Michel Le Bellac

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Quantum Physics

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Quantum Physics

Quantum physics allows us to understand the nature of the physical phenomena which govern the behavior of solids, semiconductors, lasers, atoms, nuclei, subnuclear particles, and light. In *Quantum Physics*, Le Bellac provides a thoroughly modern approach to this fundamental theory.

Throughout the book, Le Bellac teaches the fundamentals of quantum physics using an original approach which relies primarily on an algebraic treatment and on the systematic use of symmetry principles. In addition to the standard topics such as one-dimensional potentials, angular momentum and scattering theory, the reader is introduced to more recent developments at an early stage. These include a detailed account of entangled states and their applications, the optical Bloch equations, the theory of laser cooling and of magneto-optical traps, vacuum Rabi oscillations, and an introduction to open quantum systems. This is a textbook for a modern course on quantum physics, written for advanced undergraduate and graduate students.

MICHEL LE BELLAC is Emeritus Professor at the University of Nice, and a well-known elementary particle theorist. He graduated from Ecole Normale Supérieure in 1962, before conducting research with CNRS. In 1967 he returned to the University of Nice, and was appointed Full Professor of Physics in 1971, a position he held for over 30 years. His main fields of research have been the theory of elementary particles and field theory at finite temperatures. He has published four other books in French and three other books in English, including *Thermal Field Theory* (Cambridge 1996) and *Equilibrium and Non-equilibrium Statistical Thermodynamics* with Fabrice Mortessagne and G. George Batrouni (Cambridge 2004).

Quantum Physics

Michel Le Bellac University of Nice

Translated by

Patricia de Forcrand-Millard



CAMBRIDGE UNIVERSITY PRESS Cambridge, New York, Melbourne, Madrid, Cape Town, Singapore, São Paulo

Cambridge University Press The Edinburgh Building, Cambridge CB2 8RU, UK Published in the United States of America by Cambridge University Press, New York www.cambridge.org Information on this title: www.cambridge.org/9780521852777

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First published in print format 2006

 ISBN-13
 978-0-511-34556-2
 eBook (Adobe Reader)

 ISBN-10
 0-511-34556-9
 eBook (Adobe Reader)

 ISBN-13
 978-0-521-85277-7
 hardback

 ISBN-10
 0-521-85277-3
 hardback

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Foreword

Quantum physics is now one hundred years old, and this description of physical phenomena, which has transformed our vision of the world, has never been found at fault, which is exceptional for a scientific theory. Its predictions have always been verified by experiment with impressive accuracy. The basic concepts of quantum physics such as probability amplitudes and linear superpositions of states, which seem so strange to our intuition when encountered for the first time, remain fundamental. However, during the last few decades an important evolution has occurred. The spectacular progress made in observational techniques and methods of manipulating atoms now makes it possible to perform experiments so delicate that they were once considered as only "thought experiments" by the founders of quantum mechanics. The existence of "nonseparable" quantum correlations, which forms the basis of the Einstein-Podolsky-Rosen "paradox" and which violates the famous Bell inequalities, has been confirmed experimentally with high precision. "Entangled" states of two systems which manifest such quantum correlations are now better understood and even used in practical applications such as quantum cryptography. The entanglement of a measuring device with its environment reveals an interesting new pathway to better understanding of the measurement process.

In parallel with these conceptual advances, our everyday world is being invaded by devices which function on the basis of quantum phenomena. The laser sources used to read compact disks, in ophthalmology, and in optical telecommunications are based on light amplification by atomic systems with population inversion. Nuclear magnetic resonance is widely used in hospitals to obtain ever more detailed images of the organs of the human body. Millions of transistors are incorporated in the chips which allow our computers to perform operations at phenomenal speeds.

It is therefore clear that any modern course in quantum physics must cover these recent developments in order to give the student or researcher a more accurate idea of the progress that has been made and to motivate the better understanding of physical phenomena whose conceptual and practical importance is increasingly obvious. This is the goal that Michel Le Bellac has successfully accomplished in the present work.

Each of the fifteen chapters of this book contains not only a clear and concise description of the basic ideas, but also numerous discussions of the most recent conceptual and experimental developments which give the reader an accurate idea of the advances in the field and the general trends in its evolution. Chapter 6 on entangled states is typical of this method of presentation. Instead of stressing the mathematical properties of the tensor product of two spaces of states, which is rather austere and forbidding, this chapter is oriented on discussion of the idea of entanglement, and introduces several examples of theoretical and experimental developments (some of them very new) such as the Bell inequalities, tests of these inequalities and in particular the most recent ones based on parametric conversion, GHZ (Greenberger, Horne, Zeilinger) states, the idea of decoherence illustrated by modern experiments in cavity quantum electrodynamics (discussed in more detail in an appendix), and teleportation. It is difficult to imagine a more complete immersion in one of the most active current areas of quantum physics. Numerous examples of this modern presentation can be found in other chapters, too: interference of de Broglie waves realized using slow neutrons or laser-cooled atoms; tunnel-effect microscopy; quantum field fluctuations and the Casimir effect; non-Abelian gauge transformations; the optical Bloch equations; radiative forces exerted by laser beams on atoms; magneto-optical traps; Rabi oscillations in a cavity vacuum, and so on.

I greatly admire the effort made by the author to give the reader such a modern and compelling view of quantum physics. Of course, not all subjects can be treated in great detail, and the reader must make some effort to obtain a deeper comprehension of the subject. This is aided by the detailed bibliography given in the form of both footnotes to the text and a list of suggested reading at the end of each chapter. I am sure that this text will lead to better comprehension of quantum physics and will stimulate greater interest in this absolutely central discipline. I would like to thank Michel Le Bellac for this important contribution which will certainly give physics a more exciting image.

Claude Cohen-Tannoudji

Preface

This book has grown out of a course given at the University of Nice over many years for advanced undergraduates and graduate students in physics. The first ten chapters correspond to a basic course in quantum mechanics for advanced undergraduates, and the last four could serve to complement a graduate course in, for example, atomic physics. The book contains about 130 exercises of varying length and difficulty, most of which have actually been used in homework or exams.

This book should be interesting not only to students in physics and engineering, but also to a wider group of physicists: graduate students, researchers, and secondary-school teachers who wish to update their knowledge of quantum physics. It discusses recent developments not covered in the classic texts such as entangled states, quantum cryptography and quantum computing, decoherence, interactions of a laser with a two-level atom, quantum fluctuations of the electromagnetic field, laser manipulation of atoms, and so on, and it also includes a concise discussion of the current ideas about measurement in quantum mechanics as an appendix.

The organization of this book differs greatly from that of the classic texts, which typically begin with the Schrödinger equation and then proceed to study its solution in various situations. That approach makes it necessary to introduce the basic principles of quantum mechanics in a relatively complicated situation, and they end up being obscured by calculations which are often rather complex. Instead, I have striven to present the fundamentals of quantum mechanics using the simplest examples, and the Schrödinger equation appears only in Chapter 9. I follow the approach of pushing the logic adopted by Feynman (Feynman *et al.* [1965]) to its limit: developing the algebraic approach as far as possible and exploiting the symmetries, so as to present quantum mechanics within an autonomous framework without reference to classical physics. There are several advantages to this logic.

- The algebraic approach allows the solution of simple problems in finite-dimensional (for example, two-dimensional) spaces, such as photon polarization, spin 1/2, two-level atoms, and so on.
- This approach leads to the clearest statement of the postulates of quantum mechanics, as the fundamental issues are separated from the less fundamental ones (for example, the correspondence principle is not a fundamental postulate).

Preface

• The use of the symmetry properties leads to the most general introduction to fundamental physical properties such as momentum, angular momentum, and so on as the infinitesimal generators of these symmetries, without resorting to the correspondence principle or classical analogies.

Another advantage of this approach is that the reader wishing to learn about the recent developments in quantum information theory need consult only the first six chapters. These are sufficient for comprehension of the basics of quantum information, without passing through the stages of expansion of the wave function in spherical harmonics and solving the Schrödinger equation in a central potential!

I have given special attention to the pedagogical aspects. The order of chapters was carefully chosen: the early ones use only finite-dimensional spaces, and only after the basic principles have been covered do I go on to the general case in Chapter 7. Chapters 11 to 14 and the appendices involve more advanced techniques which may be of interest to professional physicists. An effort has been made regarding the vocabulary, in order to avoid certain historically dated expressions which can obstruct the understanding of quantum mechanics. Following the modernization proposed by J.-M. Lévy-Leblond (Quantum words for a quantum world, in *Epistemological and Experimental Perspectives on Quantum Physics*, D. Greenberger, W. L. Reiter and A. Zeilinger (eds.) Dordrecht: Kluwer (1999)), I use "physical property" instead of "observable" and "Heisenberg inequality" and "wave-particle duality."

The key chapters of this book, that is, those which diverge most obviously from the traditional treatment, are Chapters 3, 4, 5, 6, and 8. Chapter 3 introduces the space of states for the example of photon polarization and shows how to go from a wave amplitude to a probability amplitude. Spin 1/2 takes the reader directly to a problem without a classical analog. The essential properties of spin 1/2, namely the algebra of the Pauli matrices, the rotation matrices, and so on, are obtained using only two hypotheses: (1) twodimensionality of the space of states and (2) rotational invariance. The Larmor precession of the quantum spin allows us to introduce the evolution equation. This chapter prepares the reader for the statement of the postulates of quantum mechanics in the following chapter, and it is possible to illustrate each postulate in a concrete fashion by returning to the examples of Chapter 3. The distinction between the general conceptual framework of quantum mechanics and the modeling of a particular problem is carefully explained. In Chapter 5 quantum mechanics is applied to some simple and physically important systems with a finite number of levels, a particular case being the diagonalization of the Hamiltonian in the presence of a periodic symmetry. This chapter also uses the example of the ammonia molecule to introduce the interaction of a two-level atomic or molecular system with an electromagnetic field, and the fundamental concepts of emission and absorption.

Chapter 6 is devoted to entangled states. The practical importance of these states dates from the early 1980s, but they are often ignored by textbooks. This chapter also deals with fundamental applications such as the Bell inequalities, two-photon interference, and measurement theory, as well as potential applications such as quantum computing. Chapter 8 is devoted to the study of symmetries using the Wigner theorem, which is generally ignored in textbooks despite its crucial importance. Rotational symmetry allows the angular momentum to be defined as an infinitesimal generator, and the commutation relations of \vec{J} can be demonstrated immediately with emphasis on their geometrical origin. The canonical commutation relations of X and P are derived from the identification of the momentum as the infinitesimal generator of translations. Finally, I obtain the most general form of the Hamiltonian compatible with Galilean invariance using a hypothesis about the velocity transformation law. This Hamiltonian will be reinterpreted later on within the framework of local gauge invariance.

The other chapters can be summarized as follows. Chapter 1 has the triple goal of (1) introducing the basic notions of microscopic physics which will be used later on in the text; (2) introducing the behavior of quantum particles, conventionally called "wave–particle duality"; and (3) presenting a simple explanation, with the aid of the Bohr atom, of the notion of energy level and of level spectrum. Chapter 2 presents the essential ideas about Hilbert space in the case of finite dimension. Chapter 7 gives some information about Hilbert spaces of infinite dimension; the goal here is of course not to present a mathematically rigorous treatment, but rather to warn the reader of certain pitfalls in infinite dimension.

The final chapters are devoted to more classic applications. Chapter 9 presents wave mechanics and its usual applications (the tunnel effect, bound states in the square well, periodic potentials, and so on). The angular momentum commutation relations already presented in Chapter 8 reappear in Chapter 10 in the construction of eigenstates of \vec{J}^2 and J_z , and lead to the Wigner–Eckart theorem for vector operators. Chapter 11 develops the theory of the harmonic oscillator and motion in a constant magnetic field, which provides the occasion for explaining local gauge invariance. An important section in this chapter deals with quantized fields: the vibrational field and phonons, and the electromagnetic field and its quantum fluctuations. Chapters 12 and 13 are devoted to scattering and identical particles. In Chapter 14 I present a brief introduction to the physics of one-electron atoms, the main objective being to calculate the forces on a two-level atom placed in the field of a laser and to discuss applications such as Doppler cooling and magneto-optical traps.

The appendices deal with subjects which are a bit more technically demanding. The proof of the Wigner theorem and the time-reversal operation are explained in detail in Appendix A. Some complementary information about the theory and experiments on decoherence can be found in Appendix B along with a discussion of some current ideas about measurement. Finally, Appendix C contains a discussion of the method of Wigner and Weisskopf for unstable states.

Acknowledgments

I have benefited from the criticism and suggestions of Pascal Baldi, Jean-Pierre Farges, Yves Gabellini, Thierry Grandou, Jacques Joffrin, Christian Miniatura, and especially Michel Brune (to whom I am also indebted for Figs. 6.9, B.1, and B.2), Jean Dalibard, Fabrice Mortessagne, Jean-Pierre Romagnan, and François Rocca, who have read large parts or in some cases all of the manuscript. I also wish to thank David Wilkowski, who provided the inspiration for the text in some of the exercises of Chapter 14. Of course, I bear sole responsibility for the final text. The assistance of Karim Bernardet and Fabrice Mortessagne, who initiated me into XFIG and installed the software, was crucial for realizing the figures, and I also thank Christian Taggiasco for competently installing and maintaining all the necessary software. Finally, this book would never have seen the light of day were it not for the encouragement and unfailing support of Michèle Leduc, and I am very grateful to Claude Cohen-Tannoudji for writing the Preface.

Addendum for the English edition

In addition to minor corrections, I have included a few new exercises, partly rewritten Chapters 5 and 6, and added a new chapter on open quantum systems. I am grateful to Jean Dalibard and Christian Miniatura for their careful reading of this new chapter and for their useful comments. I would like to thank Simon Capelin and Vincent Higgs for their help in the publication and, above all, Patricia de Forcrand-Millard for her excellent translation and for her patience in our many email exchanges in order to find the right word.

Units and physical constants

The physical constants below are given v	with a relative precision of 10^{-3} which is sufficient for the
numerical applications in this book.	
Speed of light in vacuum	$c = 3.00 \times 10^8 \text{ m s}^{-1}$
Planck constant	$h = 6.63 \times 10^{-34} \text{ Js}$
Planck constant divided by 2π	$\hbar = 1.055 \times 10^{-34} \mathrm{Js}$
Electronic charge (absolute value)	$q_{\rm e} = 1.602 \times 10^{-19} {\rm C}$
Fine structure constant	$\alpha = q_{\rm e}^2/(4\pi\varepsilon_0\hbar c) = e^2/(\hbar c) = 1/137$
Electron mass	$m_{\rm e} = 9.11 \times 10^{-31} \text{ kg} = 0.511 \text{ MeV} c^{-2}$
Proton mass	$m_{\rm p} = 1.67 \times 10^{-27} \text{ kg} = 938 \text{ MeV} c^{-2}$
Bohr magneton	$\mu_{\rm B} = q_{\rm e} \hbar / (2m_{\rm e}) = 5.79 \times 10^{-5} {\rm eV}{\rm T}^{-1}$
Nuclear magneton	$\mu_{\rm N} = q_{\rm e}\hbar/(2m_{\rm p}) = 3.15 \times 10^{-8} {\rm eV}{\rm T}^{-1}$
Bohr radius	$a_0 = \hbar^2 / (m_e e^2) = 0.529 \times 10^{-8} \mathrm{m}$
Rydberg constant	$R_{\infty} = m_{\rm e} e^4 / (2\hbar^2) = 13.61 {\rm eV}$
Boltzmann constant	$k_{\rm B} = 1.38 \times 10^{-23} {\rm J} {\rm K}^{-1}$
Electron volt and temperature	$1 \text{ eV} = 1.602 \times 10^{-19} \text{ J} = k_{\text{B}} \times 11600 \text{ K}$
Gravitational constant	$G = 6.67 \times 10^{-11} \text{ N m}^2 \text{ kg}^{-2}$

Introduction

The first objective of this chapter is to briefly review some of the basic ideas about the structure of matter, in particular the concepts of microscopic physics, in order to recall the knowledge gained in previous physics (and chemistry) courses and make it more precise. Our review will be very concise, and most statements will be made without any proof or detailed discussion. A second objective is to give a brief description of some of the crucial stages in the early development of quantum physics. We shall not follow the strict historical order of this development or present the arguments used at the beginning of the last century by the founding fathers of quantum mechanics; rather, we shall stress the concepts which we shall find useful later on. Our last objective is to give an elementary introduction to some of the basic ideas, like those of a quantum particle or energy level, that will reappear throughout this text. We shall base our review on the Bohr theory, which provides a simple, though far from convincing, explanation of how energy levels are quantized and how the spectrum of the hydrogen atom arises. This chapter should be reread later on, once the basic ideas of quantum mechanics have been made explicit and illustrated by examples. From the practical point of view, it is possible to skip the general considerations of Sections 1.1 and 1.2 at the first reading and begin with Section 1.3, returning to those two sections later on as needed.

1.1 The structure of matter

1.1.1 Length scales from cosmology to elementary particles

Table 1.1 gives the length scales in meters of some typical objects, ranging from the size of the known Universe to the subatomic scale. A unit of length convenient for measuring astrophysical distances is the light-year (l.y.): $1 \text{ l.y.} = 0.95 \times 10^{16} \text{ m}$. The submeter scales commonly used in physics are the micrometer $1 \,\mu\text{m} = 10^{-6} \text{ m}$, the nanometer $1 \text{ nm} = 10^{-9} \text{ m}$, and the femtometer (or fermi, F) $1 \text{ fm} = 10^{-15} \text{ m}$. Objects at the microscopic scale are often studied using electromagnetic radiation of wavelength of the order of the characteristic size of the object under study (by means of a microscope, X-rays, etc.).¹ It is well known that

¹ Other techniques are neutron scattering (Exercise 1.6.4), electron microscopy, tunneling microscopy (Section 9.4.2), and so on.

	Size (m)
Known Universe	$1.3 imes 10^{26}$
Radius of the Milky Way	$\sim \! 5 imes 10^{20}$
Sun–Earth separation	$1.5 imes 10^{11}$
Radius of the Earth	6.4×10^6
Man	~1.7
Insect	0.01 to 0.001
E. coli (bacterium)	$\sim \! 2 \times 10^{-6}$
HIV (virus)	1.1×10^{-7}
Fullerene C ₆₀	$0.7 imes 10^{-9}$
Atom	$\sim \! 10^{-10}$
Lead nucleus	7×10^{-15}
Proton	0.8×10^{-15}

 Table 1.1 Some typical distance scales

the limiting resolution is determined by the wavelength used: it is fractions of a micrometer for a microscope using visible light, or fractions of a nanometer when X-rays are used. The wavelength spectrum of electromagnetic radiation (infrared, visible, etc.) is summarized in Fig. 1.1.

1.1.2 States of matter

We shall be particularly interested in phenomena occurring at the microscopic scale, and so it is useful to recall some of the elementary ideas about the microscopic description of matter. Matter can exist in two different forms: an ordered form, namely a crystalline solid, and a disordered form, namely a liquid, a gas, or an amorphous solid.



Fig. 1.1. Wavelengths of electromagnetic radiation and the corresponding photon energies. The boundaries between different types of radiation (for example, between γ -rays and X-rays) are not strictly defined. A photon of energy E = 1 eV has wavelength $\lambda = 1.24 \times 10^{-6}$ m, frequency $\nu = 2.42 \times 10^{14}$ Hz, and angular frequency $\omega = 1.52 \times 10^{15}$ rad s⁻¹.



Fig. 1.2. Arrangement of atoms in a crystal of sodium chloride. The chlorine ions Cl^- are larger than the sodium ions Na^+ .

A crystalline solid possesses long-range order. As an example, in Fig. 1.2 we show the microscopic structure of sodium chloride. The basic crystal pattern is repeated with periodicity l = 0.56 nm, forming the *crystal lattice*. Starting from a chlorine ion or a sodium ion and moving along one of the links of the cubic structure, we again reach a chlorine ion or a sodium ion after a distance $n \times 0.56$ nm, where *n* is an integer. This is what we mean by long-range order.

Liquids, gases, and amorphous solids do not possess long-range order. Let us take as an example a monatomic liquid, namely liquid argon. To a first approximation the argon atoms can be represented as impenetrable spheres of diameter $\sigma \simeq 0.36$ nm. In Fig. 1.3 we schematically show an atomic configuration for a liquid in which the spheres practically touch each other, but are arranged in a disordered fashion. Taking the center of one atom as the origin, the probability p(r) of finding the center of another atom at a distance r from the former is practically zero for $r \lesssim \sigma$. However, this probability reaches a maximum at $r = \sigma, 2\sigma, ...$ and then oscillates before becoming stable at a constant value, whereas in the case of a crystalline solid the function p(r) possesses peaks



Fig. 1.3. (a) Arrangement of atoms in liquid argon. (b) Probability p(r) for a liquid (dashed line) and for a gas (solid line). (c) Probability p(r) for a simple crystal.

no matter what the distance from the origin is. Argon gas has the same type of atomic configuration as liquid argon, the only difference being that the atoms are much farther apart. The difference between the liquid and the gas vanishes at the critical point, and it is possible to move continuously from the gas to the liquid and back while going around the critical point, whereas such a continuous passage to a solid is impossible because the type of order is qualitatively different.

We have chosen a monatomic gas as an example, but in general the basic object is a combination of atoms in a molecule such as N_2 , O_2 , H_2O , etc. Certain molecules like proteins may contain thousands of atoms. For example, the molecular weight of hemoglobin is something like 64 000. A chemical reaction is a rearrangement of atoms – the atoms of the initial molecules are redistributed to form the final molecules:

$$H_2 + Cl_2 \rightarrow 2HCl.$$

An atom is composed of a positively charged atomic nucleus (or simply nucleus) and negatively charged electrons. More than 99.9% of the mass of the atom is in the nucleus, because the ratio of the electron mass $m_{\rm e}$ to the proton mass $m_{\rm p}$ is $m_{\rm e}/m_{\rm p} \simeq 1/1836$. The atom is ten thousand to a hundred thousand times larger than the nucleus: the typical size of an atom is 1 Å (where 1 Å= 10^{-10} m = 0.1 nm), while that of a nucleus is several fermis (or femtometers).²

An atomic nucleus is composed of protons and neutrons. The former are electrically charged and the latter are neutral. The proton and neutron masses are identical to within 0.1%, and this mass difference can often be neglected in practice. The *atomic number* Z is the number of protons in the nucleus, and also the number of electrons in the corresponding atom, so that the atom is electrically neutral. The *mass number* A is the number of protons plus the number of neutrons N: A = Z + N. The protons and neutrons are referred to collectively as *nucleons*. Nuclear reactions involving protons and neutrons of protons and neutrons involving atoms: a nuclear reaction is a redistribution of protons and neutrons to form nuclei different from the initial ones, while a chemical reaction is a redistribution of a deuterium nucleus (²H, a proton and a neutron) and a tritium nucleus (³H, a proton and two neutrons) to form a helium-4 nucleus (⁴He, two protons and two neutrons) plus a free neutron:

$$^{2}\text{H} + ^{3}\text{H} \rightarrow ^{4}\text{He} + n + 17.6 \text{ MeV}.$$

The reaction releases 17.6 MeV of energy and in the (probably distant) future may be used for large-scale energy production (fusion energy).

An important concept pertaining to an atom formed from a nucleus and electrons, as well as to a nucleus formed from protons and neutrons, is that of the *binding energy*. Let us consider a stable object C formed of two objects A and B. The object C is termed a *bound state* of A and B. The breakup $C \rightarrow A + B$ will not be allowed if the mass m_C

² We shall often use the Ångström (Å), which is the characteristic atomic scale, rather than nm.

of C is less than the sum of the masses m_A and m_B of A and B, that is, if the binding energy $E_{\rm b}$

$$E_{\rm b} = (m_A + m_B - m_C)c^2 \tag{1.1}$$

is positive.³ Here *c* is the speed of light and E_b is the energy needed to dissociate *C* into A + B. In atomic physics this energy is called the ionization energy, and it is the energy necessary to break up an atom into a positive ion and an electron, or, stated differently, to remove an electron from the atom. In the case of molecules E_b is the dissociation energy, or the energy needed to break up the molecule into atoms. A particle or a nucleus that is unstable in a particular configuration may be perfectly stable in a different configuration. For example, a free neutron (n) is unstable: in about fifteen minutes on average it disintegrates into a proton (p), an electron (e), and an electron antineutrino ($\overline{\nu}_e$); this is the basic decay of β -radioactivity:

$$\mathbf{n}^0 \to \mathbf{p}^+ + \mathbf{e}^- + \overline{\nu}_{\mathbf{e}}^0, \tag{1.2}$$

where we have explicitly indicated the charge of each particle. This decay is possible because the masses⁴ of the particles in (1.2) satisfy

$$m_{\rm n}c^2 > (m_{\rm p} + m_{\rm e} + m_{\overline{\nu}})c^2,$$

where

$$m_{\rm n} \simeq 939.5 \,{\rm MeV}\,c^{-2}, \quad m_{\rm p} \simeq 938.3 \,{\rm MeV}\,c^{-2}, \quad m_{\rm e} \simeq 0.51 \,{\rm MeV}\,c^{-2}, \quad m_{\overline{\nu}_{\rm e}} \simeq 0.$$

On the other hand, a neutron in a stable atomic nucleus does not decay; taking as an example the deuterium nucleus (the deuteron, ²H), we have

$$m_{^{2}\mathrm{H}}c^{^{2}} \simeq 1875.6 \text{ MeV} < (2m_{\mathrm{p}} + m_{\mathrm{e}} + m_{\overline{\nu}_{e}})c^{^{2}} \simeq 1878.3 \text{ MeV},$$

and so the decay

$$^{2}\text{H} \rightarrow 2\text{p} + \text{e} + \overline{\nu}_{e}$$

is impossible: the deuteron is a proton-neutron bound state.

1.1.3 Elementary constituents

So far, we have broken up molecules into atoms, atoms into electrons and nuclei, and nuclei into protons and neutrons. Can we go even farther? For example, can we break

³ According to the celebrated Einstein relation $E = mc^2$; by simple dimensional analysis we can relate mass and energy to each other, so that, for example, masses can be expressed in Jc^{-2} or in eV c^{-2} .

⁴ Three recent experiments, those of S. Fukuda *et al.* (SuperKamiokande Collaboration), Solar B8 and hep neutrino measurements from 1258 days of SuperKamiokande data, *Phys. Rev. Lett.* **86**, 5651 (2001), Q. Ahmad *et al.* (SNO Collaboration), Interactions produced by B8 solar neutrinos at the Sudbury Neutrino Observatory, *Phys. Rev. Lett.*, **87**, 071301 (2001), and K. Eguchi *et al.* (Kamland Collaboration), First results from Kamland: evidence from reactor antineutrino disappearance, *Phys. Rev. Lett.* **90**, 021802 (2003), demonstrate convincingly that the neutrino mass is not zero, but is probably of order 10⁻² eV c⁻²; cf. Exercise 4.4.6 on neutrino oscillations. For a review, see D. Wark, Neutrinos: ghosts of matter, *Physics World* **18**(6), 29 (June 2005).

up a proton or an electron into more elementary constituents? Is it possible, for example, that a neutron is composed of a proton, an electron, and an antineutrino, as Eq. (1.2) suggests? A simple argument based on the Heisenberg inequalities shows that the electron cannot pre-exist inside the neutron (Exercise 9.7.4), but instead is *created* at the moment the decay occurs. Therefore, we cannot say that a neutron is composed of a proton, an electron, and a neutrino. One could also imagine "breaking" a proton or a neutron into more elementary constituents by bombarding it with energetic particles, just as, for example, happens when a deuteron is bombarded by electrons of several MeV in energy:

$$e + {}^{2}H \rightarrow e + p + n$$
.

The deuteron 2 H is broken up into its constituents, a proton and a neutron. However, the situation is not repeated when a proton is bombarded by electrons. When low-energy electrons are used, the collisions are elastic:

$$e + p \rightarrow e + p$$
,

and when the electron energy is high enough (several hundred MeV), the proton does not break up; instead, other particles are created, for example in reactions like

$$\begin{split} e+p &\rightarrow e+p+\pi^0, \\ e+p &\rightarrow e+n+\pi^++\pi^0, \\ e+p &\rightarrow e+K^++\Lambda^0, \end{split}$$

where the π and K mesons and the Λ^0 hyperon are new particles whose nature is not important for the present discussion. The crucial point is that these particles do not exist *ab initio* inside the proton, but are created at the instant the reaction occurs.

It therefore appears that at some point it is not possible to decompose matter into constituents which are more and more elementary. We can then ask the following question: what is the criterion for a particle to be elementary? The current idea is that a particle is elementary if it behaves as a point particle in its interactions with other particles. According to this idea, the electron, neutrino, and photon are elementary, while the proton and neutron are not: they are "composed" of quarks. These quotation marks are important, because quarks do not exist as free states,⁵ and the quark "composition" of the proton is very different from the proton and neutron composition of the deuteron. Only indirect (but convincing) evidence of this quark composition exists.

As far as is known at present,⁶ there exist three families of elementary particles or "particles of matter" of spin 1/2.⁷ They are listed in Table 1.2, where the electric charge q is expressed in units of the proton charge. Each family is composed of leptons and quarks,

⁵ What exactly is meant by the quark "mass" is quite complicated, at least for the so-called "light" quarks – the up, down, and strange quarks. Something close to the mass defined in the usual way is obtained for the heavy b and t quarks.

⁶ There is a very strong argument for limiting the number of families to three. In 1992 experiments at CERN showed that the number of families is limited to three on the condition that the neutrino masses are less than 45 GeV c^{-2} . The actual experimental value of the number of families is 2.984±0.008.

⁷ Spin 1/2 is defined in Chapter 3 and spin in general in Chapter 10.

	Lepton $q = -1$	Neutrino $q = 0$	Quark $q = 2/3$	Quark $q = -1/3$
Family 1	electron	neutrino _e	up quark	down quark
Family 2	muon	neutrino _μ	charmed quark	strange quark
Family 3	tau	neutrino _τ	top quark	bottom quark

 Table 1.2 Matter particles. The electric charges are measured in units of the proton charge.

and each particle has a corresponding antiparticle of the opposite charge. The leptons of the first family are the electron and its antiparticle the positron e^+ , as well as the electron neutrino v_e and its antiparticle the electron antineutrino \overline{v}_e . The quarks of this family are the up quark u of charge 2/3 and the down quark d of charge -1/3 plus, of course, the corresponding antiquarks \overline{u} and \overline{d} , with charges -2/3 and 1/3, respectively. The proton is the combination uud and the neutron is the combination udd. This first family is sufficient for our everyday life, as all ordinary matter is composed of these particles. The neutrino is essential for the cycle of nuclear reactions occurring in the normally functioning Sun. While the existence of this first family is justified by an anthropocentric argument (if the family did not exist, we would not be here to talk about it), the reason for the existence of the other two families remains obscure.⁸

To these particles we need to add those that "carry" the interactions: the photon for electromagnetic interactions, the W and Z bosons for weak interactions, the gluons for strong interactions, and the graviton for gravitational interactions.⁹ Now let us discuss these interactions.

1.1.4 The fundamental interactions

There are four types of fundamental interaction (forces): strong, electromagnetic, weak, and gravitational.¹⁰ The *electromagnetic interaction* will play a leading role in this book, as it governs the behavior of atoms, molecules, solids, etc. The electrical forces obeying Coulomb's law dominate. We recall that a charge q fixed at the coordinate origin exerts a force on a charge q' at rest located at a point \vec{r}

$$\vec{F} = \frac{qq'}{4\pi\varepsilon_0} \frac{\hat{r}}{r^2},\tag{1.3}$$

⁸ As I. I. Rabi reputedly said of the muon: "Who ordered that?" Nevertheless, we know that each family must be complete: this is how the existence of the top quark and the value of its mass were predicted several years before its experimental discovery in 1994. Owing to its high mass, about 175 times that of the proton, the top quark was not discovered until the proton–antiproton collider known as the Tevatron was in operation in the USA.

⁹ More rigorously, the electromagnetic and weak interactions have by now been unified as the electroweak interaction. The gluon, just like the quark, does not exist as a free state. Finally, the existence of the graviton is still hypothetical.

¹⁰ Every once in a while a "fifth force" is "discovered," but it soon disappears again!

Introduction

where \hat{r} is a unit vector \vec{r}/r , $r = |\vec{r}|$, and ε_0 is the vacuum permittivity.¹¹ If the charges move with speed v, we must also take into account the magnetic forces. However, they are weaker than the Coulomb force by a factor $\sim (v/c)^2$ (we are using \sim in the sense "of the order of"). For the electrons of the outer shells of an atom $(v/c)^2 \approx (1/137)^2 \ll 1$, but, owing to the extremely high precision of atomic physics experiments, the effects of magnetic forces are easily seen in phenomena such as the fine structure or the Zeeman effect (Section 14.2.3). The Coulomb force (1.3) is characterized by

- the $1/r^2$ force law. This is called a *long-range* force law;
- the strength of the force as measured by the *coupling constant* $qq'/4\pi\varepsilon_0$.

The modern, field-theoretic, point of view is that electromagnetic forces are generated by the exchange of "virtual" photons between charged particles.¹² Quantum field theory is the result of the (conflicting!¹³) marriage between quantum mechanics and special relativity. The interactions between atoms or between molecules are represented as effective forces, for example van der Waals forces (Exercise 14.6.1). These forces are not fundamental because they are derived from the Coulomb force – they are actually the Coulomb force in disguise in the case of complex, electrically neutral systems.

The strong interaction is responsible for the cohesion of the atomic nucleus. In contrast to the Coulomb force, it falls off exponentially with distance according to the law $\simeq (1/r^2) \exp(r/r_0)$ with $r_0 \simeq 1$ F, and therefore is termed a *short-range* force. For $r \lesssim r_0$ this force is very strong, such that the typical energies inside the nucleus are of the order of MeV, while for the outer-shell electrons of an atom they are of the order of eV. In reality, the forces between nucleons are not fundamental, because, as we have seen, nucleons are composite particles. The forces between nucleons are analogous to the van der Waals forces between atoms, and the fundamental forces are actually those between the quarks. However, the quantitative relation between the nucleon–nucleon force and the quark–quark force is far from understood. The gluon, a particle of zero mass and spin 1 like the photon, plays the same role in the strong interaction as the photon plays in the electromagnetic one. The charge is replaced by a property conventionally referred to as color, and the theory of strong interactions is therefore called (*quantum*) chromodynamics. The weak interaction is responsible for radioactive β-decay:

$$(Z, N) \to (Z+1, N-1) + e^- + \overline{\nu}_e.$$
 (1.4)

A special case is that of (1.2), which is written in the notation of (1.4) as

$$(0,1) \rightarrow (1,0) + e^- + \overline{\nu}_e$$
.

Like the strong interaction, the weak interaction is short-range; however, as suggested by its name, it is much weaker than the former. The carriers of the weak interaction are

¹¹ We shall systematically use the notation \hat{r} , \hat{n} , \hat{p} etc. for unit vectors in ordinary space.

¹² The term "virtual photons" will be explained in Section 4.2.4.

¹³ The combination of quantum mechanics and special relativity leads to infinities, which must be controlled by a procedure called renormalization. The latter was not fully understood and justified until the 1970s.

spin-1 bosons: the charged W^{\pm} and the neutral Z^0 with masses 82 MeV c^{-2} and 91 MeV c^{-2} , respectively (about 100 times the proton mass). The leptons, quarks, spin-1 bosons (also referred to as gauge bosons: the photon, gluons, W^{\pm} , and Z^0 ; see Exercise 11.5.11 for some elementary explanations), as well as a hypothetical spin-0 particle called the Higgs boson which gives masses to all the particles, are the particles of the *Standard Model* of particle physics. This model has been tested experimentally with a precision of better than 0.1% over the past ten years.

Last of all, we have the *gravitational interaction* between two masses m and m', which, in contrast to the Coulomb interaction, is always attractive:

$$\vec{F} = -Gmm' \,\frac{\hat{r}}{r^2}.\tag{1.5}$$

Here the notation is the same as in (1.2) and G is the gravitational constant. The force law (1.5) is, like the Coulomb law, a long-range law, and since the two forces have the same form we can form the ratio of these forces between an electron and a proton:

$$\frac{F_{\rm C}}{F_{\rm gr}} = \left(\frac{q_{\rm e}^2}{4\pi\varepsilon_0}\right) \left(\frac{1}{Gm_{\rm e}m_{\rm p}}\right) \sim 10^{39}.$$

In the hydrogen atom the gravitational force is negligible; in general, this force is completely negligible for all the phenomena of atomic, molecular, and solid-state physics. General relativity, the relativistic theory of gravity, predicts the existence of gravitational waves.¹⁴ These are the gravitational analog of electromagnetic waves, and the spin-2, massless graviton is the analog of the photon. Nevertheless, at present there is no quantum theory of gravity. The unification of quantum mechanics and general relativity and the explanation of the origin of mass and the three particle families are major challenges of theoretical physics in the twenty-first century.

Let us summarize our presentation of the elementary constituents and the fundamental forces. There exist three families of matter particles, the leptons and quarks, plus the carriers of the fundamental forces: the photon for the electromagnetic interaction, the gluon for the strong interaction, the W and Z bosons for the weak interaction, and, finally, the hypothetical graviton for the gravitational interaction.

1.2 Classical and quantum physics

Before introducing quantum physics, let us briefly review the fundamentals of classical physics. There are three main branches of classical physics, and each has different ramifications.

¹⁴ At present, there is only indirect, but convincing, evidence for gravitational waves from observations of binary pulsars (neutron stars). Such waves may some day be detected on Earth in the VIRGO, LIGO, and LISA experiments. The graviton will probably be observed only in the very distant future.

1. The first branch is *mechanics*, where the fundamental law is Newton's law. Newton's law is the fundamental law of dynamics; it states that in an inertial frame the force \vec{F} on a point particle of mass *m* is equal to the derivative of its momentum \vec{p} with respect to time:

$$\vec{F} = \frac{\mathrm{d}\vec{p}}{\mathrm{d}t}.$$

This form of the fundamental equation of dynamics remains unchanged when the modifications due to special relativity, introduced by Einstein in 1905, are taken into account. In the general form of (1.6) we must use the relativistic expression for the momentum as a function of the particle velocity \vec{v} and mass *m*:

$$\vec{p} = \frac{m\vec{v}}{\sqrt{1 - v^2/c^2}}.$$
(1.7)

2. The second branch is *electromagnetism*, summarized in the four Maxwell equations which give the electric field \vec{E} and magnetic field \vec{B} as functions of the charge density ρ_{em} and the current density \vec{j}_{em} , which are referred to as the *sources* of the electromagnetic field:

$$\vec{\nabla} \cdot \vec{B} = 0, \qquad \vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t},$$
(1.8)

$$\vec{\nabla} \cdot \vec{E} = \frac{\rho_{\rm em}}{\varepsilon_0}, \quad c^2 \vec{\nabla} \times \vec{B} = \frac{\partial \vec{E}}{\partial t} + \frac{1}{\varepsilon_0} \vec{J}_{\rm em}.$$
 (1.9)

These equations lead to a description of the propagation of electromagnetic waves in a vacuum at the speed of light:

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right) \begin{cases} \vec{E} \\ \vec{B} \end{cases} = 0.$$
(1.10)

Maxwell's equations allow us to make the connection to optics, which becomes a special case of electromagnetism. The connection between mechanics and electromagnetism is supplied by the *Lorentz law* giving the force on a particle of charge q and velocity \vec{v} :

$$\vec{F} = q(\vec{E} + \vec{v} \times \vec{B}). \tag{1.11}$$

3. The third branch is *thermodynamics*, in which the main consequences are derived from the second law:¹⁵ there exists no transformation whose sole effect is to extract a quantity of heat from a reservoir and convert it entirely to work. This second law leads to the concept of entropy which lies at the base of all of classical thermodynamics. The microscopic origin of the second law was understood at the end of the nineteenth century by Boltzmann and Gibbs, who were able to relate this law to the fact that a macroscopic sample of matter is made up of an enormous ($\sim 10^{23}$) number of atoms; this allows us to use probability arguments, on which statistical mechanics is founded. The principal result of statistical mechanics is the *Boltzmann law*: the

¹⁵ The first law is just energy conservation, while the third is fundamentally of quantum origin.

probability p(E) for a physical system in equilibrium at absolute temperature *T* to have energy *E* includes a factor called the *Boltzmann weight* $p_B(E)$:¹⁶

$$\mathsf{p}_{\mathrm{B}}(E) = \exp\left(-\frac{E}{k_{\mathrm{B}}T}\right) = \exp(-\beta E), \qquad (1.12)$$

where $k_{\rm B}$ is the Boltzmann constant (the gas constant *R* divided by Avogadro's number), and we have introduced the usual notation $\beta = 1/k_{\rm B}T$. However, classical statistical mechanics is not in fact a consistent theory, and it is sometimes necessary to resort to questionable arguments to obtain a sensible result, for example in computing the entropy of a perfect gas. Quantum physics removes all these difficulties.

4. To be completely rigorous, we should mention a fourth branch of classical physics: the relativistic theory of gravity, which in effect is not included in the three branches listed above. This theory is called *general relativity*, and is a geometrical description in which gravitational forces arise from the curvature of spacetime.

Equations (1.6)–(1.11) represent the fundamental laws of classical physics, which can be summarized in only seven equations! The reader may wonder what happened to all the other familiar laws of physics such as Ohm's law, Hooke's law, the laws of fluid dynamics, etc. Some of these laws are derived directly from the fundamental ones; for example, Coulomb's law is a consequence of the Maxwell equations and the Lorentz force (1.11) for static charges, and the Euler equation for a perfect fluid is a consequence of the fundamental law of dynamics. Many other laws are *phenomenological*.¹⁷ They are not universally valid, in contrast to the fundamental laws. For example, some media do not obey Ohm's law; the relation between the induction \vec{D} and the electric field $\vec{D} = \varepsilon \vec{E}$ (for an isotropic medium) does not hold when the electric field becomes strong, giving rise to the phenomena of nonlinear optics. Hooke's law does not apply if the tension becomes too large, and so on. The mechanics of solids, elasticity and fluid mechanics follow from (1.6) and various phenomenological laws like the law that relates the force, velocity gradient, and viscosity in fluid mechanics. It is important to clearly distinguish between the small number of fundamental laws and the large number of phenomenological laws which, for lack of anything better, are used in classical physics to describe matter.

Although there is no doubt that classical physics is useful, it does possess a serious shortcoming: although physics claims to be a theory of matter, classical physics is completely incapable of *explaining* the behavior of matter given its constituents and the forces between them.¹⁸ It cannot predict the existence of atoms, because it is not possible to construct a length scale using the constants of classical physics: the masses and charges

¹⁶ The probability p(E) is the product of $p_B(E)$ (1.12) and the factor $\mathcal{D}(E)$, the "energy-level density," which in classical physics is obtained by integrating over phase space; see Footnote 21. The quantum calculation of the level density is described in Section 9.6.2.

¹⁷ Quite often a phenomenological law is nothing but the first term of a Taylor series.

¹⁸ This statement should be qualified slightly. There do exist good microscopic models in classical physics: for example, the kinetic theory of gases permits reliable calculation of the transport coefficients (viscosity, thermal conductivity) of a gas. However, neither the existence of the molecules making up the gas nor the value of the effective cross section needed in the calculation can be explained by classical physics.

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of the nucleus and electrons.¹⁹ It cannot explain why the Sun shines or why sodium vapor emits yellow light, and it has nothing to say about the chemical properties of the alkalines, about the fact that copper conducts electricity while sulfur is an insulator, and so on. When the classical physicist needs a property of a material such as an electrical resistance or a specific heat, he or she has no choice but to measure it experimentally. In contrast, quantum mechanics attempts to explain the behavior of matter starting from the constituents and forces. Naturally, it is not possible to make precise predictions based on first principles except for the simplest systems, like the hydrogen or helium atoms. The complexity of the calculations does not allow, for example, prediction of the crystal structure of silver based on the data for this atom, but given the crystal structure it can explain why silver is a conductor, which classical physics is incapable of doing.

It should not be concluded from this discussion that classical physics can no longer be interesting and innovative. On the contrary, during the past twenty years classical physics has taken on new life with the development of new ideas about chaotic dynamical systems, instabilities, nonequilibrium phenomena, and so on. Moreover, such familiar problems as turbulence and friction remain poorly understood and extremely interesting. There simply exist problems that by their nature are not *suitable* for study using classical physics.

Quantum physics aspires to explain the behavior of matter on the basis of its constituents and forces, but there is a price to pay: quantum objects display radically new behavior which defies our intuition developed from the behavior of classical objects. That said, quantum mechanics proves to be a remarkable tool which so far has always given correct results and is capable of coping with problems ranging from quark physics to cosmology and all scales in between. Without quantum mechanics, most of modern technology would never have seen the light of day. All of information technology is based on our quantum understanding of solids and, in particular, semiconductors. The miniaturization of electronic devices will make quantum mechanics more and more omnipresent in modern technology.

The vast majority of physicists do not worry about the puzzling aspects of quantum mechanics, but simply use it as a tool without asking questions of principle. Nevertheless, the theoretical and, especially, experimental progress made over the past twenty years have led to a better grasp of certain aspects of the behavior of quantum objects. Although things are still far from clear, we shall see in Chapter 6 and Appendix B that we are certainly on the path to a more satisfactory understanding of quantum mechanics. Perhaps in a few years Feynman's statement, "I think it can be stated today that no one understands quantum mechanics," will become obsolete. Before discussing the recent developments, let us go back a few years to the beginning of quantum physics.

$$r_{\rm e} = \frac{q_{\rm e}^2}{4\pi\varepsilon_0} \frac{1}{m_{\rm e}c^2} \simeq 2.8 \times 10^{-15} \,{\rm m}.$$

but it is four orders of magnitude too small to be related to atomic dimensions. Another way of saying all this is to invoke the scale invariance of the classical equations; cf. Wichman [1967], Chapter 1.

¹⁹ If we include the speed of light, we can construct a length scale, the *classical electron radius*

1.3 A bit of history

1.3.1 Black-body radiation

A hot object such as a red-hot iron or the Sun emits electromagnetic radiation with a frequency spectrum that depends on temperature. The power emitted $u(\omega, T)$ per unit frequency ω and unit area depends on the absolute temperature T of the object. Purely thermodynamical arguments can be made to show that if the object is perfectly absorbing, that is, if it is a *black body*, then $u(\omega, T)$ is a universal function independent of the object at a given temperature. An excellent realization of a black body for visible light is a small opening in a cavity whose interior is painted black. A light ray which enters the cavity has practically no chance of getting out, because at each reflection there is a high probability of being absorbed by the inner wall of the cavity (Fig. 1.4).

Let us suppose that the cavity is heated to a temperature T. The atoms of the inner wall emit and absorb electromagnetic radiation, and a system of standing waves in thermodynamical equilibrium is established in the cavity. If the cavity is a parallelepiped of sides L_x , L_y , and L_z and we use periodic boundary conditions, the electric field will have the form $\vec{E}_0 \exp[i(\vec{k} \cdot \vec{r} - \omega t)]$, with the wave vector \vec{k} perpendicular to \vec{E}_0 and of the form

$$\vec{k} = \left(\frac{2\pi}{L_x}n_x, \ \frac{2\pi}{L_y}n_y, \ \frac{2\pi}{L_z}n_z\right),\tag{1.13}$$

where (n_x, n_y, n_z) are positive or negative integers and $\omega = c|\vec{k}| = ck$. It can be shown that each standing wave behaves like a harmonic oscillator²⁰ of frequency ω with energy proportional to the squared amplitude \vec{E}_0^2 . According to the Boltzmann law (1.12), the probability that this oscillator has energy *E* involves the factor



Fig. 1.4. Cavity for black-body radiation.

²⁰ This will be explained in Section 11.3.3.

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 $\exp(-E/k_{\rm B}T) = \exp(-\beta E)$. In fact, in this case the level density $\mathcal{D}(E)$ (cf. Footnote 16) is a constant,²¹ and the average energy of this oscillator is simply

$$\langle E \rangle = \frac{\int dE \, E \exp(-\beta E)}{\int dE \, \exp(-\beta E)} = -\frac{\partial}{\partial \beta} \ln \left(\int dE \, \exp(-\beta E) \right)$$
$$= -\frac{\partial}{\partial \beta} \ln \frac{1}{\beta} = \frac{1}{\beta} = k_{\rm B} T.$$
(1.14)

The average energy of each standing wave is $k_{\rm B}T$. Since there are an infinite number of possible standing waves, the energy inside the cavity is infinite!

The emitted power $u(\omega, T)$ has a simple relation to the energy density $\epsilon(\omega, T)$ per unit frequency in the cavity (Exercise 1.6.2):

$$u(\omega, T) = \frac{c}{4} \epsilon(\omega, T), \qquad (1.15)$$

so that we need to compute $\epsilon(\omega, T)$, from which we obtain the energy density:

$$\boldsymbol{\epsilon}(T) = \int_0^\infty \mathrm{d}\omega \,\boldsymbol{\epsilon}(\omega, T). \tag{1.16}$$

Thermodynamics gives the scaling law

$$\epsilon(\omega, T) = \omega^3 \varphi\left(\frac{\omega}{T}\right),$$
 (1.17)

but tells us nothing about the explicit form of the function φ except that it is independent of the shape of the cavity. Let us try to find it up to a multiplicative factor by means of dimensional analysis. A priori, $\epsilon(\omega, T)$ can only depend on ω , c, the energy $k_{\rm B}T$, and a dimensionless constant A which cannot be fixed by dimensional analysis. The only possible solution is (Exercise 1.6.2)

$$\epsilon(\omega, T) = Ac^{-3}(k_{\rm B}T)\omega^2 = \omega^3 \left[Ac^{-3}\left(\frac{k_{\rm B}T}{\omega}\right)\right],\tag{1.18}$$

which has the form (1.17). We rediscover the fact that the energy density in the cavity is infinite:

$$\epsilon(T) = \int_0^\infty \mathrm{d}\omega \,\epsilon(\omega, T) = Ac^{-3}(k_{\rm B}T) \int_0^\infty \omega^2 \mathrm{d}\omega = +\infty.$$

The constant A can be calculated in statistical mechanics (Exercise 1.6.2), but this does not resolve the problem of the infinite energy, and the dimensional analysis strongly suggests that black-body radiation cannot be explained unless a new physical constant is introduced.

$$\int \mathrm{d}x\mathrm{d}p\,\delta\left(E-\frac{p^2}{2m}-\frac{1}{2}\,m\omega^2x^2\right)f(E)=\frac{2\pi}{\omega}\,f(E),$$

where x and p are the position and momentum, and δ is a Dirac delta function.

²¹ The integration over phase space for a one-dimensional harmonic oscillator gives, for an arbitrary function f(E) (Exercise 1.6.2),

Out of all the hypotheses that could lead to the unacceptable result of infinite energy, Planck chose the one on which the calculation (1.14) of the average oscillator energy is based.²² Instead of allowing *E* to take all possible values between zero and infinity, he assumed that it can take only discrete values E_n which are integer multiples of the oscillator frequency ω with proportionality coefficient \hbar :

$$E_n = n(\hbar\omega), \quad n = 0, 1, 2, \dots$$
 (1.19)

The constant \hbar is called *Planck's constant*; more precisely, it is Planck's constant *h* divided by 2π : $\hbar = h/2\pi$.²³ Planck's constant is measured in joule seconds (J s), and it has dimensions $\mathcal{ML}^2\mathcal{T}^{-1}$ and numerical value

$$\hbar \approx 1.054 \times 10^{-34} \,\text{J s}$$
 or $h \approx 6.63 \times 10^{-34} \,\text{J s}$.

According to the Boltzmann law, the normalized probability of observing an energy E_n is

$$\mathsf{p}(E_n) = \mathrm{e}^{-\beta n \hbar \omega} \left(\sum_{n=0}^{\infty} \mathrm{e}^{-\beta n \hbar \omega} \right)^{-1} = \exp(-\beta n \hbar \omega) [1 - \exp(-\beta \hbar \omega)].$$
(1.20)

In obtaining (1.20) we have used the fact that the summation over *n* is that of a geometrical series. Setting $x = \exp(-\beta\hbar\omega)$, we easily find the average oscillator energy $\langle E \rangle$:

$$\langle E \rangle = (1-x) \sum_{n=0}^{\infty} (n\hbar\omega) x^n = (1-x)\hbar\omega x \frac{\mathrm{d}}{\mathrm{d}x} \sum_{n=0}^{\infty} x^n$$
$$= (1-x)\hbar\omega x \frac{\mathrm{d}}{\mathrm{d}x} \frac{1}{1-x} = \frac{\hbar\omega x}{1-x} = \frac{\hbar\omega}{\exp(\beta\hbar\omega) - 1}.$$
(1.21)

This expression can be used to calculate the energy density (Exercise 1.6.2)

$$\boldsymbol{\epsilon}(\boldsymbol{\omega},T) = \frac{\hbar}{\pi^2 c^3} \frac{\boldsymbol{\omega}^3}{\exp(\beta\hbar\omega) - 1}$$
(1.22)

and then $u(\omega, T)$, in perfect agreement with experiment for a suitably chosen value of \hbar and with the result (1.17) of thermodynamics. We note that the classical approximation (1.18) is valid if $k_{\rm B}T \gg \hbar \omega$, that is, for low frequencies.

The best-known example of black-body radiation is the relic 3 K background radiation filling the Universe, also called the cosmic microwave background (CMB).²⁴ The frequency distribution of this radiation is in remarkable agreement with the Planck

²² In reality, Planck applied his arguments to a "resonator," the nature of which remains obscure, and the present argument follows that of Einstein (1905). Dealing with electromagnetic field oscillations is simpler and more direct, but it does distort the historical truth. Our "historical" presentation, like that of many textbooks, is more reminiscent of a fairy tale (H. Kragh, Max Planck: the reluctant revolutionary, *Physics World* **13** (12), 31 (December 2000)) than actual history. Likewise, it does not appear that the physicists of the late nineteenth century were troubled by the infinite energy or the absence of a fundamental constant.

²³ We shall systematically use \hbar rather than h, and somewhat carelessly refer to \hbar as Planck's constant; the relation $E = \hbar \omega$ is of course the same as $E = h\nu$, where ν is the ordinary frequency measured in hertz and ω is the angular or rotational frequency measured in rad s⁻¹: $\omega = 2\pi\nu$. Since we nearly always use ω rather than ν , we shall just refer to ω as the frequency.

²⁴ A particularly good account of the Big Bang is given by S. Weinberg in, *The First Three Minutes: A Modern View of the Origin of the Universe*, New York: Basic Books (1977).



Fig. 1.5. The 3 K black-body radiation. On the vertical axis is the radiation intensity in W m⁻² sr⁻¹ Hz⁻¹. The remarkable agreement with Planck's law for T = 2.73 K is clearly seen. Taken from J. Rich, *Fundamentals of Cosmology*, New York: Springer (2001).

law (1.22) for the temperature 2.73 K \approx 3 K (Fig. 1.5), but this radiation is no longer in thermodynamical equilibrium. It was decoupled from matter about 380 000 years after the Big Bang, that is, after the birth of the Universe. At the instant of decoupling the temperature was about 10⁴ K. The subsequent expansion of the Universe has reduced this value to the present one of 3 K. Deviations from a fully isotropic black-body radiation, of the order of 10⁻³, arise from the motion of the Solar System with respect to the cosmic microwave background, owing to the Doppler effect. There are also angular dependent temperature fluctuations, ~10⁻⁵, which are much more interesting as they give us important information on the early history of the Universe.

1.3.2 The photoelectric effect

The integer *n* in (1.19) has a particularly important physical interpretation: the reason that the energy of a standing wave of frequency ω is an integer multiple $n\hbar\omega$ of $\hbar\omega$ is that it corresponds to precisely *n photons* (or "particles of light") of energy $\hbar\omega$. It is this interpretation that led Einstein to introduce the concept of photon in order to explain the photoelectric effect. When a metal is illuminated by electromagnetic radiation, some electrons escape from it and there is a threshold effect that depends on the frequency



Fig. 1.6. The Millikan experiment. (a) Schematic view of the experiment. (b) $|V_0|$ as a function of ω .

and not the intensity of the radiation. The Millikan experiment (Fig. 1.6) confirms the Einstein interpretation: the electrons emitted from the metal have kinetic energy E_k

$$E_{\rm k} = \hbar \omega - W, \tag{1.23}$$

where W is the work function. An electron of charge q_e does not reach the cathode if $|q_e V| > E_k$. If V_0 is the potential at which the current vanishes, then

$$|V_0| = \frac{\hbar}{|q_e|} \,\omega - \frac{W}{|q_e|}.$$
(1.24)

The potential $|V_0|$ as a function of ω has a constant slope $\hbar/|q_e|$, and the value of \hbar coincides with that for black-body radiation, thus confirming the Einstein hypothesis²⁵ that electromagnetic radiation is composed of photons.²⁶ The fact that the value of \hbar is the same as in the case of black-body radiation strongly suggests that one must introduce a new fundamental constant.

1.4 Waves and particles: interference

1.4.1 The de Broglie hypothesis

From Eq. (1.19) for n = 1 we find $E = \hbar \omega$, the *Planck–Einstein relation* between the energy and frequency of a photon. The photon possesses momentum

$$p = \frac{E}{c} = \frac{\hbar\omega}{c},$$

²⁵ Another rewriting of history! Some qualitative results on the photoelectric effect were obtained by Lenard in the early 1900s, but the precise measurements of Millikan were made 10 years after the Einstein hypothesis. Einstein seems to have been motivated not by the photoelectric effect, but by thermodynamic considerations. See G. Margaritondo, *Physics World* 14(4), 17 (April 2001).

²⁶ The argument is not completely convincing, because the photoelectric effect can be explained within the framework of a semiclassical theory, where the electromagnetic field is not quantized and where there is no concept of photon; cf. Section 14.3.3. However, it is not possible to explain the photoelectric effect without introducing \hbar . The fact that a photomultiplier whose operation is based on the photoelectric effect registers isolated counts can be attributed to the quantum nature of the device rather than the arrival of isolated photons.

but using $\omega = ck$ and the fact that the momentum and wave vector point in the same direction we obtain the following vector relation between the latter:

$$\vec{p} = \hbar \vec{k} \quad . \tag{1.25}$$

This equation can also be written as a relation (this time, scalar) between the momentum and wavelength λ :

$$p = \frac{h}{\lambda} \quad . \tag{1.26}$$

The de Broglie hypothesis is that the relations (1.25) and (1.26) are valid for all particles. According to this hypothesis, a particle of momentum \vec{p} possesses wave properties characterized by the de Broglie wavelength $\lambda = h/p$. If $v \ll c$ we can use $\vec{p} = m\vec{v}$, while otherwise we use the general expression (1.7), except for m = 0, when p = E/c. If this hypothesis is correct, particles must have observable wave properties; in particular, they must undergo interference and diffraction.

1.4.2 Diffraction and interference of cold neutrons

Since the 1980s, modern experimental techniques have allowed interference and diffraction of particles to be verified in experiments based on simple principles and admitting direct interpretation. Such experiments have been performed using photons, electrons, atoms, molecules, and neutrons. Here we have chosen, a bit arbitrarily, to discuss neutron experiments, as they are particularly elegant and clear. Neutron diffraction by crystals has been around for fifty years now and is a classic experiment (Exercise 1.6.4), but modern experiments are carried out using macroscopic devices with slits that can be viewed by the naked eye, rather than a crystal lattice with a spacing of a few angstroms.

The experiments were performed in the 1980s by a group in Innsbruck using the research nuclear reactor of the Laue-Langevin Institute in Grenoble. Neutrons of mass m_n are produced in the fission of uranium-235 in the reactor core, and then channeled to the experiments. The order of magnitude of their kinetic energy is $k_B T$, where $T \approx 300$ K is the ambient temperature. Such neutrons are termed thermal and have kinetic energy $\sim k_B T \approx 1/40 \text{ eV}$ for T = 300 K. The momentum $p = \sqrt{2m_nk_BT}$ corresponds to a speed $v = p/m_n$ of about 1000 m s⁻¹, and according to (1.26) the associated wavelength λ_{th} is $h/\sqrt{2m_nk_BT} \approx 1.8$ Å. The wavelength is increased when the neutrons are made to pass through a low-temperature material. For example, if the temperature of the material is 1 K, the wavelength will increase to $\lambda = \lambda_{\text{th}}\sqrt{300} \approx 31$ Å. Such neutrons are termed "cold." In the experiments of the Innsbruck group, the neutrons were cooled to 25 K using liquid deuterium.²⁷ This produced neutrons with an average wavelength of about 20 Å.

²⁷ Deuterium was chosen over hydrogen, as the latter inconveniently absorbs neutrons in the reaction $n + p \rightarrow {}^{2}H + \gamma$ (see Exercise 14.6.8). This is why in a nuclear reactor heavy water is a better moderator than ordinary water.



Fig. 1.7. Experimental setup for neutron diffraction and interference: S_1 and S_2 are collimating slits, S_3 is the entrance slit, S_4 is the object slit, and S_5 is the slit at the location of the counter *C*. From A. Zeilinger *et al.*, *Rev. Mod. Phys.* **60**, 1067 (1988).

The experimental setup is shown schematically in Fig. 1.7. The neutrons are detected by means of BF_3 counters, in which the boron absorbs neutrons in the reaction

$$^{10}\text{B} + \text{n} \rightarrow {}^{7}\text{Li} + {}^{4}\text{He}$$

with an efficiency of nearly 100%. The counter is placed behind the screen at S_5 , and counts the number of neutrons arriving in the neighborhood of S_5 .

In the diffraction experiment the slit S_4 has a width of $a = 93 \,\mu\text{m}$, which leads to a diffraction maximum of angular size

$$\theta = \frac{\lambda}{a} \approx 2 \times 10^{-5}$$
 rad.

On the screen located D = 5 m from the slit the linear size of the diffraction peak is of order 100 µm. It is possible to calculate the diffraction pattern precisely, taking into account, for example, the spread of wavelengths about the average value of 20 Å. The theoretical result is in excellent agreement with experiment (Fig. 1.8).

In the interference experiment, two 21- μ m slits have their centers separated by a distance $d = 125 \mu$ m. The separation between fringes on the screen is

$$i = \frac{\lambda D}{d} = 80 \,\mu \mathrm{m}.$$

The slits are visible with the naked eye, and the interference pattern is macroscopic. Again, the theoretical calculation taking into account the various parameters of the experiment is in excellent agreement with the experimental interference pattern (Fig. 1.9).

However, there is a crucial difference from an experiment on optical interference: the interference pattern is made up of impacts of isolated neutrons and it is reconstructed afterwards, when the experiment is completed. Actually, the counter is moved along the screen (or an array of identical counters covers the screen), and the neutrons arriving in the neighborhood of each point of the screen are recorded during identical time intervals. Let $N(x)\Delta x$ be the number of neutrons detected per second in the interval



Fig. 1.8. Neutron diffraction by a slit. The full line is the theoretical prediction. From A. Zeilinger *et al.*, *Rev. Mod. Phys.* **60**, 1067 (1988).



Position of the slit S_5

Fig. 1.9. Young's slit experiment using neutrons. The full line is the theoretical prediction. From A. Zeilinger *et al.*, *Rev. Mod. Phys.* **60**, 1067 (1988).

 $[x - \Delta x/2, x + \Delta x/2]$, where x is the abscissa of a point on the screen. The intensity $\mathcal{I}(x)$ can be defined as being equal to N(x), and the number of neutrons arriving in the neighborhood of a point of the screen is proportional to the intensity $\mathcal{I}(x)$ of the interference pattern, with statistical fluctuations of order \sqrt{N} about the average value. The isolated impacts are illustrated in Fig. 1.10 for an experiment performed using not neutrons, but cold atoms (see Section 14.4) which were allowed to fall through Young slits. The impacts of the atoms that hit the screen were recorded, giving the pattern in Fig. 1.10.



Fig. 1.10. Interference using cold atoms. From Basdevant and Dalibard [2002].

1.4.3 Interpretation of the experiments

In addition to cold neutrons and atoms, other types of particle have been used in diffraction and interference experiments:

- photons, with the light intensity reduced such that the photons arrive at the screen one by one. Nevertheless, an experiment performed under these conditions is not entirely convincing, because it can be explained semiclassically taking into account the quantum nature of the detector; see Footnote 26. However, it is now known how to construct sources that provide truly isolated photons, and experiments using such photons unarguably demonstrate interference produced by one photon at a time²⁸
- electrons
- light molecules (Na₂)
- fullerenes C₆₀ (Exercise 1.6.1).

There is every reason to assume that the results are universal, independent of the type of particle – atoms, molecules, virus particles, etc.²⁹ However, a difficulty of principle seems to arise in interpreting these experimental results. In a classical Young's slit interference experiment realized using waves, the incident wave is split into two waves which recombine and interfere, a phenomenon which is visible to the naked eye in, for example, the case of waves on the surface of water. In the case of neutrons, each neutron arrives separately, and the interval between the arrivals of two successive neutrons is such that when a neutron is detected on the screen, the next one is still in the reactor confined inside a uranium atom. Can we imagine that a neutron is split in two, with each half passing through a slit? It is easy to convince ourselves that this hypothesis is absurd: a counter always detects an entire neutron, never a fraction of one. The same situation occurs if a semi-transparent mirror is used to split a light wave of intensity

²⁸ A. Aspect, P. Grangier, and G. Roger, Dualité onde-corpuscule pour un photon unique, J. Optics (Paris) 20, 119 (1989).

²⁹ However, wave effects become more and more difficult to observe for larger particles, in practice because the wavelength becomes shorter and shorter, and more fundamentally because decoherence effects (Section 15.4.5) become more and more important as an object becomes larger. See M. Arndt, K. Hornberger, and A. Zeilinger, Probing the limits of quantum worlds, *Physics World* **18** (3), 35 (2005).



Fig. 1.11. Beam-splitting plate and photon counting by photodetectors D_1 and D_2 .

reduced enough to permit the detection of individual photons. The photodetectors D_1 and D_2 always detect an entire photon, never a fraction of one (Fig. 1.11). The photon, like the neutron, is indivisible, at least in a vacuum (though by interaction with a nonlinear medium a photon can be split into two of lower energy; see Section 6.3.2).

We therefore must assume that a quantum particle possesses wave and particle properties *simultaneously*. It is an entirely new and strange object, at least to our intuition based on experience with macroscopic objects. As Lévy-Leblond and Balibar, paraphrasing Feynman, have written, "quantum objects are completely crazy." However, they add "at least they are all crazy in the same way." Photons, electrons, neutrons, atoms, molecules – all behave the same way, like waves and particles at the same time. In order to emphasize this unity of quantum behavior, some authors have proposed the term "quanton" to refer to such an object. Here we shall continue to use "quantum particle" or simply "particle," because the particles we shall consider in this book generally display quantum behavior. We will specify "classical particle" when we need to refer to particles that behave like little billiard balls.

If the neutron is indivisible, is it possible to know which slit it has passed through? If one slit is closed, we observe on the screen the diffraction pattern corresponding to the other slit and vice versa. If the experimental situation is such that it is possible to tell which slit the neutron has passed through, then we observe on the screen the superposition of the *intensities* of the diffraction patterns of each slit: the neutrons can effectively be divided into two groups, those that passed through the upper slit and for which the lower slit could have been closed without changing the result, and those that passed through the lower slit. We observe an interference pattern only if the experimental apparatus is such that we cannot know, *even in principle*, which slit a neutron has passed through. Summarizing:

- (i) If the experimental apparatus does not permit knowledge of which slit a neutron passed through, an interference pattern is observed.
- (ii) If the apparatus permits us in principle to determine which of the two slits a neutron passed through, the interference will be destroyed independently of whether we actually bother to determine which slit it was.

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A fundamental point to note is that we cannot know a priori at which point of the screen a given neutron will arrive. We can only state that the *probability* of arriving at the screen is large at a point of an interference maximum and small at a point of an interference minimum. More precisely, the probability of arriving at an abscissa x is proportional to the intensity $\mathcal{I}(x)$ of the interference pattern at this point. Likewise, in the experiment of Fig. 1.11 each photomultiplier has a probability of 1/2 of being triggered by a given photon, but it is impossible to know in advance which of the two detectors will be triggered.

Let us try to make the preceding discussion quantitative. First of all, by analogy with waves, we shall introduce a complex function of x, $a_1(x)$ $[a_2(x)]$, associated with the passage through the upper slit [lower slit] of a neutron that reaches a point x on the screen. For reasons to be explained below, this function will be called the probability amplitude. The squared modulus of the probability amplitude gives the intensity: if slit 2 is closed $\mathcal{I}_1(x) = |a_1(x)|^2$, and, conversely, if slit 1 is closed $\mathcal{I}_2(x) = |a_2(x)|^2$. In case (i) above we add the *amplitudes* before calculating the intensity:

$$\mathcal{I}(x) \propto |a_1(x) + a_2(x)|^2,$$
 (1.27)

while in case (ii) we add the *intensities*

$$\mathcal{I}(x) \propto |a_1(x)|^2 + |a_2(x)|^2 = \mathcal{I}_1(x) + \mathcal{I}_2(x).$$
(1.28)

As above, the intensity can be defined as the number of neutrons arriving per second per unit length of the screen. To take into account the probabilistic nature of the neutron point of impact, the amplitudes a_1 and a_2 will not be wave amplitudes measuring the amplitude of a vibration, but *probability amplitudes*, with the squared modulus being the probability of arriving at a point x on the screen. The concept of probability amplitude in quantum physics will be developed and given mathematical status in Chapter 3.

A more general statement of (1.27) and (1.28) is the following. Let us suppose that starting from an initial state *i* we arrive at a final state *f*. To find the probability $p_{i \to f}$ of observing the final state *f*, we must add all the amplitudes that lead to the result *f* starting from *i*:

$$a_{i \to f} = a_{i \to f}^{(1)} + a_{i \to f}^{(2)} + \dots + a_{i \to f}^{(n)}$$

and then $p_{i \to f} = |a_{i \to f}|^2$. It should be understood that the states *i* and *f* are specified uniquely by the parameters that define the initial and final states of the full ensemble of the experimental apparatus. If, for example, we desire information about the passage of a neutron through a given slit, we can obtain it by integrating the Young's slits into a larger apparatus. Then the final state of this larger apparatus, which will be a function of other parameters in addition to the neutron point of impact, is capable of informing us whether the neutron has passed through the given slit. Just what is the final state of this larger apparatus will depend on which slit the neutron passed through.

In summary, we must sum the amplitudes for identical final states and the probabilities for different final states, even if these final states differ only by physical parameters other than those of interest. It is sufficient that these other parameters be accessible in principle, even if they are not actually observed, for us to consider the final states as being different. We shall illustrate this point by a concrete example in the following paragraph. Another way of saying this which is easier to visualize is the following: identical final states are associated with *indistinguishable paths*, and it is necessary to sum the amplitudes corresponding to all indistinguishable paths.

1.4.4 Heisenberg inequalities I

Let us return to the neutron diffraction experiment in order to extract from it a fundamental relation called the *Heisenberg inequality*, or, more commonly but ambiguously, the *Heisenberg uncertainty principle*. If the slit width is *a* and if we orient the *x* axis along the slit, perpendicular to the direction through the slit, the neutron position relative to this axis immediately on leaving the slit is known to within $\Delta x = a$. Because the angular width of the diffraction maximum is $\sim \lambda/\Delta x$, the *x* component of the neutron momentum is $\Delta p_x \approx (\lambda/\Delta x)p = h\Delta p_x$, where *p* is the neutron momentum (we assume that $p \gg \Delta p_x$). We then obtain the relation

$$\Delta p_x \Delta x \sim h. \tag{1.29}$$

In Chapter 9 we shall discuss a more accurate version of Eq. (1.29) involving the standard deviations, which we shall call simply the dispersions, of momentum and position Δp_i and Δx_i for identical values of i = x, y, z:

$$\Delta p_i \Delta x_i \ge \frac{1}{2} \hbar. \tag{1.30}$$

There are no inequalities relating different components of momentum and position, for example Δp_x and Δy . When interpreting a diffraction experiment it is often said that the passage of a neutron through a slit of width Δx allows the neutron's *x* coordinate to be measured with a precision Δx , and that this measurement perturbs the neutron's momentum by an amount $\Delta p_x \approx h/\Delta x$. We shall see in Section 4.2.4 that the inequalities (1.30) in fact have nothing to do with the experimental measurement of position or momentum, but instead arise from the mathematical description of a quantum particle as a wave packet, and we shall also elaborate on the precise meaning of these relations.

We are now going to use (1.29) to discuss the question of observing trajectories in a neutron interference experiment. Einstein proposed the apparatus of Fig. 1.12 for determining the neutron trajectory, i.e., for determining whether the neutron passes through the upper or the lower slit. When the neutron passes through the first slit S_0 , owing to momentum conservation it transfers a downward momentum to the screen E_0 if it passes through the upper slit S_1 and an upward momentum to the screen if it passes through the lower slit S_2 . It is then possible to determine which slit the neutron has passed through. Bohr's response was the following. If the screen E_0 receives a momentum δp_x which can be measured, this means that the *initial* momentum Δp_x of the screen was much less than δp_x , and the initial position is determined with an uncertainty at least of order



Fig. 1.12. The Bohr–Einstein controversy. Slits S_1 and S_2 are Young's slits. Slit S_0 is located in a screen which can move vertically.

 $h/\Delta p_x$. Such an inaccuracy in the position of the source is sufficient to make the interference pattern disappear (Exercise 1.6.3). All the various types of apparatus that can be imagined for determining the neutron trajectory are either efficient, in which case there is no interference pattern, or inefficient, in which case there is an interference pattern, but the slit through which the neutron has passed cannot be known. The interference pattern becomes more and more fuzzy as the apparatus becomes more and more efficient.

The above discussion is completely correct, but one should not conclude that it is the perturbation of the neutron trajectory on hitting the first screen that spoils the interference pattern.³⁰ The crucial point is the possibility of tagging the trajectory. It is possible to imagine and even experimentally construct an apparatus that tags trajectories without disturbing the observed degrees of freedom at all, and yet this tagging is sufficient to destroy the interference pattern. Let us briefly describe an apparatus which has not yet been realized experimentally, but may become feasible when technology has evolved further. Other types of apparatus that tag trajectories without perturbing them have been *effectively* realized and are discussed in Exercise 3.3.9, Section 6.3.2, and Appendix B. However, the principle governing such devices is based on ideas which we have not yet introduced, and so for now we shall return to the familiar example of Young's slits. The proposed

³⁰ The same remark applies to the apparatus imagined by Feynman for a Young's slit experiment using electrons (Feynman *et al.* [1965], Vol. III, Chapter 1). A photon source placed behind the slits makes it possible in theory to observe the electron passage. When short-wavelength photons are used the electron-photon collisions permit the two slits to be distinguished, but the collisions perturb the trajectories enough to spoil the interference pattern. If the photon wavelength is increased, the impacts are less violent, but the resolving power of the photons decreases. The interference fringes reappear when the resolution becomes such that it is no longer possible to distinguish between the slits.

apparatus uses atoms,³¹ so that it is possible to play with their internal degrees of freedom without affecting the trajectory of their center of mass. Before passing through the slits, the atoms are raised to an excited state by a laser beam (Fig. 1.13). Behind each slit is a superconducting microwave cavity, described in more detail in Section 6.4.1 and Appendix B. In passing through the cavity the atom returns to its ground state and with nearly 100% probability emits a photon which remains confined in the cavity. The presence of a photon in one or the other cavity allows the atom's trajectory to be tagged, which destroys the interference pattern. The perturbation to the trajectory of the atom's center of mass is completely negligible: there is practically no momentum transfer between the photon and the atom. However, the two final states – the atom arriving at abscissa x on the screen and a photon in cavity 1, and the atom arriving at x on the screen and a photon in cavity 2 -are different. It is therefore necessary to take the squared modulus of each of the corresponding amplitudes and add the probabilities. We note that it is not necessary to detect the photon, a requirement which moreover would introduce an additional experimental complication. It is sufficient to know that the atom has emitted a photon in a quasi-certain way in its passage through the cavity. As we have already emphasized, it is not at all necessary that the final state is effectively observed, it is only necessary that it can be observed in principle, even if the present or future state of technology does not permit such observation. In the terminology to be defined in Chapters 6 and 15, we can say that interference is destroyed if "which path" information is encoded in the environment. We shall return to this subject in Appendix B.1, where we will discuss it in a mathematical context.



Fig. 1.13. Tagging of trajectories in Young's slit experiments. Taken from B. Englert, M. Scully, and H. Walther, Origin of quantum mechanical complementarity probed by a "which way" experiment in an atom interferometer. *Nature* **351**, 111 (1991).

³¹ This has been imagined by B. Englert, M. Scully, and H. Walther, Quantum optical tests of complementarity, *Nature* 351, 111 (1991), and they present a popularized description of it in *Scientific American* 271, 86 (December 1994). The atoms are assumed to be in Rydberg states (cf. Exercise 14.5.4). A related experiment based on the same principle but with a more complicated realization has been performed by S. Dürr, T. Nonn, and G. Rempe, Origin of quantum mechanical complementarity probed by a "which way" experiment in an atom interferometer, *Nature* 395, 33 (1998). See also P. Bertet *et al.*, A complementarity experiment with an interferometer at the quantum–classical boundary, *Nature* 411, 166–170 (2001).

1.5 Energy levels

The goal of this section is to define the concept of energy level, first on the basis of the classical notion. Taking as an example the Bohr atom, we can then proceed in a simple way to the quantum notion, after which we shall examine radiative transitions between levels.

1.5.1 Energy levels in classical mechanics and classical models of the atom

Let us imagine a classical particle which we take, for the sake of simplicity, to be moving along the x axis and which has potential energy U(x). In quantum mechanics, U(x) is referred to in general as the *potential*. It is well known that the mechanical energy E, the sum of the kinetic energy K and the potential energy U, is constant: E = K + U =const. Let us assume that the potential energy has the form shown in Fig. 1.14, that of a "potential well" which tends to the same constant value for $x \to \pm \infty$. It will be convenient to fix the zero of the energy such that E = 0 for a particle of kinetic energy that vanishes at infinity.

There are two possible situations.

- (i) The particle has energy E > 0. Then if, for example, it leaves from $x = -\infty$, it is first accelerated and then decelerated in passing through the potential well, and at $x = +\infty$ it reaches a final velocity equal to the initial one. Such a particle is said to be in a *scattering state*.
- (ii) The particle has negative energy $U_0 < E < 0$. Then the particle cannot escape from the well, but travels back and forth inside it between the points x_1 and x_2 satisfying $E = U(x_{1,2})$. It is confined inside a finite region of the x axis, $x_1 \le x \le x_2$, and is said to be in a *bound state*.

When the potential energy is positive (Fig. 1.15) we have the case of a "potential barrier."³² In this case E > 0 and only scattering states are observed. If $E < U_0$, a particle leaving from $x = -\infty$ is at first decelerated, and when it arrives at the point x_1 satisfying $U(x_1) = E$ it is reflected by the potential barrier. If $E > U_0$ the particle passes over the potential barrier and reaches $x = +\infty$ with its initial velocity.



Fig. 1.14. A potential well.

³² Naturally, situations more complex than the ones in these figures can be imagined, for example a double well. Here we shall discuss only the simplest cases.



Fig. 1.15. A potential barrier.

In classical mechanics the energy of a bound state can take all possible values between U_0 and 0. In quantum mechanics, we shall see in Chapter 9 that it can take only discrete values. On the other hand, as in classical mechanics, the energy of a scattering state is arbitrary. However, there are still notable differences (Sections 9.3 and 9.4) from the case of classical mechanics. For example, the particle can pass over a potential barrier even if $E < U_0$. This is called "tunneling." Moreover, the particle can be reflected even if $E > U_0$.

Let us apply these ideas from classical mechanics to atoms. The first atomic model was proposed by Thomson (Fig. 1.16a). Here the atom is represented as a sphere of uniform positive charge, with electrons moving around inside this charge distribution. It is a result of elementary electrostatics that the electrons here experience a harmonic potential, and their ground (stable) energy level is the state in which they are at rest at the bottom of the potential well. Excited states correspond to vibrations about the equilibrium position. This model was ruled out by the experiments of Geiger and Marsden, who showed that α -particle (⁴He nucleus) scattering by atoms is incompatible with it.³³ Rutherford deduced from his experiments the existence of an atomic nucleus of size less than 10 F, and proposed a planetary model of the atom (Fig. 1.16b): the electrons orbit the nucleus like the planets orbit the Sun, with the Coulomb interaction playing the role of gravitational attraction. This model possesses two major, related shortcomings: there is no scale which fixes the atomic size, and the atom is unstable, because the orbiting electrons radiate and end up falling onto the nucleus. In this process a continuous frequency spectrum is emitted, whereas experiments performed in the late nineteenth century showed that (Fig. 1.17)

- the frequencies of radiation emitted or absorbed by an atom are discrete. They are expressed as a function of two integers *n* and *m* and can be written as differences, $\omega_{nm} = A_n A_m$;
- there exists a ground-state configuration of the atom in which it does not radiate.

³³ Though atomic physicists still often make use of it ...



Fig. 1.16. Models of the atom. (a) Thomson: the electrons are located inside a uniform distribution of positive charge. (b) Rutherford: the electrons orbit a nucleus.



Fig. 1.17. Emission and absorption of radiation between two levels E_n and E_m .

These results suggest that the atom emits or absorbs a photon in passing from one level to another, with the photon frequency ω_{nm} given by $(E_n > E_m)$

$$\hbar\omega_{nm} = E_n - E_m. \tag{1.31}$$

The frequencies ω_{nm} are called the Bohr frequencies. According to these arguments, only certain levels labeled by a discrete index can exist. This is referred to as the quantization of energy levels.

1.5.2 The Bohr atom

In order to explain this quantization, Bohr imposed an ad hoc quantization rule on classical mechanics and the Rutherford atom. We shall follow an argument slightly different from his original one. Taking for simplicity the hydrogen atom with an electron of mass m_e

and charge q_e in a circular orbit of radius *a*, we postulate that the circumference $2\pi a$ of the orbit must be an integer multiple of the de Broglie wavelength λ :

$$2\pi a = n\lambda, \quad n = 1, 2, \dots \tag{1.32}$$

This postulate is intuitive; it means that the phase of the de Broglie wave of the electron returns to its initial value after one complete orbit and a standing wave is formed. From (1.32) and (1.26) we deduce

$$2\pi a = n\frac{h}{p} = \frac{nh}{m_{\rm e}v}$$

According to Newton's law,

$$\frac{m_{\rm e}v^2}{a} = \frac{q_{\rm e}^2}{4\pi\varepsilon_0 a^2} = \frac{e^2}{a^2}, \quad {\rm from \ which} \quad v^2 = \frac{e^2}{m_{\rm e}a},$$

where we have defined the quantity $e^2 = q_e^2/4\pi\varepsilon_0$. Eliminating the speed v between the two equations, we obtain the orbital radius:

$$a = \frac{n^2 \hbar^2}{m_e e^2}.$$
 (1.33)

The case n = 1 corresponds to the orbit of smallest radius, and this radius, denoted a_0 , is called the *Bohr radius*:

$$a_0 = \frac{\hbar^2}{m_{\rm e} e^2} \simeq 0.53 \text{ Å}$$
 (1.34)

The energy level labeled by n is

$$E_n = \frac{1}{2} m_{\rm e} v^2 - \frac{e^2}{a} = -\frac{e^2}{2a} = -\frac{m_{\rm e} e^4}{2n^2 \hbar^2} = -\frac{R_{\infty}}{n^2}.$$

The energy levels E_n are expressed as a function of the *Rydberg constant* $R_{\infty}^{,34}$

$$R_{\infty} = \frac{m_e e^4}{2\hbar^2} \simeq 13.6 \text{ eV}$$
(1.35)

as

$$E_n = -\frac{R_\infty}{n^2} \quad . \tag{1.36}$$

This formula gives the *level spectrum* of the hydrogen atom. The ground state corresponds to n = 1 and the ionization energy of the hydrogen atom is R_{∞} . The photons emitted by the hydrogen atom have frequencies

$$\hbar\omega_{nm} = -R_{\infty} \left(\frac{1}{n^2} - \frac{1}{m^2}\right), n > m, \qquad (1.37)$$

³⁴ The subscript ∞ is used because the theory described here assumes that the proton is infinitely heavy. When the finite mass m_p of the proton is taken into account, R_{∞} is changed to $R_{\infty}[1/(1+m_e/m_p)]$; cf. Exercise 1.6.5.

in perfect agreement with the spectroscopic data for hydrogen. However, the simplicity with which the spectrum of the hydrogen atom can be calculated using the Bohr theory should not be allowed to mask the artificial nature of this theory.

Sommerfeld's generalization of the Bohr theory consists of the postulate

$$\int p_i \,\mathrm{d}q_i = nh,\tag{1.38}$$

where q_i and p_i are coordinates and momenta conjugate in the sense of classical mechanics and n is an integer ≥ 1 . However, we now know that the conditions (1.38) are valid only for certain very special systems and for large n, with some exceptions. The Bohr– Sommerfeld theory cannot describe atoms with many electrons, or scattering states. The success of the Bohr theory in the case of the hydrogen atom is only a happy accident.

1.5.3 Orders of magnitude in atomic physics

Metre/Kilogram/Second units, which are adapted to measuring things at the human scale, are not convenient in atomic physics. A priori, a convenient system of units should feature the fundamental constants \hbar and c, as well as the electron mass m_{e} . The proton can be considered infinitely heavy, or, more precisely, the electron mass can be replaced by the reduced mass (cf. Footnote 34). Let us recall the values of these constants with an accuracy of $\sim 10^{-3}$ sufficient for the numerical applications in this book:

$$\hbar = 1.054 \times 10^{-34} \,\mathrm{J \ s},$$

 $c = 3 \times 10^8 \,\mathrm{m \ s^{-1}},$
 $m_e = 0.911 \times 10^{-30} \,\mathrm{kg}.$

From these constants we can form the following natural units:

- The unit of length:³⁵ $\frac{\hbar}{m_e c} = 3.86 \times 10^{-13} \text{ m};$ The unit of time: $\frac{\hbar}{m_e c^2} = 1.29 \times 10^{-21} \text{ s};$
- The unit of energy: $m_e c^2 = 5.11 \times 10^5 \text{ eV}.$

These units are much closer than MKS units to the orders of magnitude characteristic of atomic physics, though a few orders of magnitude are still lacking. This is fixed by introducing a quantity which measures the strength of the electromagnetic force, the

³⁵ Called the *Compton wavelength* of the electron.

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coupling constant $e^2 = q_e^2/4\pi\varepsilon_0$. From \hbar , *c*, and e^2 we can form a dimensionless quantity called the *fine-structure constant* α :³⁶

$$\alpha = \frac{e^2}{\hbar c} = \frac{q_{\rm e}^2}{4\pi\varepsilon_0\hbar c} \simeq \frac{1}{137}.$$
 (1.39)

The relations between atomic units and natural units are now easy to find. For the Bohr radius, the natural unit of length in atomic physics, we obtain

$$a_0 = \frac{\hbar^2}{m_e e^2} = \frac{\hbar c}{e^2} \frac{\hbar}{m_e c} = \frac{1}{\alpha} \frac{\hbar}{m_e c} \approx 0.53 \text{ Å.}$$
(1.40)

The Rydberg, the natural unit of energy in atomic physics, is related to $m_e c^2$ as

$$R_{\infty} = \frac{1}{2} \frac{m_{\rm e} e^4}{\hbar^2} = \frac{1}{2} \left(\frac{e^2}{\hbar c}\right)^2 m_{\rm e} c^2 = \frac{1}{2} \alpha^2 m_{\rm e} c^2 \approx 13.6 \text{ eV}.$$
 (1.41)

The speed of the electron in the ground state is $v = \alpha c = e^2/\hbar$, and the period of this orbit, which is the atomic unit of time, is

$$T = \frac{2\pi a_0}{v} = 2\pi \frac{1}{\alpha} \frac{\hbar}{m_{\rm e}c} \frac{1}{\alpha c} = \frac{2\pi}{\alpha^2} \frac{\hbar}{m_{\rm e}c^2} \approx 1.5 \times 10^{-16} \,\,{\rm s.} \tag{1.42}$$

Equations (1.40)–(1.42) show that the natural units and atomic units are related by powers of α .

As a final example, let us estimate the average lifetime of an electron in an excited state. We shall use a classical picture, viewing the electron as traveling in an orbit of radius a.³⁷ We shall push this picture until it breaks down, and then we shall attempt to correct it by taking into account quantum considerations; this is called *semiclassical reasoning*. A calculation in classical electromagnetism shows that an electron in a circular orbit which moves with speed $v = \omega a \ll c$ radiates a power

$$P = \frac{2}{3c^3}e^2a^2\omega^4 = \frac{2}{3}\left(\frac{e^2}{\hbar c}\right)\frac{a^2\hbar\omega^4}{c^2} \sim \alpha\omega^2\hbar\left(\frac{a\omega}{c}\right)^2.$$
 (1.43)

In a purely classical picture, the electron will lose energy in a continuous fashion by emitting electromagnetic radiation. This is where an admittedly ad hoc quantum argument

³⁶ This terminology arose for historical reasons and is somewhat confusing; it would be better to say "atomic constant" α . This is the *coupling constant of electrodynamics*, although it is not really constant owing to subtleties of quantum field theory. The quantum fluctuations of the electron–positron field have the effect of screening electric charges: owing to (virtual) electron–positron pair production, the charge of a particle measured far from the particle is smaller than the charge measured close to it. Owing to the Heisenberg inequality (1.30), short distance implies large momentum and therefore high energy, i.e., particles of high energy must be used to explore short distances. It can therefore be concluded that the fine-structure constant is an increasing function of energy, and in fact at energies of the order of the Z⁰ boson rest energy, $m_Z c^2 \approx 90$ GeV, we have $\alpha \approx 1/129$ instead of the low-energy value $\alpha \approx 1/137$. The renormalization procedure of eliminating infinities allows us to choose an arbitrary energy (or distance) scale for defining α . In sun, α depends on the energy scale characteristic of the process under study, and also on details of the renormalization procedure (cf. Footnote 13). This energy dependence of α has been observed for several years now in precision experiments in high-energy physics. See also Exercise 14.6.3.

³⁷ One can also view an atom as a dipole oscillating with frequency ω , as in the Thomson model. The only difference is that the factor of 2/3 in (1.43) becomes 1/3, which has no effect on the orders of magnitude.

enters: the atom emits a photon when it has accumulated an energy $\sim \hbar \omega$, which takes a time τ corresponding to the *lifetime of the excited state*:

$$\frac{1}{\tau} \sim \frac{P}{\hbar\omega} \sim \alpha \omega \left(\frac{a\omega}{c}\right)^2. \tag{1.44}$$

However, we have seen that $a\omega/c = v/c \sim \alpha$, and the relation between the period T and the average lifetime τ is

$$\frac{T}{\tau} \sim \frac{1}{\tau\omega} \sim \alpha^3 \sim 10^{-6}.$$
(1.45)

The electron orbits about a million times before emitting a photon, and so an excited state is well defined. For the ground state of the hydrogen atom where the energy is ~10 eV we have seen that $T \sim 10^{-16}$ s, while for an outer-shell electron of an alkaline atom with energy ~1 eV we have instead $T \sim 10^{-15}$ s and the order of magnitude of the lifetime of an excited state is ~10⁻⁷-10⁻⁹ s. For example, the first excited state of rubidium (D_2 line) has an average lifetime of 2.7×10^{-8} s.

The reasoning we have followed in this section has the merit of simplicity, but it is not satisfying. We had to impose a somewhat ad hoc quantum constraint on the classical arguments when they became untenable, and the reader can justly fail to be convinced by this sort of reasoning. It is therefore necessary to develop an entirely new theory which is no longer guided by classical physics, but instead develops in an autonomous fashion, *without reference to classical physics*.

1.6 Exercises

1.6.1 Orders of magnitude

- 1. We would like to explore distances at the atomic scale, that is, 1 Å, using photons, neutrons, or electrons. What should the order of magnitude of the energy of these particles be in eV?
- 2. When the wavelength λ of a sound wave is large compared with the lattice spacing of the crystal in which the vibration propagates, the frequency ω of the wave is linear in the wave vector $k = 2\pi/\lambda$: $\omega = c_s k$, where c_s is the speed of sound (cf. Section 11.3.1). In the case of steel $c_s \simeq 5 \times 10^3$ m s⁻¹. What is the energy $\hbar \omega$ of a sound wave for k = 1 nm⁻¹? The particle analogous to the photon in the case of sound waves is called the *phonon* (see Section 11.3.1), and $\hbar \omega$ is the phonon energy. Using the fact that a phonon can be created in an inelastic collision with a crystal, should neutrons or photons be used to study phonons?
- 3. In an interference experiment using fullerenes C_{60} , which are at present the largest objects for which wave behavior has been verified experimentally,³⁸ the average speed of the molecules is about 220 m s⁻¹. What is their de Broglie wavelength? How does it compare with the size of the molecule?
- 4. A diatomic molecule is composed of two atoms of masses M_1 and M_2 and has the form of a dumb-bell. The two nuclei are located a distance $r_0 = ba_0$ apart, where a_0 is the Bohr radius (1.34)

³⁸ M. Arndt, O. Nairz, J. Vos-Andreae, C. Keller, G. van der Zouw, and A. Zeilinger, Wave–particle duality of C₆₀ molecules, *Nature* **401**, 680 (1999). For more recent results see M. Arndt, K. Hornberger, and A. Zeilinger, *Physics World* **18**(3), 35 (2005).

and *b* is a numerical coefficient ~1. It is assumed that the molecule rotates about its center of inertia, through which passes the axis perpendicular to the line joining the nuclei, referred to as the nuclear axis. Show that the moment of inertia is $I = \mu r_0^2$, where $\mu = M_1 M_2 / (M_1 + M_2)$ is the reduced mass. If we assume that the angular momentum is \hbar , what is the angular speed of rotation and the corresponding energy ε_{rot} ? Show that this energy is proportional to $(m_e/\mu)R_{\infty}$, where m_e is the electron mass and $R_{\infty} = m_e c^4 / (2\hbar^2) = e^2 / (2a_0)$.

- 5. The molecule can also vibrate along the nuclear axis about the equilibrium position $r = r_0$, where the restoring force has the form $-K(r - r_0)$, with $Kr_0^2 = dR_\infty$ and *d* a numerical coefficient ~1. What are the vibrational frequency ω_v and the corresponding energy $\hbar \omega_v$? Show that this energy is proportional to $\sqrt{m_e/\mu} R_\infty$. An example is the H³⁵Cl molecule, for which the experimental values are $r_0 = 1.27$ Å, $\varepsilon_{rot} = 1.3 \times 10^{-3}$ eV, and $\hbar \omega_v = 0.36$ eV. Calculate the numerical values of *b* and *d*. What will the wavelengths of photons of energy ε_{rot} and $\hbar \omega_v$ be? In which regions do these wavelengths lie?
- 6. The absence of a quantum theory of gravity makes it necessary to restrict all theories to energies lower than $E_{\rm P}$, the Planck energy. Use a dimensional argument to construct $E_{\rm P}$ as a function of the gravitational constant G (Eq. (1.5)), \hbar , and c and find its numerical value. What is the corresponding wavelength (or Planck length) $l_{\rm P}$?

1.6.2 The black body

1. Prove the following equation (Footnote 21):

$$\int \mathrm{d}x\mathrm{d}p\,\delta\left(E-\frac{p^2}{2m}-\frac{1}{2}\,m\omega^2x^2\right)f(E)=\frac{2\pi}{\omega}\,f(E).$$

2. We want to relate the energy density per unit frequency $\epsilon(\omega, T)$ to the emitted power $u(\omega, T)$, Eq. (1.15). We consider a cavity maintained at temperature *T* (Fig. 1.4). Let $\tilde{\epsilon}(k, T)d^3k$ be the energy density in a volume d^3k about \vec{k} , which depends only on $k = |\vec{k}|$. Show that

$$\tilde{\boldsymbol{\epsilon}}(k,T) = \frac{c}{4\pi k^2} \, \boldsymbol{\epsilon}(\omega,T).$$

The Poynting vector of a wave with wave vector \vec{k} escaping from the cavity is $c\tilde{\epsilon}(k, T)\hat{k}$. Show that the flux of the Poynting vector through an opening of area S is

$$\Phi = \frac{1}{4} c \mathcal{S} \int_0^\infty \epsilon(\omega, T) \mathrm{d}\omega$$

and derive (1.15).

3. Show by dimensional analysis that in classical physics the energy density of a black body is given by

$$\boldsymbol{\epsilon}(T) = A(k_{\rm B}T)c^{-3}\int_0^\infty \omega^2\,\mathrm{d}\omega,$$

where A is a numerical coefficient.

4. Each mode k of the electromagnetic field inside the cavity is a harmonic oscillator. In classical statistical mechanics the energy of such a mode is $2k_{\rm B}T$ (where does the factor of 2 come from?). Show that the energy density inside the cavity is

$$\epsilon(T) = \frac{1}{\pi^2} (k_{\rm B} T) c^{-3} \int_0^\infty \omega^2 \,\mathrm{d}\omega$$

and compute A.

5. Demonstrate (1.22) and show that the classical expression is recovered for $\hbar \omega \ll k_{\rm B}T$, that is, for a sufficiently high temperature with ω fixed. This is a very general result: *the classical approximation is valid at high temperature*.

1.6.3 Heisenberg inequalities

In the thought experiment of Fig. 1.12, show that the momentum δp_x transferred to the screen must be pa/(2D), where *a* is the spacing between the slits S_1 and S_2 (Fig. 1.12) and *p* is the neutron momentum. Determination of the trajectory implies that $\Delta p_x \ll \delta p_x$, where Δp_x is the spread in the *initial* momentum of the screen. What is the dispersion Δx at the location of S_0 ? Show that in this case the interference pattern is destroyed.³⁹

1.6.4 Neutron diffraction by a crystal

Neutron diffraction is one of the principal techniques used to analyze crystal structure. For simplicity, let us consider a two-dimensional crystal composed of identical atoms with wave vectors lying in the plane of the crystal.⁴⁰ The atoms of the crystal are located at the lattice sites (Fig. 1.18)

$$\vec{r}_i = na\hat{x} + mb\hat{y}, \quad n = 0, 1, \dots, N-1, \quad m = 0, 1, \dots, M-1.$$

The neutrons interact with the atomic nuclei via the nuclear interaction.⁴¹ We use $f(\theta)$ to denote the probability amplitude that a neutron of momentum $\hbar \vec{k}$ is scattered in the direction \hat{k}' by an atom located at the origin, where θ is the angle between \hat{k} and \hat{k}' . Since



Fig. 1.18. Neutron diffraction by a crystal. The incident neutron has momentum $\hbar \vec{k}$ and the scattered neutron $\hbar \vec{k'}$. The Bragg angle $\theta_{\rm B}$ is defined in question 4.

⁴¹ There is also an interaction between the neutron magnetic moment and the atomic magnetism. It plays a very important role in studies of magnetism, but is not relevant to the present discussion.

³⁹ See W. Wootters and W. Zurek, Complementarity in the double slit experiment: quantum nonseparability and a quantitative statement of Bohr's principle, *Phys. Rev.* D19, 473–484 (1979).

⁴⁰ One can also imagine 3D scattering by a 2D crystal; cf. Wichman [1974], Chapter 5, where a model for diffraction by the surface of a crystal is presented.

the neutron energy is very low, $\sim 0.01 \text{ eV}$, $f(\theta)$ is independent of θ (Section 12.2.4): $f(\theta) = f$. The collision between a neutron and an atomic nucleus is elastic and leaves the state of the crystal unchanged: it is impossible to know which atom has scattered the neutron.

1. Show that the amplitude for scattering by an atom located at a site \vec{r}_i is

$$f_i = f e^{i(\vec{k} - \vec{k}') \cdot \vec{r}_i} = f e^{-i\vec{q} \cdot \vec{r}_i}$$

with $\vec{q} = \vec{k}' - \vec{k}$.

2. Show that the amplitude f_{tot} for scattering by a crystal has the form

$$f_{\rm tot} = fF(aq_x, bq_y),$$

with the function $F(aq_x, bq_y)$ given by

$$F(aq_x, bq_y) = \exp\left(-i\frac{aq_x(N-1)}{2}\right) \exp\left(-i\frac{bq_y(M-1)}{2}\right) \\ \times \left[\frac{\sin(aq_xN/2)}{\sin(aq_x/2)}\right] \left[\frac{\sin(bq_yM/2)}{\sin(bq_y/2)}\right].$$

3. Show that for $N, M \gg 1$ the scattering probability is proportional to $(NM)^2$ when \vec{q} has components

$$q_x = \frac{2\pi n_x}{a}, \quad q_y = \frac{2\pi n_y}{b}$$

 n_x and n_y being integers. When the components of \vec{q} are of this form, it is said that \vec{q} belongs to the *reciprocal lattice* of the crystal lattice. Diffraction maxima are obtained if \vec{q} is a reciprocal lattice vector. What is the width of a diffraction peak about the maximum? Show that the intensity inside the peak is proportional to *NM*.

4. The elastic nature of the scattering must be taken into account. Show that the condition for elastic scattering is

$$2\vec{k}.\vec{q} + q^2 = 0.$$

A reciprocal lattice vector does not give a diffraction maximum unless this condition is satisfied. For fixed wavelength, this condition cannot be satisfied unless the angle of incidence takes special values, called the *Bragg angles* $\theta_{\rm B}$. A simple analysis is possible if $n_x = 0$. Show that in this case an angle of incidence $\theta_{\rm B}$ gives rise to diffraction when

$$\sin \theta_{\rm B} = \frac{\pi n}{bk}, \quad n = 1, 2, \dots$$

In general, it is convenient to interpret the Bragg condition geometrically: the tip of the vector \vec{k} is located at a point of the reciprocal lattice and traces a circle of radius k. If this circle passes through another point of the reciprocal lattice a diffraction maximum is obtained. In general, a beam of neutrons incident on a crystal will not give rise to a diffraction peak. The angle of incidence and/or wavelength must be chosen appropriately. Why doesn't this phenomenon occur in diffraction by a one-dimensional lattice? What happens if only the first vertical column of atoms on the line y = 0 is present?

5. Now let us assume that the crystal is composed of atoms of two types. The basic crystal pattern, or *cell*, is formed as follows. Two atoms of type 1 are respectively located at

$$\vec{r}_1 = 0$$
 and $\vec{r}_1' = a\hat{x} + b\hat{y}$,

and two atoms of type 2 at

$$\vec{r}_2 = a\hat{x}$$
 and $\vec{r}_2' = b\hat{y}_2$

The pattern is repeated with periodicity 2a in the x direction and 2b in the y direction. Let $f_1 [f_2]$ be the amplitude for neutron scattering by an atom of type 1 [2] located at the origin; these amplitudes can be taken to be real. If NM is the number of cells, show that the amplitude for scattering by the crystal is proportional to $F(2aq_x, 2bq_y)$. Find the proportionality factor as a function of f_1 and f_2 . Show that if q_x and q_y correspond to a diffraction maximum, this proportionality factor must be

$$f_1 \left[1 + (-1)^{n_x + n_y} \right] + f_2 \left[(-1)^{n_x} + (-1)^{n_y} \right].$$

Discuss the result as a function of the parity of n_x and n_y .

6. The atoms 1 and 2 form an alloy.⁴² At low temperatures the atoms are in the configuration described in question **5** above, but above a certain temperature each atom has a 50% probability of occupying any site, and all sites are equivalent. How will the diffraction picture change?

1.6.5 Hydrogen-like atoms

Calculate, as a function of R_{∞} , the ground-state energy of the ordinary hydrogen atom, the deuterium atom, and the singly ionized helium atom taking into account the fact that nucleons have finite mass. Hint: what are the reduced masses?

1.6.6 The Mach–Zehnder interferometer

In a Mach–Zehnder interferometer (Fig. 1.19), a light beam arrives at the first beam splitter BS_1 . The two resulting beams are then reflected by two mirrors and recombined



Fig. 1.19. The Mach–Zehnder interferometer.

⁴² An example of the phenomenon described in this exercise is brass with composition 50% copper and 50% zinc.

Introduction

by a second beam splitter BS_2 . The intensity of the incident light is reduced to the level at which the photons arrive one by one. More precisely, the time between the arrival of two successive photons is very large compared with the resolution times of the photodetectors D_1 and D_2 . If a photon arrives at a beam splitter with probability amplitude a_0 , it will be transmitted with an amplitude ta_0 and reflected with an amplitude ra_0 , where t and r are complex numbers

$$t = |t| e^{i\alpha}, \quad r = |r| e^{i\beta}$$

and $|t| = |r| = 1/\sqrt{2}$. A phase shift δ can be introduced into, for example, the upper path of the interferometer by means of a plate with parallel faces of variable thickness. In the absence of this plate $\delta = \delta_0 \neq 0$ because the two beam paths in the interferometer are never exactly equal. Let p_1 and p_2 denote the probabilities of detecting a photon by D_1 and D_2 .

- 1. Calculate p_1 and p_2 as functions of α , β , and δ . What is observed when δ is varied?
- 2. What is the relation between p_1 and p_2 ? Derive the expression

$$\alpha - \beta = \frac{\pi}{2} \pm n\pi$$
, integer *n*.

1.6.7 Neutron interferometry and gravity

A neutron interferometer is realized in the following way (Fig. 1.20). A monochromatic (i.e., fixed wavelength) incident beam arrives at the first crystal at point *A*, with the angle of incidence and wavelength chosen such that a diffraction maximum is obtained (see Exercise 1.6.4, question 4); this angle of incidence is the Bragg angle $\theta_{\rm B}$. Part of the beam is transmitted as beam I with probability amplitude *t* and the rest is refracted as beam II



Fig. 1.20. Neutron interferometry.

with probability amplitude r. These amplitudes satisfy $|t|^2 + |r|^2 = 1$. Beams I and II arrive at a second crystal at points B and D, respectively, and the refracted parts of I and II are recombined by a third crystal at point C. The neutrons are detected by the two counters D_1 and D_2 . On trajectory II the neutrons undergo a phase shift χ which can have various origins (a difference between the lengths of the trajectories, gravity, passage through a magnetic field, etc.), and the objective of neutron interferometry is to measure this phase shift.

1. Show that the probability amplitude a_1 for a neutron to arrive at D_1 is

$$a_1 = a_0 (e^{i\chi} trr + rrt),$$

and that the probability of detection by D_1 is

$$p_1 = 2|a_0|^2|t|^2|r|^4(1 + \cos \chi) = A(1 + \cos \chi),$$

where a_0 is the amplitude incident on the first crystal.

2. What is the amplitude a_2 for a neutron to reach detector D_2 as a function of r, t, and a_0 , and the corresponding probability p_2 ? Why must we have $p_1 + p_2 = \text{constant}$? Show that

$$\mathsf{p}_2 = B - A\cos\chi.$$

What is *B* as a function of *t*, *r*, and a_0 ? Letting

$$t = |t| \mathrm{e}^{\mathrm{i}\alpha}, \quad r = |r| \mathrm{e}^{\mathrm{i}\beta},$$

show that

$$\alpha - \beta = \frac{\pi}{2} \pm n\pi, \quad n = 0, 1, 2, \dots$$

3. We now take gravity into account. How does the wave vector $k = 2\pi/\lambda$ of a neutron vary with height z when the neutron is located in a gravitational field with gravitational acceleration g? Compare the numerical values of the neutron kinetic energy and gravitational energy⁴³ $m_n gz$ (where m_n is the neutron mass), and derive an approximation for k. Assuming that the plane *ABCD* is initially horizontal, it can be rotated about the axis *AB* such that it becomes vertical. Show that such a rotation induces the following phase difference between the two trajectories:

$$\Delta \phi = \frac{m_{\rm n}^2 g \mathcal{S}}{\hbar^2 k} = \frac{2\pi m_{\rm n}^2 g \mathcal{S} \lambda}{h^2},$$

where S is the area of the rhombus *ABCD*.

 $^{^{43}}$ The energy is defined up to an additive constant, with the zero of energy fixed according to the following convention: a neutron of zero velocity and height z = 0 has zero energy.