

Quantum Transport

Introduction to Nanoscience

Yuli V. Nazarov
and **Yaroslav M. Blanter**

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Quantum Transport

Introduction to Nanoscience

Quantum transport is a diverse field, sometimes combining seemingly contradicting concepts – quantum and classical, conducting and insulating – within a single nano-device. Quantum transport is an essential and challenging part of nanoscience, and understanding its concepts and methods is vital to the successful design of devices at the nano-scale.

This textbook is a comprehensive introduction to the rapidly developing field of quantum transport. The authors present the comprehensive theoretical background, and explore the groundbreaking experiments that laid the foundations of the field. Ideal for graduate students, each section contains control questions and exercises to check the reader's understanding of the topics covered. Its broad scope and in-depth analysis of selected topics will appeal to researchers and professionals working in nanoscience.

Yuli V. Nazarov is a theorist at the Kavli Institute of Nanoscience, Delft University of Technology. He obtained his Ph.D. from the Landau Institute for Theoretical Physics in 1985, and has worked in the field of quantum transport since the late 1980s.

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Preface

This book provides an introduction to the rapidly developing field of quantum transport. Quantum transport is an essential and intellectually challenging part of nanoscience; it comprises a major research and technological effort aimed at the control of matter and device fabrication at small spatial scales. The book is based on the master course that has been given by the authors at Delft University of Technology since 2002. Most of the material is at master student level (comparable to the first years of graduate studies in the USA). The book can be used as a textbook: it contains exercises and control questions. The program of the course, reading schemes, and education-related practical information can be found at our website www.hbar-transport.org.

We believe that the field is mature enough to have its concepts – the key principles that are equally important for theorists and for experimentalists – taught. We present at a comprehensive level a number of experiments that have laid the foundations of the field, skipping the details of the experimental techniques, however interesting and important they are. To draw an analogy with a modern course in electromagnetism, it will discuss the notions of electric and magnetic field rather than the techniques of coil winding and electric isolation.

We also intended to make the book useful for Ph.D. students and researchers, including experts in the field. We can liken the vast and diverse field of quantum transport to a mountain range with several high peaks, a number of smaller mountains in between, and many hills filling the space around the mountains. There are currently many good reviews concentrating on one mountain, a group of hills, or the face of a peak. There are several books giving a view of a couple of peaks visible from a particular point. With this book, we attempt to perform an overview of the whole mountain range. This comes at the expense of detail: our book is not at a monograph level and omits some tough derivations. The level of detail varies from topic to topic, mostly reflecting our tastes and experiences rather than the importance of the topic.

We provide a significant number of references to current research literature: more than a common textbook does. We do not give a representative bibliography of the field. Nor do the references given indicate scientific precedences, priorities, and relative importance of the contributions. The presence or absence of certain citations does not necessarily reflect our views on these precedences and their relative importance.

This book results from a collective effort of thousands of researchers and students involved in the field of quantum transport, and we are pleased to acknowledge them here. We are deeply and personally indebted to our Ph.D. supervisors and to distinguished senior colleagues who introduced us to quantum transport and guided and helped us, and to comrades-in-research working in universities and research institutions all over the world.

This book would never have got underway without fruitful interactions with our students. Parts of the book were written during our extended stays at Weizmann Institute of Science, Argonne National Laboratory, Aspen Center of Physics, and Institute of Advanced Studies, Oslo.

It is inevitable that, despite our efforts, this book contains typos, errors, and less comprehensive discourses. We would be happy to have your feedback, which can be submitted via the website www.hbar-transport.org. We hope that it will be possible thereby to provide some limited “technical” support.

Contents

Preface

page vii

Introduction	1
1 Scattering	7
1.1 Wave properties of electrons	7
1.2 Quantum contacts	17
1.3 Scattering matrix and the Landauer formula	29
1.4 Counting electrons	41
1.5 Multi-terminal circuits	49
1.6 Quantum interference	63
1.7 Time-dependent transport	81
1.8 Andreev scattering	98
1.9 Spin-dependent scattering	114
2 Classical and semiclassical transport	124
2.1 Disorder, averaging, and Ohm's law	125
2.2 Electron transport in solids	130
2.3 Semiclassical coherent transport	137
2.4 Current conservation and Kirchhoff rules	155
2.5 Reservoirs, nodes, and connectors	165
2.6 Ohm's law for transmission distribution	175
2.7 Spin transport	187
2.8 Circuit theory of superconductivity	193
2.9 Full counting statistics	205
3 Coulomb blockade	211
3.1 Charge quantization and charging energy	212
3.2 Single-electron transfers	223
3.3 Single-electron transport and manipulation	237
3.4 Co-tunneling	248
3.5 Macroscopic quantum mechanics	264
3.6 Josephson arrays	278
3.7 Superconducting islands beyond the Josephson limit	287

4	Randomness and interference	299
4.1	Random matrices	299
4.2	Energy-level statistics	309
4.3	Statistics of transmission eigenvalues	324
4.4	Interference corrections	336
4.5	Strong localization	363
5	Qubits and quantum dots	374
5.1	Quantum computers	375
5.2	Quantum goodies	386
5.3	Quantum manipulation	397
5.4	Quantum dots	406
5.5	Charge qubits	427
5.6	Phase and flux qubits	436
5.7	Spin qubits	445
6	Interaction, relaxation, and decoherence	457
6.1	Quantization of electric excitations	458
6.2	Dissipative quantum mechanics	470
6.3	Tunneling in an electromagnetic environment	487
6.4	Electrons moving in an environment	499
6.5	Weak interaction	513
6.6	Fermionic environment	523
6.7	Relaxation and decoherence of qubits	538
6.8	Relaxation and dephasing of electrons	549
	<i>Appendix A Survival kit for advanced quantum mechanics</i>	562
	<i>Appendix B Survival kit for superconductivity</i>	566
	<i>Appendix C Unit conversion</i>	569
	<i>References</i>	570
	<i>Index</i>	577

Introduction

It is an interesting intellectual game to compress an essence of a science, or a given scientific field, to a single sentence. For natural sciences in general, this sentence would probably read: *Everything consists of atoms*. This idea seems evident to us. We tend to forget that the idea is rather old: it was put forward in Ancient Greece by Leucippus and Democritus, and developed by Epicurus, more than 2000 years ago. For most of this time, the idea remained a theoretical suggestion. It was experimentally confirmed and established as a common point of view only about 150 years ago.

Those 150 years of research in atoms have recently brought about the field of *nanoscience*, aiming at establishing control and making useful things at the *atomic scale*. It represents the common effort of researchers with backgrounds in physics, chemistry, biology, material science, and engineering, and contains a significant technological component. It is technology that allows us to work at small spatial scales. The ultimate goal of nanoscience is to find means to build up useful artificial devices – *nanostructures* – atom by atom. The benefits and great prospects of this goal would be obvious even to Democritus and Epicurus.

This book is devoted to *quantum transport*, which is a distinct field of science. It is also a part of nanoscience. However, it is a very unusual part. If we try to play the same game of putting the essence of quantum transport into one sentence, it would read: *It is not important whether a nanostructure consists of atoms*. The research in quantum transport focuses on the properties and behavior regimes of nanostructures, which do not immediately depend on the material and atomic composition of the structure, and which cannot be explained starting by classical (that is, non-quantum) physics. Most importantly, it has been experimentally demonstrated that these features do not even have to depend on the size of the nanostructure. For instance, the transport properties of quantum dots made of a handful of atoms may be almost identical to those of micrometer-size semiconductor devices that encompass billions of atoms.

The two most important scales of quantum transport are conductance and energy scale. The measure of conductance, G , is the conductance quantum $G_Q \equiv e^2/\pi\hbar$, the scale made of fundamental constants: electron charge e (most of quantum transport is the transport of electrons) and the Planck constant \hbar (this indicates the role of quantum mechanics). The energy scale is determined by flexible experimental conditions: by the temperature, $k_B T$, and/or the bias voltage applied to a nanostructure, eV . The behavior regime is determined by the relation of this scale to internal energy scales of the nanostructure. Whereas physical principles, as stressed, do not depend on the size of the nanostructure, the internal scales do. In general, they are *bigger* for smaller nanostructures.

This implies that the important effects of quantum transport, which could have been seen at room temperature in atomic-scale devices, would require helium temperatures (4.2 K), or even sub-kelvin temperatures, to be seen in devices of micrometer scale. This is not a real problem, but rather a minor inconvenience both for research and potential applications. Refrigeration techniques are currently widely available. One can achieve kelvin temperatures in a desktop installation that is comparable in price to a computer. The cost of creating even lower temperatures can be paid off using innovative applications, such as quantum computers (see Chapter 5).

Research in quantum transport relies on the nanostructures fabricated using nanotechnologies. These nanostructures can be of atomic scale, but also can be significantly bigger due to the aforementioned scale independence. The study of bigger devices that are relatively easy to fabricate and control helps to understand the quantum effects and their possible utilization before actually going to atomic scale. This is why quantum transport tells what can be achieved if the ultimate goal of nanoscience – shaping the world atom by atom – is realized. This is why quantum transport presents an indispensable “*Introduction to nanoscience*.”

Historically, quantum transport inherits much from a field that emerged in the early 1980s known as *mesoscopic physics*. The main focus of this field was on quantum signatures in semiclassical transport (see, e.g., Refs. [1] and [2], and Chapter 4). The name *mesoscopic* came about to emphasize the importance of intermediate (meso) spatial scales that lie between micro-(atomic) and macroscales. The idea was that quantum mechanics reigns at microscales, whereas classical science does so at macroscale. The mesoscale would be a separate kingdom governed by separate laws that are neither purely quantum nor purely classical; rather, a synthesis of the two. The mesoscopic physics depends on the effective dimensionality of the system; the results in one, two, and three dimensions are different. The effective dimensionality may change upon changing the energy scale. In these terms, quantum transport mostly concentrates on a zero-dimensional situation where the whole nanostructure is regarded as a single object characterized by a handful of parameters; the geometry is not essential. Mesoscopics used to be a very popular term in the 1990s and used to be the name of the field reviewed in this book. However, intensive experimental activity in the late 1980s and 1990s did not reveal any sharp border between meso- and microscales. For instance, metallic contacts consisting of one or a few atoms were shown to exhibit the same transport properties and regimes as micron-scale contacts in semiconductor heterostructures. This is why the field is called now quantum transport, while the term *mesoscopic* is now most commonly used to refer to a cross-over regime between quantum and classical transport.

The objects, regimes, and phenomena of quantum transport are various and may seem unlinked. The book comprises six chapters that are devoted to essentially different physical situations. Before moving on to the main part of the book, let us present an overview of the whole field (see the two-dimensional map, Fig. 1). For the sake of presentation, this map is rather Procrustean: we had to squeeze and stretch things to fit them on the figure. For instance, it does not give important distinctions between normal and superconducting systems. Still, it suffices for the overview.

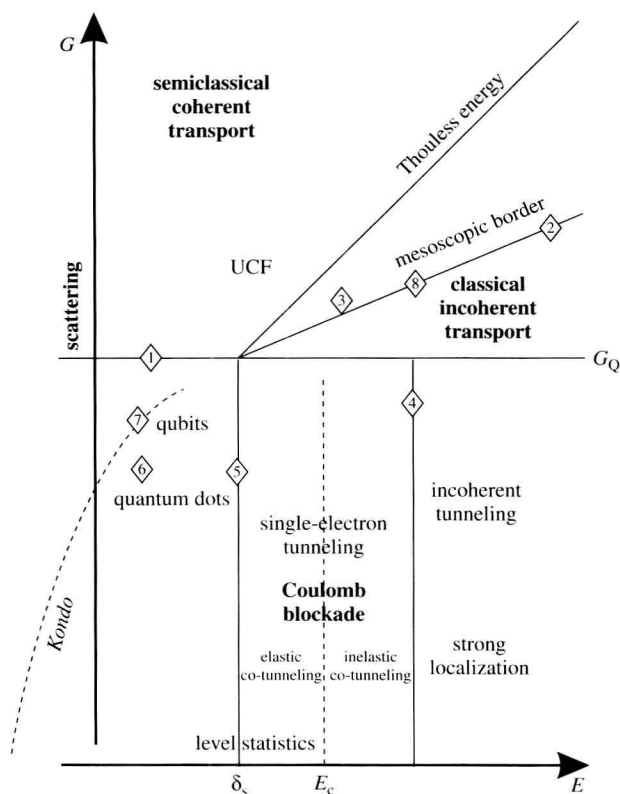


Fig. 1.

Map of quantum transport. Various important regimes are given here in a log-log plot. The numbered diamonds show the locations of some experiments described in the book (see the end of this Introduction for a list).

The axes represent the conductance of a nanostructure and the energy scale at which the nanostructure is operated; i.e. that set by temperature and/or voltage. This is a log-log plot, and allows us to present in the same plot scales that differ by several orders of magnitude. There is a single universal measure for the conductance – the conductance quantum G_Q . If $G \gg G_Q$, the electron conductance is easy: many electrons traverse a nanostructure simultaneously and they can do this in many ways, known as *transport channels*. For $G \ll G_Q$, the transport takes place in rare discrete events: electrons tunnel one-by-one. The regions around the cross-over line $G \simeq G_Q$ attract the most experimental interest and are usually difficult to comprehend theoretically.

There are several internal energy scales characterizing the nanostructure. To understand them, let us consider an example nanostructure that is of the same (by order of magnitude) size in all three dimensions and is connected to two leads that are much bigger than the nanostructure proper. If we isolated the nanostructure from the leads, the electron energies become discrete, as we know from quantum mechanics. Precise positions of the energy levels would depend on the details of the nanostructure. The energy measure of such quantum discreteness is the *mean level spacing* δ_s – a typical energy distance between the adjacent

levels. Another energy scale comes about from the fact that electrons are charged particles carrying an elementary charge e . It costs finite energy – the *charging energy* E_C – to add an extra electron to the nanostructure. This charging energy characterizes the interactions of electrons. At atomic scale, $\delta_S \simeq 1$ eV and $E_C \simeq 10$ eV. These internal scales are smaller for bigger structures, and E_C is typically much bigger than δ_S .

As seen in Fig. 1, these scales separate different regimes at low conductance $G \ll G_Q$. At high conductance, $G \gg G_Q$, the electrons do not stay in the nanostructure long enough to feel E_C or δ_S . New scales emerge. The time the electron spends in the nanostructure gives rise to an energy scale: the *Thouless energy*, E_{Th} . This is due to the quantum uncertainty principle, which relates any time scale to any energy scale by $(\Delta E)(\Delta t) \sim \hbar$. The Thouless energy is proportional to the conductance of the nanostructure, $E_{Th} \simeq \delta_S G / G_Q$, and this is why the corresponding line in the figure is at an angle in the log–log plot.

Another slanted line in the upper part of Fig. 1 is due to the electron–electron interaction, which works destructively. It provides intensive energy relaxation of the electron distribution in a nanostructure and/or limits the quantum-mechanical *coherence*. On the right of the line, the quantum effects in transport disappear: we are dealing with classical incoherent transport. At the line, the inelastic time, τ_{in} , equals the time the electron spends in the nanostructure, that is, $\hbar/\tau_{in} \simeq E_{Th}$. The corresponding energy scale can be estimated as $\simeq \delta_S (G/G_Q)^2 \gg E_{Th}$. In the context of mesoscopes, Thouless has suggested that extended conductors are best understood by subdividing a big conductor into smaller nanostructures. The size of such nanostructure is chosen to satisfy the condition $\hbar/\tau_{in} \simeq E_{Th}$. This is why all experiments where mesoscopic effects are addressed are actually located in the vicinity of the line; we call it the *mesoscopic border*.

Once we have drawn the borders, we position the material contained in each chapters on the map. Chapter 1 is devoted to the *scattering* approach to electron transport. It is an important concept of the field that at sufficiently low energies any nanostructure can be regarded as a (huge) scatterer for electron waves coming from the leads. At $G \gg G_Q$, the validity of the scattering approach extends to the mesoscopic border. At energies exceeding the Thouless energy, the energy dependence of the scattering matrix becomes important. In Chapter 1, we explain how the scattering approach works in various circumstances, including a discussion of superconductors and time-dependent and spin-dependent phenomena. We relate the transport properties to the set of transmission eigenvalues of a nanostructure – its “pin-code.” The basics explained in Chapter 1 relate, in one way or another, to all chapters.

If we move up along the conductance axis, $G \gg G_Q$, the scattering theory becomes progressively impractical owing to a large number of transport channels resulting in a bigger scattering matrix. Fortunately, there is an alternative way to comprehend this *semi-classical coherent regime* outlined in Chapter 2. We show that the properties of nanostructures are determined by *self-averaging* over the quantum phases of the scattering matrix elements. Because of this, the laws governing this regime, being essentially quantum, are similar to the laws of transport in classical electric circuits. We explain the machinery necessary to apply these laws – quantum *circuit theory*. The quantum effects are frequently concealed in this regime; for instance, the conductance is given by the classical Ohm’s law. Their

manifestations are most remarkable in superconductivity, the statistics of electron transfers, and spin transport. Remarkably, there is no limitation to quantum mechanics at high conductances as soon as one remains above the mesoscopic border.

Chapter 3 brings us to the lower part of the map – to conductances much lower than G_Q . There, the charging energy scale E_C becomes relevant, manifesting a strong interaction between the electrons (the *Coulomb blockade*). This is why we concentrate on the energies of the order of E_C , disregarding the mean level spacing δ_S . Transport in this *single-electron tunneling* regime proceeds via incoherent transfer of single electrons. However, the transfers are strongly correlated and can be precisely controlled – one can manipulate electrons one-by-one. The quantum correction to single-electron transport is *co-tunneling*, i.e. cooperative tunneling of two electrons. The energy scale $\sqrt{E_C \delta_S}$ separates inelastic and elastic co-tunneling. In the elastic co-tunneling regime, the nanostructure can be regarded as a scatterer in accordance with the general principles outlined in Chapter 1. The combination of the Coulomb blockade and superconductivity restores the quantum coherence of elementary electron transfers and provides the opportunity to build quantum devices of almost macroscopic size.

The material discussed in Chapter 4 is spread over several areas of the map. In this chapter, we address the statistics of persistent fluctuations of transport properties. We start with the statistics of discrete electron levels – this is the domain of low conductances, $G \ll G_Q$, and low energies, of the order of the mean level spacing. Then we go to the different corner, to $G \gg G_Q$ and the energies on the left from the mesoscopic border, to discuss fluctuations of transmission eigenvalues – the *universal conductance fluctuations* (UCF) – and the interference correction to transport, *weak localization*. The closing section of Chapter 4 is devoted to strong localization in disordered media, where electron hopping is the dominant mechanism of conduction. This implies $G \ll G_Q$ and high energies.

A fascinating development of the field is the use of nanostructures for quantum information purposes. Here, we do not need a flow of quantum electrons, but rather a flow of quantum information. Chapter 5 presents qubits and quantum dots, perhaps the most popular devices of quantum transport. For both devices, the discrete nature of energy levels is essential. This is why they occupy the energy area left of the level spacing δ_S on the map. We also present in Chapter 5 a comprehensive introduction to quantum information and manipulation.

In Chapter 6 we discuss interaction effects that do not fit into the simple framework of the Coulomb blockade. Such phenomena are found in various areas of the map. We start this chapter with a discussion of the underlying theory, called *dissipative quantum mechanics*. We study the effects of an electromagnetic environment on electron tunneling, remaining in the area of the Coulomb blockade. We go up in conductance to understand the fate of the Coulomb blockade at $G \gtrsim G_Q$ and the role of interaction effects at higher conductances. The electrons in the leads provide a specific (fermionic) environment responsible for the *Kondo effect* in quantum dots. The Kondo energy scale depends exponentially on the conductance and is given by the curve on the left side of the map. Finally, we discuss energy dissipation and dephasing separately for qubits and electrons. In the latter case, we are at the mesoscopic border.

At high energies one leaves the field of quantum transport: transport proceeds as commonly taught in courses of solid-state physics.

We have not yet mentioned the numbered diamonds in the map. These denote the location of several experiments presented in various chapters of the book.

- (1) Discovery of conductance quantization (Section 1.2);
- (2) interference nature of the weak localization (Section 1.6);
- (3) universal conductance fluctuations (Section 1.6);
- (4) single-electron transistor (Section 3.2);
- (5) discrete states in quantum dots (Section 5.4);
- (6) early qubit (Section 5.5);
- (7) Kondo effect in quantum dots (Section 6.6);
- (8) energy relaxation in diffusive wires (Section 6.8).

1.1 Wave properties of electrons

Quantum mechanics teaches us that each and every particle also exists as a wave. Wave properties of macroscopic particles, such as brickstones, sand grains, and even DNA molecules, are hardly noticeable to us; we deal with them at a spatial scale much bigger than their wavelength. Electrons are remarkable exceptions. Their wavelength is a fraction of a nanometer in metals and can reach a fraction of a micrometer in semiconductors. We cannot ignore the wave properties of electrons in nanostructures of this size. This is the central issue in quantum transport, and we start the book with a short summary of elementary results concerning electron waves.

A quantum electron is characterized by its *wave function*, $\Psi(\mathbf{r}, t)$. The squared absolute value, $|\Psi(\mathbf{r}, t)|^2$, gives the probability of finding the electron at a given point \mathbf{r} at time t . Quantum states available for an electron in a vacuum are those with a certain wave vector \mathbf{k} . The wave function of this state is a *plane wave*,

$$\Psi_{\mathbf{k}}(\mathbf{r}, t) = \frac{1}{\sqrt{\mathcal{V}}} \exp(i\mathbf{k} \cdot \mathbf{r} - iE(\mathbf{k})t/\hbar), \quad (1.1)$$

$E(\mathbf{k}) = \hbar^2 \mathbf{k}^2 / 2m$ being the corresponding energy. The electron in this state is spread over the whole space of a very big volume \mathcal{V} ; the squared absolute value of Ψ does not depend on coordinates. The prefactor in Eq. (1.1) ensures that there is precisely one electron in this big volume. There are *many* electrons in nanostructures. Electrons are spin 1/2 fermions, and the Pauli principle ensures that each one-particle state is either empty or filled with one fermion. Let us consider a cube in k -space centered around \mathbf{k} with the sides $dk_x, dk_y, dk_z \ll |\mathbf{k}|$. The number of available states in this cube is $2_s \mathcal{V} dk_x dk_y dk_z / (2\pi)^3$. The factor of 2_s comes from the fact that there are two possible spin directions. The fraction of states filled in this cube is called an electron *filling factor*, $f(\mathbf{k})$. The particle density n , energy density \mathcal{E} , and density of electric current \mathbf{j} are contributed to by all electrons and are given by

$$\begin{bmatrix} n \\ \mathcal{E} \\ \mathbf{j} \end{bmatrix} = \int 2_s \frac{d^3 \mathbf{k}}{(2\pi)^3} \begin{bmatrix} 1 \\ E(\mathbf{k}) \\ e\mathbf{v}(\mathbf{k}) \end{bmatrix} f(\mathbf{k}). \quad (1.2)$$

Here we introduce the electron charge e and the velocity $\mathbf{v}(\mathbf{k}) = \hbar \mathbf{k} / m$. Quantum mechanics puts no restriction on $f(\mathbf{k})$. However, the filling factor of electrons in an *equilibrium* state at a given electrochemical potential μ and temperature T is set by Fermi–Dirac statistics:

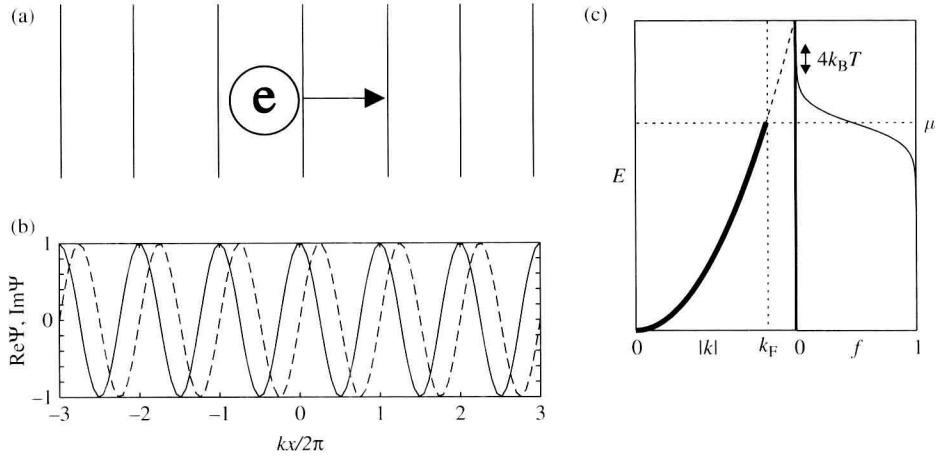


Fig. 1.1.

Electrons as waves. (a) An electron in a vacuum is in the plane wave state with the wave vector \mathbf{k} . (b) The profile of its wave function Ψ . (c) At zero temperature, the electrons fill the states with energies below the chemical potential μ ($|\mathbf{k}| < k_F$). At a given temperature, the filling factor f is a smoothed step-like function of energy.

$$f_{\text{eq}}(\mathbf{k}) = f_F(E(\mathbf{k}) - \mu) \equiv \frac{1}{1 + \exp((E - \mu)/k_B T)}. \quad (1.3)$$

The chemical potential at zero temperature is known as the Fermi energy, E_F .

Control question 1.1. What is the limit of $f_F(E)$ at $T \rightarrow 0$? Hint: see Fig. 1.1.

Next, we consider electrons in the field of electrostatic potential, $U(\mathbf{r}, t)/e$. The wave function $\Psi(\mathbf{r}, t)$ of an electron is no longer a plane wave. Instead, it obeys the time-dependent Schrödinger equation, given by

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \hat{H} \Psi(\mathbf{r}, t); \quad \hat{H} \equiv -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}, t). \quad (1.4)$$

This is an evolutionary equation: it determines Ψ in the future given its instant value. The evolution operator \hat{H} is called the *Hamiltonian*. For the time being, we concentrate on the stationary potential, $U(\mathbf{r}, t) \equiv U(\mathbf{r})$. The wave functions become stationary, with their time dependence given by the energy

$$\Psi(\mathbf{r}, t) = \exp(-iEt/\hbar) \psi_E(\mathbf{r}).$$

The Schrödinger equation reduces to

$$E \psi_E(\mathbf{r}) = \hat{H} \psi_E(\mathbf{r}) = \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right] \psi_E(\mathbf{r}). \quad (1.5)$$

The Hamiltonian becomes the operator of energy, while the equation becomes a linear algebra relation defining the eigenvalues E and the corresponding eigenfunctions Ψ_E of this operator. These eigenfunctions form a *basis* in the Hilbert space of all possible wave

functions, so that an arbitrary wave function can be expanded, or represented, in this basis. The first (gradient) term in the Hamiltonian describes the kinetic energy; the second term, $U(\mathbf{r})$, represents the potential energy.

A substantial part of quantum mechanics deals with the above equation. It cannot be readily solved for an arbitrary potential, and our qualitative understanding of quantum mechanics is built upon several simple cases when this solution can be obtained explicitly. Following many good textbooks, we will concentrate on the one-dimensional motion, in which the potential and the wave functions depend on a single coordinate x . However, we pause to introduce a key concept that makes this one-dimensional motion more physical.

1.1.1 Transmission and reflection

Let us confine electrons in a tube – a *waveguide* – of rectangular cross-section that is infinitely long in the x direction. We can do this by setting the potential U to zero for $|y| < a/2$, $|z| < b/2$ and to $+\infty$ otherwise. We thus create walls that are impenetrable to the electron and are perpendicular to the y and z axes. We expect a wave to be reflected from these walls, changing the sign of the corresponding component of the wave vector, $k_y \rightarrow -k_y$ or $k_z \rightarrow -k_z$. This suggests that the solution of the Schrödinger equation is a superposition of incident and reflected waves of the following kind:

$$\psi(x, y, z) = \exp(ik_x x) \sum_{s_y, s_z = +, -} C_{s_y, s_z} \exp(s_y i k_y y) \exp(s_z i k_z z). \quad (1.6)$$

Since the infinite potential repels the electron efficiently, the wave function must vanish at the walls, $\psi(x, y = \pm a/2, z) = \psi(x, y, z = \pm b/2) = 0$. This gives a linear relation between C_{s_y, s_z} that determines these superposition coefficients. To put it simply, the walls have to be in the nodes of a standing wave in both y and z directions. This can only happen if $k_{y,z}$ assume quantized values $k_y^n = \pi n_y/a$, $k_z^n = \pi n_z/b$, with integers $n_y, n_z > 0$ corresponding to the number of half-wavelengths that fit between the walls. The notation we use throughout the book here we introduce for the compound index $n = (n_y, n_z)$. The wave function reads as follows:

$$\begin{aligned} \psi_{k_x, n}(x, y, z) &= \psi_{k_x}(x) \Phi_n(y, z); \\ \psi_{k_x}(x) &= \exp(ik_x x); \\ \Phi_n(y, z) &= \frac{2}{\sqrt{ab}} \sin(k_y^n (y - a/2)) \sin(k_z^n (z - b/2)). \end{aligned} \quad (1.7)$$

The transverse motion of the electron is thus *quantized*. The electron in a state with the given n (these states are called *modes* in wave theory and *transport channels* in nanophysics) has only one degree of freedom corresponding to one-dimensional motion. The energy spectrum consists of one-dimensional branches shifted by a channel-dependent energy E_n (see Fig. 1.2), given by

$$E_n(k_x) = \frac{(\hbar k_x)^2}{2m} + E_n; \quad E_n = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_y^2}{a^2} + \frac{n_z^2}{b^2} \right). \quad (1.8)$$