Electron Transport in Nanostructures and Mesoscopic Devices

An Introduction

Thierry Ouisse

Series Editor
Mireille Mouis
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Chapter 1

Introduction

1.1. Introduction and preliminary warning

Matter stability and the way in which rigid crystalline or amorphous arrays of atoms can be formed are ruled by two pillars of physics: electromagnetism and quantum mechanics; nothing else, provided that we admit the existence of elementary constituents such as atom nuclei without having to derive their internal structure from the first principles (then we need to add nuclear forces to our bunch of tools). The postulates and basic equations of these two theories can be written on a couple of pages, and everything can be derived from them\(^1\). If the world was ruled by classical mechanics, it would simply be impossible to obtain stable atoms\(^2\) or stable chemical bonding to ensure the existence of matter as we all experience it in our everyday life. Thus, it is something of a misnomer to say that we are going to study quantum devices as opposed to devices which would not be quantum. Everything is ruled by quantum mechanics, from the insulating or conducting character to the color of any piece of matter or object that you can see inside the room where you are now reading this introduction (see also Figure 1.1). To understand our macroscopic world, we often feel that once we admit the existence of stable matter, we can content ourselves with using the second Newton’s law of motion and classical gravitational forces. An aeronautics engineer does not put too much quantum mechanics in his calculations, but this is certainly no longer the case

\(^1\) Of course with a substantial amount of hard work and mathematics, and adding some thermodynamics. Note also that if quantum mechanical predictions can be verified with an astonishingly high precision, their interpretation was (and is) the source of thousands of scientific articles and books.

\(^2\) Classical electrons accelerated over orbits radiate electromagnetic waves and thus lose energy. Thus, bound electrons would collapse onto the atoms.
if we want to justify the way in which electrons and therefore the electrical current behaves in a bulk semiconductor. Without a periodic atomic lattice and quantum mechanics, we could not find free electrons able to carry a current in a $p$-$n$ junction, or in the channel of transistors which form the integrated circuits inside our computers. Thus, the reason why the devices under study in this book are called quantum is that we can straightforwardly apply to them the basic quantum effects that students are accustomed to calculating in an introductory quantum mechanics course.

In nanostructures, electrons can be confined in potential wells narrow enough to obtain energy quantization along the confining direction. Their dimension is small enough for probing the dual wave-particle nature of the electron in a straightforward manner, because the electron wave function phase can be kept coherent over the whole device length. Thus, it becomes possible to observe wave interference effects just by measuring the average current which can be passed through such components, and particle-like properties from current noise data. As once stated by the physicist Esaki, this looks like some kind of “do-it-yourself” quantum mechanics: you are not required to become a specialist in group theory and irreducible representations, or of field-theoretic methods to get in touch with the essence of the topic (see also Figure 1.2). In addition, other specific effects, although not quantum-mechanical, are also due to reduced dimensions: if you can inject a few electrons into a nanostructure and if the capacitance between this nanostructure and the rest of the world is very small, we can probe effects which are due to charge granularity (we cannot divide the electron charge), and which are known as Coulomb blockade. Such effects are the subject of intensive research in R&D laboratories, because many people hope to put them to good use to produce new types of memories and devices that are smaller, faster and require a smaller amount of operating power. The aim of this book is to give an introduction to the basic concepts which govern the conduction mechanisms taking place in such small devices.

**Figure 1.1. The ubiquitous character of quantum mechanics**
Many (not to say most) of the phenomena described in this book usually take place at quite low temperatures, or in devices not yet (and for some of them never) used in the industry. The physics described here is not useful for understanding how industrial semiconductor devices behave in most applications right now, with the notable exception of resonant tunneling. Nevertheless, “today’s” silicon ($\text{Si}$) Metal-Oxide-Semiconductor Field-Effect Transistors (MOSFETs) definitely exhibit non-stationary and ballistic transport effects. Explaining these effects requires us to use some of the concepts developed in this book, even the high electric fields involved in MOSFET operation make the application of such concepts much more complicated than what is described in this introduction. At room temperature, the electron mean free path in silicon is in the 5-10 nm range, not far from the 45 nm channel length of the current CMOS technology, and integrated chips using a 32 nm process technology have already been demonstrated by the INTEL corporation in 2007. Figure 1.3 shows the picture of a 20 nm channel length prototype MOSFET produced in 2006 by LETI-CEA. Thus, even at room temperature some commercial electronic devices are close to the ballistic regime. Those industrial MOSFET’s are fabricated with an incredibly high reproducibility in order to form extremely complex integrated circuits (and as a side note such precision and reproducibility are actually far from being achieved in most research laboratories working in the realm of mesoscopic physics and nanostructures, or with semiconductors more exotic and physically more appealing than silicon). Device-modeling based on ballistic properties has thus become an active research field, even in the case of silicon devices (see, e.g., [NAT 94] for one of the pioneering Si papers).
In addition, mesoscopic effects are important in four respects:

(i) they are often of great physical significance, and give a deep and straightforward insight into some of the most striking implications of quantum mechanics (for instance, they provide unambiguous and clear demonstrations of the dual electron nature, particle and wave);

(ii) although often obtained at low temperatures or high magnetic fields they are very useful for extracting physical parameters dealing with (nano)structures actually used in applications;

(iii) some of the effects are already used in (e.g. resonant tunneling) or potentially useful for (e.g. Coulomb blockade) applications;

(iv) although still difficult to engineer, devices made from graphene or carbon nanotubes exhibit truly ballistic and quantum-coherent effects even at room temperature. Thus, it is quite possible that not only ballistic, but also quantum-coherent effects may be present in electronic applications in the near future.

---

Figure 1.3. A transmission electron microscope view of a planar double-gate MOSFET fabricated by LETI-CEA with a 20 nm channel length; reproduced by permission after J. Widiez et al., IEEE Transactions on nanotechnology, vol. 5, p. 643 (2006), copyright ©2006IEEE ([WID 06])

As a consequence, in most of the largest semiconductor companies, and in a very large number of university labs, intensive research work is devoted to such structures. Scarcely applied though it may seem at first sight, this field of activity is in fact the leading edge of semiconductor research.

This book is designed to be accessible to the independent reader, and to students not having a strong background in solid-state physics (e.g. issued from engineering disciplines). As a matter of fact, this book is an attempt to answer the following question: what must be taught to students starting from scratch to make them
understand the bases of electron transport in mesoscopic devices? A professor
placed in such a situation soon realizes that a good deal of solid-state physics and
quantum mechanics is required. This explains the incorporation of chapters which
are usually absent from the more specialized, already-existing books, and marks the
difference between them and this. In addition, to follow the classification once given
by J.M. Ziman, this book does not fall into the category of a “treatise” but into that
of a “textbook”, with the purpose of introducing and explaining concepts. The text
has been written with the aim of being as self-contained as possible, and is based on
an oral course delivered at an international European master’s degree course
involving three technical universities (GrenobleINP, EPFLausanne and
Polit’oTorino). It is a deliberate choice of the author to keep in the book the spirit of
the oral course, and this is the reason why the reader should not be surprised to be
sometimes interpellated or hailed in a somewhat familiar way.

Assimilating the quantum-mechanical rules summarized at the very beginning of
the book suffices to derive any subsequent result, but should by no means be
considered as enough to master quantum mechanics itself. Hence, and despite the
fact that the text remains at an introductory level, a complete understanding of the
course probably requires a minimum prior knowledge and self-maturation of the
basic quantum-mechanical concepts. A reader not acquainted with this field will
certainly feel the need to consult more authoritative manuals, due to the innumerable
number of questions, either technical or fundamental, that a concise and incomplete
presentation of quantum mechanics must arouse in any normally constituted mind.
Some knowledge of solid-state and semiconductor physics certainly help as well, but
all concepts useful for understanding the book can in principle be found in the book
itself, and since this book is an introduction dedicated to a broad audience, maybe
some of you are probably already acquainted with the required solid-state physics
notions. For those who are experienced in solid-state physics it is possible to simply
skip most of the reminders which make up Chapter 2. Besides, many of those
reminders are not always quite rigorously demonstrated. All undemonstrated or
heuristically-derived quantum-mechanical formulae can be found and are rigorously
derived in a self-contained, encyclopedic textbook: [COH 77]. Solid-state physics
has its self-contained book too: [ASH 76]. For bulk semiconductor physics and
transport, an advanced and quite remarkable and complete textbook was written by
[RID 82], but it is not essential for understanding this book. Eventually, we can find
books specifically devoted to mesoscopic electron transport, which can be of great
support for a better understanding or for gaining more information (the list below is
not exhaustive): [BEE 91], [KEL 95], [DAT 95] and [FER 97]. The book which is
the closest in spirit to this course is the one by Datta. It includes many exercises and
also contains more advanced formalisms (e.g. Green’s functions) and discussions.

---

3 As you may have already noticed, the familiar way of addressing the reader began in the
very first lines of this introduction.
which are not necessarily required at this introductory level. The book by Kelly presents a very large amount of data and also deals with aspects which are either more related to technological aspects or closer to the applications.

This book is an introduction and as such a number of important aspects have been omitted, mainly those which imply the use of mathematical concepts too involved to be developed in front of an audience new to the field. In particular, the reader will not find here a rigorous description of Green’s function formalism, which is necessary to include electron-electron interactions in transport modeling. A general discussion and study of many-body effects is also absent, which would be mandatory to understand a physical phenomenon such as the fractional quantum Hall effect, metal-based mesoscopic devices, carbon nanotubes operating in the 1D form of a Luttinger liquid and many others. Justice has not been done to the electron spin and its possible applications. This book could thus be given a second title: how far can we go using only independent electrons and the exclusion Pauli principle (see also Figure 1.4)? Surprising though it may seem, a good deal of nanostructure physics can still be grasped that way, but the reader will not find in this book a wealth of phenomena associated with electron-electron interactions. If they are not discouraged by this introductory text their study should constitute the next step, to be achieved by studying more specialized treatises and articles. Thus, if after studying the various chapters the student decides to read further and deeper, the main objective of this book will have been fulfilled. In the same spirit, we shall skip some difficult demonstrations which would be required for a rigorous derivation of some important solid-state physics results. However, even if difficult theoretical techniques have been deliberately banished from the text, “the language of physics is mathematics”, and none of the chapters escape from the rule.

![Figure 1.4. The quantum society and Pauli's exclusion principle](image)

4 Whenever this occurs, the unsatisfied reader will always be left with the possibility of consulting the more advanced textbooks or specialized articles mentioned in the bibliography.
Most exercises proposed at the end of each chapter are easy and their purpose is to provide the reader with a means of checking that they have correctly assimilated the chapter content and concepts. However, some of them require more time, and have been inserted to complete points not detailed in the main text.

Not all the sections were dealt with during the original oral course. I have put indicators at the beginning of each section:

- This section is a reminder. Thus it can be skipped if the reader is already familiar with the corresponding field.
- This section is essential to the book (and, quite accessorily, it may be helpful to prepare an exam). Some reminders belong to this category.
- This section is not a reminder, but is not considered as essential to understand the other parts.
- This section can be skipped at first reading.

1.2. Bibliography


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Chapter 2

Some Useful Concepts and Reminders

2.1. Quantum mechanics and the Schrödinger equation

2.1.1. A more than brief introduction

The following is only a summary which includes the basic quantum-mechanical (QM) equations required for understanding the book. It is by no means a rigorous introduction to the topics, and if you want to go further, a wise thing to do would be to immerse yourself, e.g., in the introductory textbook by R.P. Feynman [FEY 65], and then in the book by Cohen-Tannoudji et al. [COH 77] for a while\(^1\). Besides, several formulations can be used to describe quantum mechanics, and here we shall not really make the effort of differentiating them from one another. A concise description of those different formulations can be found in [STY 02].

In classical mechanics the elementary constituents of matter are massive point particles whose movement is controlled by electromagnetic or gravitational forces. At any instant we can precisely define the particle position and, provided that at a time \( t \) we are given the position and velocity of all the system particles, we can calculate everything at any other time, and obtain well-defined trajectories (with a powerful enough computer if the particles are numerous, etc.), even if the system remains isolated. Thus, the whole picture is \textit{in principle} perfectly deterministic. In quantum mechanics the situation is far more subtle. Experimentally, it appears that if we let a system evolve isolated for a while, the maximum information concerning

\(^1\) Of course these are not the only useful introductory QM textbooks, and the reader can also consult, e.g., [DIR 58], [SCH 68], [MES 62], [BOH 54], [MER 70], [LAN 65], among which many present a historical interest in addition to their scientific value, and there are many others.
this system that is physically accessible to human knowledge does not allow us to predict in a deterministic and unique way the result which will be obtained once we act on this system to measure some of its properties.

Figure 2.1. Quantum-mechanical interference experiment illustrating the dual wave-particle nature of the electron

The celebrated double-slit interference experiment is probably one of the more striking and meaningful illustrations of the quantum nature of matter. This effect figures in due place in almost any introduction chapter on quantum mechanics, and we shall respect this very justified habit. Interference experiments such as that illustrated by Figure 2.1 reveal that it is no longer possible to consider an entity such as an electron or a proton as a particle, and that it is not possible to consider it as a pure wave either [FEY 65]. “Identically prepared” electrons propagating through double slits exhibit interference patterns like waves [JON 61], but if we put a screen behind the plane of those slits we always obtain localized spots, as for particles [TON 89]. It is the statistical collection of a large number of such individual events which forms the interference pattern. Thus, in quantum mechanics (and in the real world) we have to assign a dual nature to electrons, whose behavior can be modeled only as a combination of both a particle and a wave. Suppress one slit and we lose the interference pattern. The wave really passes through both slits. Try to detect the electron at one of the two slits and we also lose the pattern, because the particle-like detection at one slit instantaneously reduces the extended propagating wave.
In some textbooks it is stated that quantum mechanics does not allow us, even in principle, to calculate any trajectory, and that it is a probabilistic theory in essence. This is not a correct statement, because one interpretation, known as the de Broglie-Bohm theory, gives a perfectly deterministic picture of quantum mechanics (at least for massive particles). In such an interpretation both a wave and a particle co-exist. The wave guides the particle, and in Bohm’s version the only guiding rule states that the particle momentum is equal to the phase gradient of the complex wave obeying the Schrödinger equation multiplied by $\hbar$, a physical quantity known as the Planck constant [HOL 93]. In such a picture we can calculate well-defined trajectories (which are quite weird compared to classical ones, due to the action of the guiding wave). The unknown parameters, or “hidden variables”, which make experiments exhibit a statistical aspect are nothing but the initial particle coordinates with respect to the wave. Thus, it is not possible to say from quantum mechanics that the basic facts of nature are undeterministic in principle. However, since this interpretation does not provide any new prediction with respect to the usual quantum rules, and exhibits the moral drawback of being obviously non-local, it has not attracted the favor of most physicists².

The “orthodox” interpretation of the quantum-mechanical formalism is that in between measurements we cannot precisely define a thing such as a particle; the experimental indeterminacy obtained when repeating the same experiment a large number of times with identically prepared systems results from the indeterminacy of nature itself, and not from a difference in system preparation which would be unknown to the observer. This was quite an incredible statement when quantum mechanics emerged, but it has now become a common “philosophical” view among scientists. In this book we shall not enter into those considerations any longer. We shall just use the quantum-mechanical rules, which up to now have always been experimentally validated with a numerical precision unprecedented by any other physical theory.

² Non-locality, or the possibility of instantaneous action-at-a-distance, does not agree with another pillar of modern physics, special relativity, so physicists are reluctant to accept it in other theories. In Bohm’s interpretation experiments conducted on space-separated but correlated particles make this non-locality quite explicit. Note that in private most scientists would admit that quantum mechanics is deeply non-local, whatever the interpretation, but in public they see it as an unforgivable flaw, as soon as this non-locality is no longer buried in the mysteries of the “Copenhagen’s school” or “orthodox” interpretation, and is given a straightforward meaning. Note that Bohm’s interpretation also has its “weaknesses”. For instance, if at some time $t$ the particle distribution is given by the square modulus of the wave function, this implies that it will be true forever; however, there is nothing which rigorously justifies when and how it began to be so.
2.1.2. The postulates of quantum mechanics

Here we reproduce the postulates as they are expressed in most quantum mechanics textbooks (see, e.g., [COH 77]). Maybe some of you are already acquainted with them, but for others it is perhaps not completely useless to give a reminder. If you already followed a good course in quantum mechanics just skip this part; you will learn nothing from it. If you are more inexperienced and require further explanation consult any quantum mechanics textbook.

**First postulate:** At a given time \( t \), the state of a physical system is described by an abstract state vector \( |\psi(t)\rangle \), also called a ket, which belongs to the state space.

In practice, we shall essentially appeal to the “quantum mechanics of the poor man”, most often contenting ourselves with identifying those states with the wave functions \( \psi(\vec{r}, t) \) obtained by solving the Schrödinger equation inside our nanostructures. Before a position measurement, the nature of the electron wave prevents us from assigning a uniquely defined space-time position to the particle. These wave functions are mathematical devices associated with a given electron and link to each point of space a complex number. As with any wave, they can propagate or lead to stationary phenomena. The scalar product of two kets \( |\phi\rangle \) and \( |\psi\rangle \) is defined as

\[
\langle \phi | \psi \rangle = \int \phi^*(\vec{r})\psi(\vec{r})d^3r
\]  
(2.1)

where \( \phi^* \) is the complex conjugate of \( \phi \) (the state space is a mathematical, complex Hilbert space; it is formed by complex functions operating on real space, and not using simple real vectors). The notation \( \langle \phi | \) allows us to manipulate easily scalar products such as in equation (2.1). This was proposed by Dirac and is called a bra. The wave nature of an electron forbids its precise localization as long as it is not subject to a position measurement, during which it reveals its particle nature. Therefore, it is clear that in a quantum system, classical measurable quantities which depended on position, or on position and velocity (such as, for instance, the energy), cannot be assigned a precise and unique value unless they are specifically measured. Their description thus requires an operation which can act on the whole wave field, and this leads us to the formulation of the second postulate.

**Second postulate:** Any measurable physical quantity \( M \) (such as, e.g., a position, or a momentum, or an energy) is described by an operator \( M \) which acts on the state vector \( |\psi(t)\rangle \). This operator is called an observable.

We can apply to a state vector the operator \( B \), and then another operator \( A \). The operator corresponding to those two successive actions is noted \( AB \), but this product...
is not always commutative. \( AB \) is not necessarily equal to \( BA \), and when these two operator products differ we say that \( A \) and \( B \) do not commute. A famous example of non-commuting operators is the couple formed by position and momentum. Non-commutativity of some operators is indeed at the heart of many strange consequences of quantum mechanics. The quantity \( AB-BA \) is called the commutator of \( A \) and \( B \), and is denoted \([AB]\).

**Third postulate:** The result of a measurement of a physical quantity \( \mathcal{M} \) is always an eigenvalue of the corresponding observable \( M \).

Consider for instance the position operator. Its eigenvalues are formed by the ensemble of all three-dimensional real vectors \( \vec{r}_0 \). The corresponding eigenstates are Dirac peaks centered at \( \vec{r}_0 \), which are written under the form \( |\vec{r}_0\rangle = \delta(\vec{r} - \vec{r}_0) \). For the next postulate we shall limit ourselves to the case of a non-degenerate spectrum (i.e. we assume that to one eigenvalue corresponds one and only one eigenstate).

**Fourth postulate:** If the spectrum of the observable \( \mathcal{M} \) is discrete, and if the state vector is normalized, the probability \( P(m_n) \) of obtaining the eigenvalue \( m_n \) as a measurement result is equal to \( P(m_n) = |\langle u_n | \psi \rangle|^2 \), where \( |u_n\rangle \) is the normalized eigenvector of \( M \) associated with the eigenvalue \( m_n \). If the spectrum is continuous, the probability \( dP(\mu) \) of obtaining a result between \( \mu \) and \( \mu + d\mu \) is equal to \( dP(\mu) = |\langle u_\mu | \psi \rangle|^2 \), where \( |u_\mu\rangle \) is the eigenvector of the eigenvalue \( \mu \).

An example of a continuous spectrum is the position, and an example of a discrete spectrum is the energy inside a quantum well. From this postulate we can give a probabilistic interpretation of the wave function (initially proposed by M. Born): if we make a position measurement, from the fourth postulate the probability of finding the particle at a position \( \vec{r}_0 \) is given by \( P(\vec{r}_0) = |\langle \vec{r}_0 | \psi \rangle|^2 = \int d^3r |\psi(\vec{r}_0)|^2 \). Thus, from the fourth postulate \( |\psi(\vec{r}_0)|^2 \) is nothing but the probability density of finding the particle at a position \( \vec{r}_0 \). However, be careful: in the “orthodox” interpretation this is not the probability of the particle being at \( \vec{r}_0 \), and we cannot say that we do not know its position before the measurement simply because we are missing some information. Before a measurement the entity “electron” exists, but your particle is literally “nowhere”. Otherwise we could not obtain any wave interference effect. No matter how strange nature may seem, it is really the “measurement process” which turns an entity such as an electron into a corpuscle. In between measurements (or energy exchange with the macroscopic external world) the only relevant physical entity to prescribe the system evolution is the electron wave and nothing else.
**Fifth postulate (also called the measurement postulate):** If the measurement result of the physical quantity $M$ gives the result $m_n$, the state vector of the system immediately after the measurement is the normalized projection

$$\frac{P_n |\psi\rangle}{\sqrt{|\psi \rangle P_n |\psi\rangle}}$$

of $|\psi\rangle$ onto the sub-eigenspace associated with $m_n$ ($P_n$ is the projection operator).

If the spectrum is non-degenerate this means that just after a measurement the state vector is necessarily equal to the normalized eigenstate corresponding to the obtained eigenvalue $m_n$. This postulate has caused more ink to flow than all the newspaper issues devoted to Princess Diana and Madonna put together. Nevertheless, in this book we shall not even try to discuss the subtle issues which are attached to it.

**Sixth (and final) postulate:** The time evolution of the state vector obeys Schrödinger’s equation

$$H(t) |\psi(t)\rangle = i\hbar \frac{d|\psi\rangle}{dt},$$

in which the Hamiltonian $H(t)$ is the operator associated with the energy of the system.

### 2.1.3. Essential properties of observables

An operator $A$ is **Hermitian** or **self-adjoint** if it verifies the property

$$\int \phi^* A \psi \, d^3r = \int (A \phi)^* \psi \, d^3r.$$

As a matter of fact, in quantum mechanics all observables are both **linear** and **Hermitian**. Linearity ensures the validity of the superposition principle of our wave functions, which derives from the form of the Schrödinger equation. Hermiticity is required because if we measure something, we always obtain a real number, not a complex one, even if the scalar products are calculated using complex waves. Now from equation (2.3) and the fifth postulate, it is easy to demonstrate that this is achieved with Hermitian operators, because we have
Some Useful Concepts and Reminders

\[ m_n = \langle u_n | M u_n \rangle = \int u_n^* M u_n \, d^3 r \]  \hspace{1cm} (2.4)

\[ = \int (M u_n)^* u_n \, d^3 r = (\int u_n^* M u_n \, d^3 r)^* = m_n^*. \]

Since the eigenvalue is equal to its complex conjugate, it must be real.

It is worth noting that the eigenstates of an observable always form an orthogonal basis of the state space, even if it is of infinite dimension (in fact this should be taken as the definition of an observable). Thus, it is possible to develop any state vector as a linear combination of the observable eigenstates \(|u_n\):

\[ |\psi\rangle = \sum \langle u_n | \psi \rangle |u_n\rangle \]  \hspace{1cm} (2.5)

A useful relation can be easily derived from that property. The unity operator \(I\) (i.e. the operator which leaves any state vector unchanged) can be expressed as

\[ I = \sum |u_n\rangle \langle u_n| \]  \hspace{1cm} (2.6)

where the sum runs over all eigenstates (this is immediately demonstrated by making this operator act on a state vector, since this gives its expansion in terms of the eigenfunctions).

Assume that \(M\) is an observable and that the state vector is \(|\psi\rangle\). By expressing the ket \(|\psi\rangle\) in the eigenstate basis \(|u_n\rangle\) the action of \(M\) upon \(|\psi\rangle\) can be written as

\[ M|\psi\rangle = M \sum \langle u_n | \psi \rangle |u_n\rangle = \sum m_n \langle \psi | u_n \rangle |u_n\rangle \]  \hspace{1cm} (2.7)

Using the fourth postulate and equation (2.7), the quantity \(\langle \psi | M |\psi\rangle\) can thus be transformed as

\[ \langle \psi | M |\psi\rangle = \langle \psi | M |\psi\rangle = \sum m_n \langle \psi | u_n \rangle^2 = \langle M \rangle \]  \hspace{1cm} (2.8)

Thus, \(\langle \psi | M |\psi\rangle\) is nothing but the expectation value of \(M\) (i.e. the average value which would be approached after carrying out many measurements with identically prepared systems, all described by the state \(|\psi\rangle\)).
2.1.4. Momentum operator

The relation between momentum and wavevector $\vec{p} = \hbar \vec{k}$ proposed by de Broglie is one of the key ideas which paved the way for the advent of a rigorous version of quantum mechanics. His proposal was to associate both a wave and a particle to describe an entity such as an electron, and that a plane wave function of the form $\exp(i\vec{k}\vec{r})$ carries a momentum $\vec{p} = \hbar \vec{k}$. A heuristic way\(^3\) to find again the expression of the momentum operator

$$p = -i\hbar \nabla$$

(2.9)

is to apply operator $p$ to a plane wave $\exp(i\vec{k}\vec{r})$, and to state that we must find the eigenvalue $\hbar \vec{k}$. It immediately appears that the momentum operator must have the form above. An important relation links the momentum operator to the position operator, that we can also easily find again using a plane wave. Apply the operator $r p$ to a plane wave, and then apply $p r$. The difference between both results is not equal to zero and we will easily find the non-commutation relation

$$[r, p] = rp - pr = i\hbar ,$$

(2.10)

which can be shown to lead in turn to the famous Heisenberg’s uncertainty relation (see section 10.1 for a demonstration based on simple mathematics):

$$\Delta p \Delta x \geq \hbar$$

(2.11)

Equation (2.11) means that it is not possible to measure with an arbitrary precision both the momentum and position. This can also be viewed another way: from the de Broglie relation the momentum is proportional to the wavevector, and thus happens to be the Fourier transform of the position, within a constant proportionality factor $\hbar$. If the reader has followed a course in signal processing they will already know that the more something is bounded (e.g. in time), the more its Fourier transform spreads (e.g. in frequency), and reciprocally. Thus, we cannot restrict one without extending the uncertainty of the other. The momentum and position are not the only non-commuting observables. For instance, two orthogonal

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\(^3\) This note will not really help us to understand, but this relation can indeed be derived from general arguments, which show that the Hamiltonian of a particle is expressed in a unique way as a function of the generator of the space translations $-i\hbar \nabla$ and of the position, because on quite general grounds this Hamiltonian must satisfy the commutation relations of the Galilei transformation group (see [JOR 75]; note that this reference is not an article that can be read quickly).
components of an orbital angular momentum do not commute. From our comment on the Fourier transform we can also understand that time and energy, whose unit appears as a \textit{frequency} multiplied by a constant action $\hbar$ in the Schrödinger equation, cannot be measured simultaneously with an arbitrary precision. Even if time is not an operator, we can also write

$$\Delta E \Delta t \geq \hbar .$$ \hspace {1cm} (2.12)

\subsection*{2.1.5. Stationary states}

Assume that the potential energy $V(\vec{r})$ does not depend on time. The Hamiltonian is $H=p^2/2m + V(\vec{r})$, and along with equation (2.9) the Schrödinger equation can be written as

$$-\frac{\hbar^2}{2m} \nabla^2 \psi (\vec{r},t) + V(\vec{r}) \psi (\vec{r},t) = i\hbar \frac{\partial \psi (\vec{r},t)}{\partial t} .$$ \hspace {1cm} (2.13)

Here we are going to show that it is possible to separate the space and time dependence. If we look for solutions of the form

$$\psi (\vec{r},t) = \phi(\vec{r}) \zeta (t) ,$$ \hspace {1cm} (2.14)

after a few manipulations we can obtain from equation (2.13) that

$$i\hbar \frac{1}{\zeta (t)} \frac{d \zeta (t)}{dt} = -\frac{\hbar^2}{2m \phi (\vec{r})} \nabla^2 \phi (\vec{r}) + V(\vec{r}) .$$ \hspace {1cm} (2.15)

The left-hand side is a function of $t$ only, and the right-hand side is a function of $\vec{r}$. Thus, to be equal for any value of $t$ and $\vec{r}$ these two quantities must be a constant, which we shall note $\hbar \omega$. Then we can integrate the left-hand side to obtain

$$\zeta (t) = Ce^{-i\omega t}$$ \hspace {1cm} (2.16)

and the right-hand side leads to

$$-\frac{\hbar^2}{2m} \nabla^2 \phi (\vec{r}) + V(\vec{r}) \phi (\vec{r}) = \hbar \omega \phi (\vec{r}) ,$$ \hspace {1cm} (2.17)
which can also be written under the form

$$H \varphi (\vec{r}) = E \varphi (\vec{r})$$  \hspace{1cm} (2.18)$$

defining $E=h\omega$. We can incorporate the $C$ factor in function $\varphi$, because if we do so $\varphi$ will still be a solution of equation (2.15), and we find that

$$\psi (\vec{r},t) = \varphi (\vec{r}) e^{-i \omega t}$$  \hspace{1cm} (2.19)$$

is a solution to the stationary Schrödinger’s equation. This type of solution is called a stationary solution, because with a form such as equation (2.19) it is clear that the probability density $|\psi (\vec{r})|^2$ does not depend on time and is just a function of position. Since the function $\varphi (\vec{r})$ satisfies equation (2.18) it is an eigenstate of the Hamiltonian operator, and $E=h\omega$ is an energy eigenvalue.

Equation (2.18) is nothing but the eigenvalue equation of the Hamiltonian operator. From the fifth postulate, after an energy measurement on such a system we can only obtain one of the eigenvalues of $H$. This is the famous energy quantization phenomenon, which is an essential ingredient of semiconductor nanostructures and devices such as semiconductor quantum wells. Be careful: the fact that we can only obtain one energy eigenvalue does not mean that before the measurement the electron is in the corresponding eigenstate, even though the scalar product between the actual state vector and the eigenstate must be different from zero (see the fifth postulate). The stationary eigenstates do form a basis onto which can be expanded any other state, but if the actual state vector is a linear combination of several stationary states its evolution becomes time-dependent, because if we add several complex functions such as equation (2.19) the time does not only appear in the phase factor.

2.1.6. Probability current

In the general case the wave function depends on time and thus the probability density to find the particle somewhere also depends on time. This means that there is a probability density flow $\vec{J}$, and to calculate an average electron current we must be able to express this flow as a function of the wave function. Since probability should be conserved we expect to find a relation such as the charge conservation equation established from Maxwell’s equations. In this section we limit ourselves to the case of a scalar potential.