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量子输运
——纳米科学导论

(影印版)

〔荷〕纳扎罗夫(Y. V. Nazarov)
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序 言

物理学是研究物质、能量以及它们之间相互作用的科学。她不仅是化学、生命、材料、信息、能源和环境等相关学科的基础,同时还是许多新兴学科和交叉学科的前沿。在科技发展日新月异和国际竞争日趋激烈的今天,物理学不仅囿于基础科学和技术应用研究的范畴,而且在社会发展与人类进步的历史进程中发挥着越来越关键的作用。

我们欣喜地看到,改革开放三十多年来,随着中国政治、经济、教育、文化等领域各项事业的持续稳定发展,我国物理学取得了跨越式的进步,做出了很多为世界瞩目的研究成果。今日的中国物理正在经历一个历史上少有的黄金时代。

在我国物理学科快速发展的背景下,近年来物理学相关书籍也呈现百花齐放的良好态势,在知识传承、学术交流、人才培养等方面发挥着无可替代的作用。从另一方面看,尽管国内各出版社相继推出了一些质量很高的物理教材和图书,但系统总结物理学各门类知识和发展,深入浅出地介绍其与现代科学技术之间的渊源,并针对不同层次的读者提供有价值的教材和研究参考,仍是我国科学传播与出版界面临的一个极富挑战性的课题。

为有力推动我国物理学研究、加快相关学科的建设与发展,特别是展现近年来中国物理学者的研究水平和成果,北京大学出版社在国家出版基金的支持下推出了“中外物理学精品书系”,试图对以上难题进行大胆的尝试和探索。该书系编委会集结了数十位来自内地和香港顶尖高校及科研院所的知名专家学者。他们都是目前该领域十分活跃的专家,确保了整套丛书的权威性和前瞻性。

这套书系内容丰富,涵盖面广,可读性强,其中既有对我国传统物理学发展的梳理和总结,也有对正在蓬勃发展的物理学前沿的全面展示;既引进和介绍了世界物理学研究的发展动态,也面向国际主流领域传播中国物理的优秀专著。可以说,“中外物理学精品书系”力图完整呈现近现代世界和中国物理

科学发展的全貌，是一部目前国内为数不多的兼具学术价值和阅读乐趣的经典物理丛书。

“中外物理学精品书系”另一个突出特点是，在把西方物理的精华要义“请进来”的同时，也将我国近现代物理的优秀成果“送出去”。物理学科在世界范围内的重要性不言而喻，引进和翻译世界物理的经典著作和前沿动态，可以满足当前国内物理教学和科研工作的迫切需求。另一方面，改革开放几十年来，我国的物理学研究取得了长足发展，一大批具有较高学术价值的著作相继问世。这套丛书首次将一些中国物理学者的优秀论著以英文版的形式直接推向国际相关研究的主流领域，使世界对中国物理学的过去和现状有更多的深入了解，不仅充分展示出中国物理学研究和积累的“硬实力”，也向世界主动传播我国科技文化领域不断创新的“软实力”，对全面提升中国科学、教育和文化领域的国际形象起到重要的促进作用。

值得一提的是，“中外物理学精品书系”还对中国近现代物理学科的经典著作进行了全面收录。20 世纪以来，中国物理界诞生了很多经典作品，但当时大都分散出版，如今很多代表性的作品已经淹没在浩瀚的图书海洋中，读者们对这些论著也都是“只闻其声，未见其真”。该书系的编者们在这方面下了很大工夫，对中国物理学科不同时期、不同分支的经典著作进行了系统的整理和收录。这项工作具有非常重要的学术意义和社会价值，不仅可以很好地保护和传承我国物理学的经典文献，充分发挥其应有的传世育人的作用，更能使广大物理学人和青年学子切身体会我国物理学研究的发展脉络和优良传统，真正领悟到老一辈科学家严谨求实、追求卓越、博大精深的治学之美。

温家宝总理在 2006 年中国科学技术大会上指出，“加强基础研究是提升国家创新能力、积累智力资本的重要途径，是我国跻身世界科技强国的必要条件”。中国的发展在于创新，而基础研究正是一切创新的根本和源泉。我相信，这套“中外物理学精品书系”的出版，不仅可以使所有热爱和研究物理学的人们从中获取思维的启迪、智力的挑战和阅读的乐趣，也将进一步推动其他相关基础科学更好更快地发展，为我国今后的科技创新和社会进步做出应有的贡献。

“中外物理学精品书系”编委会 主任
中国科学院院士，北京大学教授
王恩哥
2010 年 5 月于燕园

Quantum Transport

Introduction to Nanoscience

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CAMBRIDGE
UNIVERSITY PRESS

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

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 nanostuctures 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.

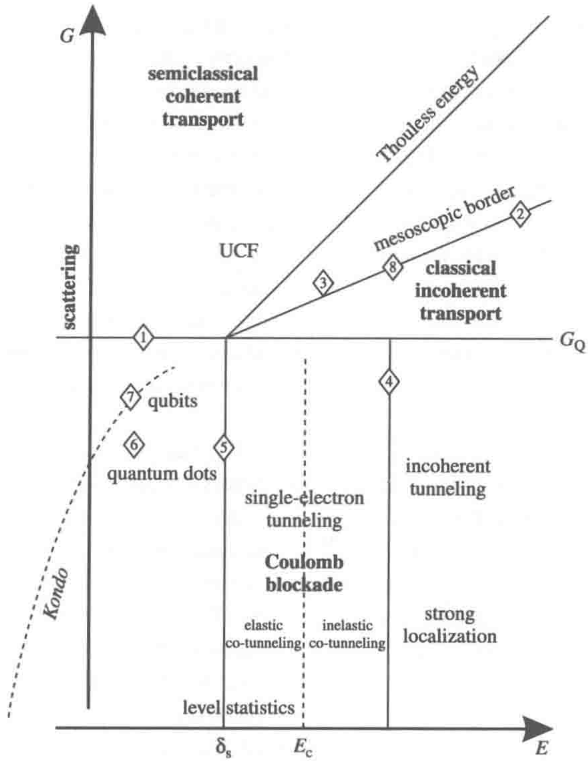

Fig. 1. **Map of quantum transport. Various important regimes are given here in a log–log plot. The numbered diamonds show the locations of some experiments described in the book (see the end of this Introduction for a list).**

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 change 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, $\delta_S \simeq 1\,\text{eV}$ and $E_C \simeq 10\,\text{eV}$. 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 mesoscopics, 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