louis de Broglie made the bold but remarkable assumption that any particle of mass m and of velocity $\boldsymbol{v}$ possesses an "associated" wave of wavelength

$$\lambda = \frac{h}{p} ; \tag{2.7}$$

where $\boldsymbol{p} = m\boldsymbol{v}$ is the momentum of the particle and p its norm.

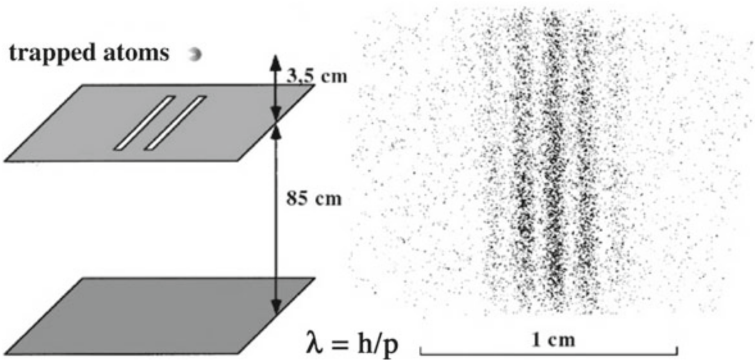

Fig. 2.3 Double slit Young interference experiment performed with neon atoms cooled down to a milliKelvin (*left part*). Each point of the figure (*right part*) corresponds to the impact of an atom on the detector. Interference fringes are clearly visible

Louis de Broglie had many reasons to propose this. In particular he had in mind that the discrete energy levels of Bohr might come from a stationary wave phenomenon. This aspect struck the minds of people, in particular that of Einstein, who was enthusiastic.

In order to verify such an assumption, it is natural to perform interference and diffraction experiments. The first experimental confirmation is due to Davisson and Germer in 1927. It is a diffraction experiment of an electron beam on a nickel crystal.

It is more difficult to perform a Young double-slit interference experiment with electrons. However, a group of Japanese physicists from Nippon Electronics (NEC) performed in 1994 a beautiful interference experiment of cold atoms in Young slits. Neon atoms are initially trapped in stationary laser waves (so-called optical molasses). They are then released and undergo free fall across a two-slit device. The slits are 2 μm large, they are 6 μm apart. The scale in Fig. 2.3 is distorted.

What do we observe in Fig. 2.3? The distribution of impacts of atoms on the detecting plate is similar to the optical intensity in the same device. The fringes are at the same positions provided Louis de Broglie's relation is satisfied $\lambda = h/p$. (Of course, one must take care of the uniform acceleration in this particular setup.)

The same phenomenon can be observed with other particles: neutrons, helium atoms, hydrogen molecules, the same relation holds between the wavelength and the momentum. The present record is to perform interferences with large molecules such as fullerenes, that is, C_{60} molecules.[3]

Therefore matter particles exhibit a wave behavior with a wavelength given by de Broglie's formula.

[3] O. Nairz, M. Arndt, A. Zeilinger, American Journal of Physics, Vol. 71, 319 (2003), and references therein.

2.1.3 Analysis of the Phenomenon

Now, a number of questions are in order.

What is this wave? And why is this result so extraordinary?

It is extraordinary because atoms are known to be particles. An atom has a size of the order of an angström (0.1 nm) and it is pointlike at the scales of interest (μm or mm). With a counter, one can measure whether an atom has arrived at some point with an accuracy as fine as one wishes. When an atom is detected, it has a well-defined position; it does not break up into pieces; it is point-like.

But a wave fills all space. A wave, on the surface of water, is the whole set of deformations on all points of that surface.

So, what is a particle? Is it a pointlike object or is it spread out in the entire space? A simple glance at Fig. 2.4 shows that we are facing a conceptual contradiction.

How can we escape this contradiction? Actually, the phenomenon is much richer than a simple wave phenomenon; we must observe experimental facts and use our critical minds.

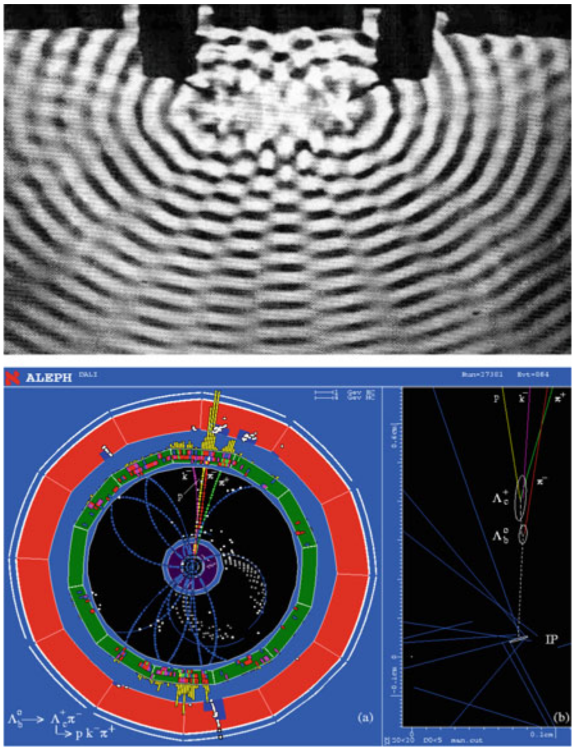

Fig. 2.4 *Top* two source interferences on the surface of water; the radial lines are nodes of interferences. *Bottom* tracks of particles in the Aleph detector of LEP at CERN

Since atoms are particles, we can send them individually, one at a time, and all in the same way.

This proposition is perfectly decidable; it is feasible experimentally. We can trigger the device so that it releases atoms one after the other and that they are all released in the same way.

2.2 Probabilistic Nature of Quantum Phenomena

2.2.1 Random Behavior of Particles

What do we observe? Actually, we can guess that from Fig. 2.3.

- Each atom has a well-defined impact; an atom does not break into pieces.
- But the positions of the impacts are distributed at random. In other words, to the same initial conditions, there correspond different impacts.

In other words, atoms, or particles in general, have a random behavior. Each atom arrives where it wants, but the whole lot is distributed with a probability law similar to the intensity observed in optics or acoustics:

$$P(z) \propto I_{(optical)}(\lambda = h/p).$$

Therefore, there is a second difference with classical physics: to identical initial conditions, there correspond different final conditions. The impact of a single particle is unpredictable, the whole set of impacts has a well defined probability distribution.

But, one can object that random, or probabilistic, phenomena exist in classical physics, such as playing dice, or heads and tails, and so on.

True, but the big problem is that this is by no means a classical probabilistic phenomenon, as in usual probability theory. Why is that?

2.2.2 A Nonclassical Probabilistic Phenomenon

If we block one of the slits, the atoms will pass through the other one and their distribution on the detector shows no sign of any interference. If we block the other slit, the distribution is approximately the same, up to a small global shift (1 μm/1 mm) Now let's make a logical reasoning and perform the critique of what we say.

1. We send the atoms one by one. These are independent phenomena; atoms don't bother each other; they do not act on each other's trajectory.
2. Each atom has certainly gone through one of the slits.
3. We can measure which slit each atom went through. There exist techniques for this; send light on the slits, put counters, and so on. It is feasible.

4. If we perform this measurement, we can separate the outgoing atoms in two samples, those that have passed through the first slit, and those that have passed through the second one. And we know where each atom arrived.
5. For those that passed through the first slit, everything is as if the second slit were blocked, and vice versa. Each sample shows no interference.

Now, we have two independent samples, and we can bring them together. Classically, the result we would obtain by opening the two slits should be the sum, the superposition of the two distributions such as (2.5). But not at all!

It's even worse! Opening a second slit (i.e., giving an extra possibility for the atoms to reach the detector) has prevented the atoms from arriving at certain points. That's really incredible to be able to stop some people from entering your house by opening another door!

We must admit that the usual logical ideas of probability theory do not apply. We cannot explain the phenomenon in classical terms. It is a non-classical probabilistic phenomenon.

2.3 Conclusions

At this point, it seems we are at a logical dead end. How can we find our way? Our argument, however logical it may seem, leads to wrong conclusions. There is something we haven't thought about. Because physics is consistent. The answer is experimental. What actually happens is the following.

1. If we measure by which slit each atom passed, we can indeed make the separation and indeed we observe the sum of two distributions such as in Fig. 2.5. Therefore we no longer observe interferences; they disappear.
   It is another experiment!

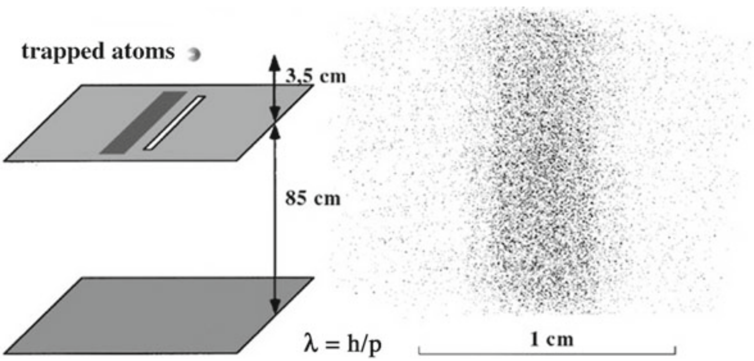

Fig. 2.5 Same experiment as in Fig. 2.3 but opening only one slit. The interference fringes disappear and one observes a diffraction pattern (this figure is not experimental)

2. Conversely, if we do observe interferences, it is not possible to know through which slit each atom passed. We can talk about it, but we can't do anything with it.
   Knowing by which slit an atom has passed in an interference experiment is a proposition that has no physical meaning; it is undecidable. It is perfectly correct to say that an atom passed through both holes at the same time, which seems paradoxical or absurd classically.

What was wrong was to assume implicitly that, at the same time, we could measure by which slit each atom passed and observe interferences. We assumed that without checking it.

We can draw the following conclusions.

• First, *a measurement perturbs the system*. If we do not measure by which slit they pass, the atoms are capable of interfering. After we perform this measurement, they are in another state where they are no longer capable of interfering. They have been perturbed by the measurement.

• Secondly and consequently, *there is no trajectory* in the classical sense. If we observe an atom in an interference experiment, we know when and where it was emitted and where and when it was detected, but we cannot say where it was in the meantime.

However, these two ideas seemed obvious in classical physics. The fact that we can make a measurement as accurate as we wish without affecting the system is an old belief of physics. Physicists used to say that they just needed to improve the measuring apparatus. Quantum physics tells us that there is a absolute lower bound to the perturbation that a measurement produces.

The notion of a trajectory, namely that there exists a set of points by which we can claim and verify that a particle has passed at each moment, is as old as mankind. Cavemen knew that intuitively when they went hunting. It took centuries to construct a theory of trajectories, to predict a trajectory in terms of initial conditions. Newton's classical mechanics, celestial mechanics, ballistics, rests entirely on that notion, but its starting point is beaten up by the simple quantum phenomenon we just examined.

Classically, we understand the motion of a particle by assuming that, at each moment one can measure the position of a projectile, that the collection of the results consists of a trajectory, and that we can draw a reproducible conclusion independent of the fact that we measure the positions at any moments. We learn these ideas as if they were obvious, but they are wrong. More precisely: in order to penetrate the quantum world, one must get rid of such ideas. Figure 2.6, or analogous ones, is completely wrong in quantum mechanics.

Of course, one mustn't go too far. These are very good approximations in the classical world. If a policeman stops you on a freeway saying you were driving at 80 miles an hour, the good attitude is to claim, "Not at all! I was driving peacefully at 35 mph on the little road under the bridge, and your radar perturbed me!" Unfortunately, he won't believe you even if he knows some physics. Because it is Planck's constant $\hbar$ that governs such effects. However, in quantum driving one must change the rules. Changing the rules consists of constructing the theory of all that.

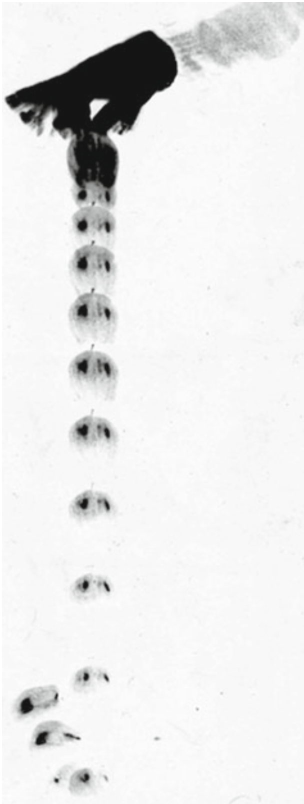

Fig. 2.6 Stroboscopic picture of the free fall of an apple which then bounces on the floor. This is a good example of the a priori representation of an intuitive phenomenon that cannot show up in quantum mechanics (William McLaughlin, "The resolution of Zeno's paradoxes," *Sci. Amer.*, 1994)

Phenomenological Description

The interference phenomenon would be very complicated to explain if we did not have the luck that it so closely resembles usual interference, with, in addition, a simple formula for the wavelength $\lambda = h/p$.

So, let's try and use the analogy with wave physics in order to formalize Louis de Broglie's idea. Here, we should be able to explain the interference experiment in the following way.

- The behavior of an atom of velocity v and momentum $p = mv$ in the incoming beam corresponds to that of a monochromatic plane wave

$$\psi_{\text{incident}} = e^{-i(\omega t - \mathbf{p}\cdot\mathbf{r}/\hbar)}, \quad \boldsymbol{k} = \boldsymbol{p}/\hbar,\ \lambda = 2\pi/k = h/p, \qquad (2.8)$$

  which has the good wave vector $\boldsymbol{k} = \boldsymbol{p}/\hbar$ and the good wavelength.

- After the two slits, the behavior is that of the sum of two waves each of which has been diffracted by a slit

$$\psi_{\text{outgoing}}(x) = \psi_1 + \psi_2, \tag{2.9}$$

which would describe, respectively, the behavior of the atom if it passed through one of the slits, the other one being blocked. We can calculate the phase shift of these waves at any point because we know the wavelength.
- Finally, the probability for an atom to reach some point C of the detector is simply the modulus squared of that sum

$$P(C) = |\psi_C|^2. \tag{2.10}$$

We just follow the same argument as for usual interferences.

We now have an answer to one of our questions above; what is the physical meaning of these waves?

In usual wave physics, one manipulates electromagnetic or acoustic wave amplitudes which add up and whose modulus squared gives intensities, that is, energy densities.

Our quantum waves are *probability amplitudes*. They add up and the modulus squared of the sum gives us probabilities, or probability densities.

One does not work directly with probabilities but with these intermediate tools, these probability amplitudes that add up.

The interference experiment gives us the wavelength, but not the frequency ω of the waves. Louis de Broglie made a good choice by assuming that this frequency is related to the energy of the particles in the same way as for Einstein's photons

$$\omega = E/\hbar, \quad \text{that is,} \quad \nu = E/h, \tag{2.11}$$

where $E = p^2/2m$ is the kinetic energy of the atoms. This leads to the complete structure of *de Broglie waves*:

$$\psi_{\text{incident}} = e^{-(i/\hbar)(Et-\mathbf{p}\cdot\mathbf{r})}, \text{ where } E = p^2/2m \ , \tag{2.12}$$

which is the probability amplitude for the presence of a particle at point $\mathbf{r}$ and time t of a particle of momentum $\mathbf{p} = m\mathbf{v}$.

Remark Notice that because the kinetic energy and the momentum are related by $E = p^2/2m$, one can find with this expression a wave equation, which is satisfied whatever the value of the momentum p. Indeed, if we take the time derivative on one hand, and the Laplacian on the other, we obtain

$$\frac{\partial}{\partial t}\psi_{\text{incident}} = -\frac{iE}{\hbar}\psi_{\text{incident}}, \quad \text{and} \quad \Delta\psi_{\text{incident}} = -\frac{p^2}{\hbar^2}\psi_{\text{incident}},$$

therefore, because $E = p^2/2m$, we have the wave equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi, \tag{2.13}$$

which is nothing but the Schrödinger equation for a free particle.[4]

Of course, we are not completely finished. For instance, atoms have a particlelike behavior that is obscure in all that. But we're getting closer.

2.4 Appendix: Notions on Probabilities

Probabilistic Phenomena

Consider a set of phenomena of the same nature on which we repeatedly make the same observation or measurement. For instance, play dice, measure a temperature or an economic parameter etc. Each observation belongs to some set Ω of *outcomes*. This set can be discrete, continuous, or a more complicated object such as a set of functions.

The set Ω is the set of a priori possible outcomes of the experiment. One also speaks of *events*: "the roulette number is even", "the observed temperature is between T_0 and T_1", etc.

Suppose we repeat an experiment a large number of times N, Ω being the set of possible outcomes. Consider a specific event α and N_α the number of times, among N, where α occurs. The observed number N_α depends on the specific sequence of experiments. One calls the *empirical frequency* of the event α in this sequence of experiments, the ratio:

$$f_\alpha(N) = N_\alpha/N.$$

The fundamental empirical observation is that when N becomes large, if the successive repetitions of the experiment are done *independently* (the result of an experiment has no a priori influence on the conditions in which the other experiments are done), the frequencies $f_\alpha(N)$ tend, for each event α, to a well defined limit. To each event α there corresponds a number $P(\alpha)$ called the *probability* of event α, related to the empirical frequency by the relation:

$$P(\alpha) = \lim_{N\to\infty} f_\alpha(N).$$

[4] It is surprising that de Broglie didn't think of writing this equation, or its relativistic equivalent—since he used the relativistic energy-momentum relation $E^2 = (p^2c^2 + m^2c^4)$.

Clearly, one has $P(\alpha) \geq 0$, $P(\Omega) = 1$, $P(\emptyset) = 0$, and if $(A_i)_{i \in I}$ is a finite family of disjoint events:

$$P(\bigcup_{i \in I} A_i) = \sum_{i \in I} P(A_i).$$

Examples of Probability Laws

Discrete Laws

The Simple Alternative

In this case, there are only two possible outcomes, $\alpha = 1$ or 2 (example: heads or tails). We note p the probability of the outcome 1 and q that of the outcome 2. We obviously have $p + q = 1$.

The Generalized Alternative

There are n outcomes $\alpha = 1, 2 \ldots n$. For instance one can place in an urn m_1 balls marked with the sign 1, m_2 balls marked 2, ... If the draw does not distinguish the balls, the probability law consists in the set of numbers p_1, p_2, ..., p_n such that:

$$p_\alpha = \frac{m_\alpha}{\sum_{\beta=1}^{n} m_\beta} \qquad \text{with} \qquad \sum_{\alpha=1}^{n} p_\alpha = 1.$$

Probability Laws on $\mathcal{R}$ or $\mathcal{R}^n$

A probability law P on $\mathcal{R}$ (resp. $\mathcal{R}^n$) is said to be of density p, p being a positive integrable function such that $\int_{-\infty}^{+\infty} p(x)\, dx = 1$ (resp. $\int_{R^n} p(x)\, d^n x = 1$), if, for any interval (resp. any volume) I:

$$P(I) = \int_I p(x)\, dx.$$

It is useful to treat the discrete and continuous cases in the same formalism by working with the distribution function:

$$F(t) = P(]-\infty, t]).$$

Examples

1. Exponential law:

$$p(x) = \begin{cases} \lambda e^{-\lambda x} & \text{if } x \geq 0 \quad (\lambda > 0) \\ 0 & \text{if } x < 0. \end{cases},$$

   which yields:

$$F(t) = \int_{-\infty}^{t} p(x) dx = \begin{cases} 0 & \text{if } t < 0 \\ 1 - e^{-\lambda t} & \text{if } t > 0 \end{cases}.$$

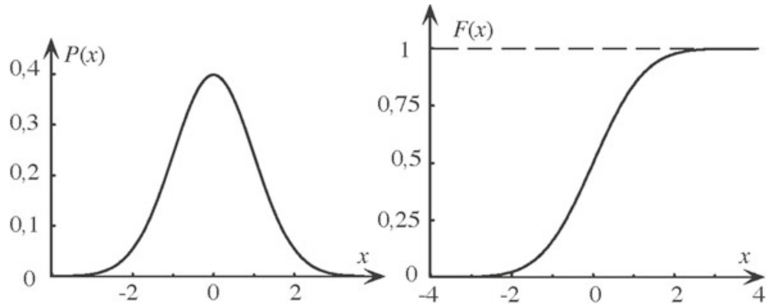

Fig. 2.7 The Gaussian probability law for $\mu = 0$ and $\sigma = 1$

2. Gauss's law of parameters μ, σ (Fig. 2.7):

$$p(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp -\frac{(x-\mu)^2}{2\sigma^2} \quad \text{with } \mu \in \mathcal{R}, \sigma \in \mathcal{R}^*. \tag{2.14}$$

Random Variables

Definition

Consider the example of the game with n outcomes $\alpha_1, \ldots, \alpha_n$ of respective probabilities $p_1, \ldots, p_n$. If, in this game, we win some amount of money x_α when the outcome is α, the number x_α which is a function of the (random) outcome of the experiment is called a *random variable*.

In the above example, the set of the $\{x_\alpha\}$ is discrete. One calls a discrete random variable x a set of numbers x_α (positive, negative, complex) each of which is associated to an outcome of a discrete random event. The couples $\{x_\alpha, p_\alpha\}$ define the *probability law* of the random variable x.

In the same way, one can consider continuous random variables. Let x be a random variable which takes its values in an interval $[a, b]$. The probability density $p(x)$ (positive or zero) defines the probability law of this random variable if the probability to find, in an experiment, a value between x and $x + dx$ is $p(x)\,dx$. We obviously have $\int_a^b p(x)\,dx = 1$. The generalization to $\mathcal{R}^n$ is straightforward.

Conditional Probabilities

Consider two types of events $[A]$ and $[B]$. We are led to defining the *conditional probability* of the event B knowing A, noted $P(B/A)$ by

$$P(B/A) = \frac{P(B \cap A)}{P(A)} \quad \text{as long as } P(A) > 0.$$

If X is a discrete random variable, one can define the *conditional probability $P(B|X = x)$ of the event B when $X = x$*, i.e. knowing the event $\{X = x\}$.

Example: The Exponential Decay Law

When a radioactive particle exists at time t, its probability to decay in the time interval $]t, t+\Delta t]$ is independent of its past history. Therefore the conditional probability that the time X at which the particle decays is between t and $t+\Delta t$, knowing that $\{X > t\}$, is independent of t and equal to $P\{0 < X \leq \Delta t\}$:

$$P\{0 < X \leq \Delta t\} = \frac{P\{t < X \leq t+\Delta t\}}{P\{X > t\}}.$$

If we call F the distribution function of X we obtain the functional relation:

$$F(\Delta t) = \frac{F(t+\Delta t) - F(t)}{1 - F(t)}.$$

The function F therefore satisfies the differential equation:

$$F'(t) = F'(0)\ (1 - F(t)).$$

Therefore, setting $\lambda = p(0) = F'(0)$ (λ is a decay rate), we get $F(t) = 1 - e^{-\lambda t}$. The density of the law of X is then:

$$p(x) = \begin{cases} \lambda e^{-\lambda x} & \text{for } x \geq 0 \\ 0 & \text{for } x < 0 \end{cases}.$$

Since λ has the dimension of the inverse of a time, we can note it $1/\tau$ where τ is the *lifetime* (or *mean life*). This exponential law is met in many practical applications (physics, pharmacology, reliability, etc.).

Independent Random Variables

Consider two discrete random variables X and Y with values in E_1 and E_2 respectively. One says that X and Y are two independent variables if the observation of X does not give any information on Y, and vice-versa. In other words, the conditional probability to find x if one knows y is independent of y (and vice versa).

This can be expressed in a symmetric form in x and y by:

$$P(\{X = x, Y = y\}) = P(\{X = x\})\ P(\{Y = y\}).$$

The variables X and Y are independent if and only if the law of the couple (X, Y) is the product of the laws of X and of Y.

Binomial Law and the Gaussian Approximation

Consider an experiment consisting in repeating N consecutive times and independently an experiment with two outcomes (for instance heads or tails). The first outcome, noted 1, has a probability p to happen, and the second, noted 0, has the probability $q = 1 - p$ to happen. Such a sequence of experiments is called a *Bernoulli sequence*.

Since the successive partial experiments are assumed to be independent, the probability for a given sequence $(x_1, \ldots, x_N)$ is given by:

$$P(x_1, \ldots, x_n) = P[X_1 = x_1] \ldots P[X_N = x_N] = p^k \, q^{N-k},$$

where k is the number of 1 in the sequence $(x_1 \ldots x_N)$. We now consider the random variable $X = X_1 + \cdots + X_N$ representing the number of times 1 appears in the N successive draws:

$$P[X = k] = \binom{N}{k} \, p^k q^{N-k} \equiv b(k; N, p).$$

This law $b(k; N, p)$ is called the *binomial law* of parameters N and p.

Normal Approximation of the Binomial Law

Using Stirling's formula: $n! \sim \sqrt{2\pi n} \, n^n \, e^{-n}$, we obtain for $n \gg 1$:

$$b(k; n, p) \sim \sqrt{\frac{1}{2\pi npq}} \exp -\frac{(k - np)^2}{2npq},$$

i.e. a Gaussian law for k, with $\mu = np$ and $\sigma = \sqrt{npq}$.

Moments of a Probability Distribution

Mean Value or Expectation Value

Consider a function $\varphi(x)$ of the random variable x ($\varphi(x)$ is a new random variable). We define its *mean value* or equivalently *expectation value* $\langle\varphi\rangle$ as

$$\langle\varphi\rangle = \begin{cases} \sum_\alpha \varphi(x_\alpha) \, p_\alpha & \text{discrete case} \\ \int_a^b \varphi(x) \, p(x) \, dx & \text{continuous case} \quad (a < x < b) \end{cases}$$

We note $\langle x \rangle$ the mean value of the variable x itself:

$$\langle x \rangle = \int x \, p(x) \, dx.$$

This quantity is equivalently called the mathematical expectation, or *expectation value*: if we gain the amount x_α when the result is α, then we expect to gain on the average $\langle x \rangle$.

Expectation Values of Usual Laws

1. Variable of the simple alternative: $\langle X \rangle = p$.
2. Binomial law $b(k; n, p)$: $\langle k \rangle = np$.

3. Geometric law $P\{X = k\} = (1 - p)p^k$ $(k \geq 0)$: $\langle X \rangle = p/(1 - p)$.
4. Poisson law $P\{X = k\} = e^{-\lambda}\, \lambda^k / k!$ $(k \geq 0)$: $\langle X \rangle = \lambda$.

Example

In the exponential decay above, the mean time that the particle spends before it decays, or the expectation value of its lifetime, is:

$$\langle t \rangle = \int_0^\infty \frac{t}{\tau} e^{-t/\tau} dt = \tau.$$

Variance and Mean Square Deviation

Consider a real random variable x whose expectation value is $\langle x \rangle = m$. The *mean square deviation* of x, noted σ or Δx, is defined by:

$$(\Delta x)^2 = \sigma^2 = \langle (x - \langle x \rangle)^2 \rangle,$$

σ^2 is also called the *variance* of the probability law. One readily checks, by expanding the square term, that:

$$\sigma^2 = \langle x^2 \rangle - 2\langle x \rangle \langle x \rangle + \langle x \rangle^2 = \langle x^2 \rangle - \langle x \rangle^2.$$

The smaller σ is, the more probable it is to find a value of x close to the mean value. The quantity σ measures the deviation from the mean value.

Variance of Usual Laws

1. The simple alternative: $\sigma^2 = p(1 - p)$.
2. Binomial law: $\sigma^2 = np(1 - p)$. Note that the relative dispersion $\sigma / \langle X \rangle$ tends to zero as $n^{-1/2}$ when $n \to \infty$.
3. Gaussian law: the variance coincides with the parameter σ^2 of (2.14).
4. Geometric law: $\sigma^2 = p/(1 - p)^2$.
5. Poisson law of parameter $\lambda : \sigma^2 = \lambda$.

Bienaymé–Tchebycheff Inequality

Note m the mean value and σ^2 the variance of the discrete real variable X. One can show that:

$$P(\{|X - m| \geq \tau\sigma\}) \leq 1/\tau^2, \tag{2.15}$$

which proves that for a small variance, there is a small probability to find X far from its expectation value.

Error Function

In the particular case of the Gaussian law (m, σ), one calls *error function* $\Phi(\tau)$ the quantity $P(\{|X - m| \leq \tau\sigma\})$. One has:

$$\Phi(\tau) = \int_{\tau\sigma}^{+\tau\sigma} \frac{1}{\sigma\sqrt{2\pi}} e^{-x^2/2\sigma^2}\, dx.$$

Some values of $\Phi(\tau)$ are the following

τ	1	2	3
$\Phi(\tau)$	0.68	0.95	0.99

2.5 Exercises

1. Distribution of impacts

We observe the impacts on a target in the xy plane. The observable is assumed to obey a probability law of density $p(x, y) = (2\pi\sigma^2)^{-1} \exp(-\rho^2/(2\sigma^2))$ where $\rho = (x^2 + y^2)^{1/2}$ is the distance from the origin of the impact point. What is the probability law of ρ?

2. Is this a fair game?

Suppose that one offers you the following game: *Bet one euro and throw three dice. If number 6 (or any number you choose in advance) does not show up, you lose your bet; you get paid 2 euros if it shows up on one dice, 3 euros if it shows up on two, and 6 euros if it shows up on the three of them.* Calculate the expectation value of what you gain (which is negative if you lose) and see if it is reasonable to play.

3. Spatial distribution of the molecules in a gas

Consider in a volume V (22.41 for instance) N molecules (6×10^{23} for instance). Consider an enclosed volume v ($10^{-3}\,\mathrm{cm}^3$). How many molecules are there on the average in v? What are the fluctuations of this number?

http://www.springer.com/978-3-319-43478-0

Lectures on Quantum Mechanics
With Problems, Exercises and their Solutions
Basdevant, J.-L.
2016, XVI, 501 p. 122 illus. in color., Hardcover
ISBN: 978-3-319-43478-0