Quantum Mechanics for Nanostructures

The properties of new nanoscale materials, their fabrication and applications, as well as the operational principles of nanodevices and systems, are solely determined by quantum-mechanical laws and principles. This textbook introduces engineers to quantum mechanics and the world of nanostructures, enabling them to apply the theories to numerous nanostructure problems.

The book covers the fundamentals of quantum mechanics, including uncertainty relations, the Schrödinger equation, perturbation theory, and tunneling. These are then applied to a quantum dot, the smallest artificial atom, and compared with the case of hydrogen, the smallest atom in nature. Nanoscale objects with higher dimensionality, such as quantum wires and quantum wells, are introduced, as well as nanoscale materials and nanodevices. Numerous examples throughout the text help students to understand the material.

VLADIMIR V. MITIN is SUNY Distinguished Professor at the Department of Electrical Engineering and Adjunct Professor of Physics at the University at Buffalo, The State University of New York. He is the author of eight textbooks and monographs and more than 490 professional publications and presentations.

DMITRY I. SEMENTSOV is Professor of Physics at Ulyanovsk State University, Russia. He is the author of more than 420 papers in peer-reviewed journals.

NIZAMI Z. VAGIDOV is Research Assistant Professor of Electrical Engineering at the University at Buffalo, The State University of New York. He is the author of about 90 professional publications in the fields of solid-state electronics, nanoelectronics, and nanotechnology.

Quantum Mechanics for Nanostructures

Vladimir V. Mitin
University at Buffalo, The State University of New York

Dmitry I. Sementsov
Ulyanovsk State University

Nizami Z. Vagidov
University at Buffalo, The State University of New York

CAMBRIDGE
UNIVERSITY PRESS

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

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/9780521763660

First published 2010

Printed in the United Kingdom at the University Press, Cambridge

A catalog record for this publication is available from the British Library

Library of Congress Cataloging in Publication data
Mitin, V. V. (Vladimir Vasil'evich)
Quantum mechanics for nanostructures / Vladimir V. Mitin, Dmitry I. Sementsov,
Nizami Z. Vagidov.
p. cm.
Includes index.
ISBN 978-0-521-76366-0 (hardback)
1. Quantum theory. 2. Nanostructured materials. I. Sementsov, Dmitry I.
II. Vagidov, Nizami Z. III. Title.
TA357.M58 2010
620′.5 – dc22 2010000700

ISBN 978 0 521 76366 0 Hardback

Contents

Preface

Nanoelectronics is a field of fundamental and applied science, which is rapidly progressing as a natural development of microelectronics towards nanoscale electronics. The modern technical possibilities of science have reached such a level that it is possible to manipulate single molecules, atoms, and even electrons. These objects are the building blocks of nanoelectronics, which deals with the processes taking place in regions of size comparable to atomic dimensions. However, the physical laws which govern electron behavior in nanoobjects significantly differ from the laws of classical physics which define the operation of a large number of complex electronic devices, such as, for example, cathode-ray tubes and accelerators of charged particles. The laws that govern electron behavior in nanoobjects, being of quantum-mechanical origin, very often seem to be very strange from a common-sense viewpoint. The quantum-mechanical description of electron (or other microparticle) behavior is based on the idea of the *wave–particle duality of matter*. The wave properties of the electron, which play a significant role in its motion in small regions, require a new approach in the description of the electron's dynamic state on the nanoscale. Quantum mechanics has developed a fundamentally new probabilistic method of description of particle motion taking into account its wave properties. This type of description is based on the notion of a wavefunction, which is not always compatible with the notion of a particle's trajectory. This makes electron behavior harder to understand.

The main objects of research in nanoelectronics are quantum-dimensional structures such as *quantum wells*, *quantum wires*, and *quantum dots*, where electron motion is limited in one, two, and three directions, respectively. The size of these quantum-mechanical objects is comparable to the *electron de Broglie wavelength*. In such structures electronic properties become different from those of bulk materials: new so-called low-dimensional effects become apparent. Quantum-mechanical laws govern various processes and define a significant modification of the energy spectrum, which is the main characteristic of an electronic system. The energy spectrum which characterizes the electron motion in the limited region becomes discrete. The structures with such an energy spectrum are the basis for the development of new types of nanoelectronic devices.

The physics of quantum-dimensional structures is currently developing rapidly and is beginning to form a separate field with quantum mechanics

as its basis. Only a small number of undergraduate engineering students take quantum-mechanics courses. However, there are only a few textbooks that are simple enough to understand for a wide range of engineering students, who would like to learn theoretical methods of analysis of the electronic properties of low-dimensional structures. While writing the current textbook we pursued two main goals: to present the main low-dimensional structures clearly from the physical point of view and to teach the reader the basics of quantum-mechanical analysis of the properties of such structures. Therefore, the experimental and theoretical material which will help the reader to understand the quantum-mechanical concepts applied to *nanostructures* is presented. Special attention is paid to the physical interpretation of quantum-mechanical notions. Theoretical material as well as the mathematical apparatus of quantum mechanics necessary for carrying out quantum-mechanical calculations independently is presented.

The book is written in such a way that it can be used by students who have studied classical physics to a sufficient extent as well as by students who have not had such an opportunity. The book consists of eight chapters and three appendices. The appendix material contains the main aspects of classical physics (particle dynamics, oscillations and waves in crystals, and electromagnetic fields and waves) which students can use while studying quantum mechanics.

In Chapter 1 we give a review of milestones in the development of *nanotechnology* and *nanoscience*. The main types of nanostructures are described and it is substantiated why it is necessary to use quantum physics for the description of their properties.

In Chapter 2 the main experimental facts which required the introduction of such unusual (for classical physics) notions as *wave–particle duality and uncertainty relationships*, among others, are described. The main notions and principles of the quantum-mechanical description are introduced. The Schrödinger equation – the main equation of non-relativistic quantum mechanics – is discussed in detail and its validity for the description of nanostructures is presented.

In Chapter 3 the solutions of the stationary Schrödinger equation are obtained for several important cases of one-dimensional motion. The main peculiarities of free electron motion as well as confined electron behavior are discussed. The main advantage of these solutions is in explanation and quantitative definition of the discrete energy levels of an electron when it moves in potential wells of various profiles.

In Chapter 4 the peculiarities of electron motion for structures wherein electron motion is confined in two and three dimensions are considered. It is shown that the discrete electron energy levels are characteristic for electron motion in potential wells of particular dimensionalities, in contrast to the continuous energy spectrum of a free electron. The structure's dimensionality and potential profile define the positioning of energy levels in the discrete energy spectrum.

The calculation of electron quantum states in various types of nanostructures generally encounters big mathematical difficulties. Therefore, approximate methods become very important for finding solutions of the Schrödinger equation. We consider in Chapter 5 several important and widely used approximate methods for calculation of electron wavefunctions, energy states, and transition probabilities between quantum states.

Chapter 6 is dedicated to finding wavefunctions, the geometry of electron clouds corresponding to them, and energy spectra of the simplest atoms and molecules using approximate methods.

When the size of the potential well is several times larger than the distance between atoms in a crystal, a fundamental reconstruction of the energy spectrum, which leads to a change in the physical properties of nanostructures, takes place. In Chapter 7 the main peculiarities of the electron energy spectrum in low-dimensional quantum structures (quantum wells, wires, and dots) as well as in periodic structures (superlattices) consisting of these low-dimensional nanostructures are considered.

In the last chapter – Chapter 8 – we consider the main methods of fabrication and characterization of nanostructures as well as their prospective applications in modern nanoelectronics.

Practically all chapters and appendices contain a large number of detailed examples and homework problems, which the authors hope will help students to acquire a deeper understanding of the material presented.

The authors have many professional colleagues and friends from different countries who must be acknowledged. Without their contributions and sacrifices this work would not have been completed. Special thanks go to the Division of Undergraduate Education of the National Science Foundation for the partial support of this work through its Course, Curriculum and Laboratory Improvement Program (Program Director Lance Z. Perez). The authors would like especially to thank Professor Athos Petrou for his editorial efforts in a critical reading of this book and for many valuable comments and suggestions. The authors also would like to thank undergraduate student Brian McSkimming for his thorough reading of the manuscript and helpful comments. We would like to thank undergraduate student Jonathan Bell for his help in preparation of figures.

Vladimir Mitin acknowledges the support and active encouragement of the faculty of the Department of Electrical Engineering and the Dean of the School of Engineering and Applied Sciences, Harvey G. Stenger Jr., as well as the members of the Center on Hybrid Nanodevices and Systems at the University at Buffalo, The State University of New York. He is also grateful to his family and friends for their strong support and encouragement, as well as for their understanding and forgiveness that he did not devote enough time to them while working on the book, and especially to his mother, grandson Anthony, and granddaughter Christina whom he missed the most.

Dmitry Sementsov thanks Tatiana Sementsova for her encouragement and help during the work on the manuscript.

Nizami Vagidov thanks his wife Saadat, his sons Garun, Timur, and Chingiz, his sisters Rukijat and Aishat, his brother Aligadji and their extended families for their constant support. Last but not least, he would like to thank his dissertation advisor, Professor Zinovi Gribnikov, for his encouragement and help.

Notation

Symbols

A – amplitude
A_{wf} – work function
a – lattice constant
a – acceleration
$\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$ – basis vectors
$\mathbf{B}$ – magnetic flux density
$\mathbf{C}$ – wrapping vector
C – capacitance
c – speed of light in vacuum
D – superlattice period
$\mathbf{D}$ – electric displacement
$\mathbf{d}$ – translation vector
E – energy of a particle
E_{c} – bottom of conduction band
E_{g} – bandgap
E_{i} – ionization energy
E_{v} – bottom of valence band
E_{F} – Fermi energy
$\mathbf{E}$ – electric field intensity
e – elementary charge
$\mathbf{e}_r$ – unit vector directed along radius vector $\mathbf{r}$
$\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ – unit coordinate vectors
$\mathbf{F}_{\mathrm{gr}}$ – gravitational force
$\mathbf{F}_{\mathrm{L}}$ – Lorentz force
$\mathbf{F}_{\mathrm{m}}$ – magnetic force
$\mathbf{F}_{\mathrm{e}}$ – electric force
g – acceleration due to gravity; density of states
$\mathbf{H}$ – magnetic field intensity
H_n – Hermite polynomials
$\hat{\mathcal{H}}$ – Hamiltonian operator
h – Planck's constant
$\hbar$ – reduced Planck constant

I – current
I_T – tunneling current
i, **j**, **k** – unit coordinate vectors
K – kinetic energy; superlattice wavenumber
k – spring constant; wavenumber
k – wavevector
k_B – Boltzmann's constant
$k_e = 1/(4\pi\epsilon_0)$ – coefficient in SI system
l – orbital quantum number
L – angular momentum
L_x, L_y, L_z – dimensions of a sample
m – orbital magnetic quantum number
m^* – effective mass of an electron
m_0 – mass of particle at rest
m_e – electron mass in vacuum
m_s – magnetic quantum number
N – number of states
N_A – Avogadro constant
n – principal quantum number; concentration
P – Poynting vector
$\mathcal{P}$ – pressure
P – probability
p – momentum
q – wavevector
Q – charge
q – charge of a particle
R – universal gas constant
r – magnitude of radius vector
r_1 – first Bohr radius
r – coordinate vector
R_∞ – Rydberg's constant
$\mathbf{R}_c$ – radius vector of center of mass
S – spin
S – cross-section
t – time
T – time period; ambient temperature
$\mathcal{T}_d$ – translation operator
U – potential energy; applied voltage
U_0 – height of potential barrier
U_G – gate voltage
u – displacement of atoms from their equilibrium positions
V – volume
v – velocity

v_{gr} – group velocity
v_{ph} – phase velocity
V_c – velocity of center of mass
W – work done by a force
$X(r)$ – radial function
x, y, z – spatial coordinates
Y_{ml} – spherical harmonics
α – angle; Madelung constant
β – force constant; $b/(2m)$
γ – gyromagnetic ratio
δ – logarithmic decrement of damping
$\delta(x)$ – Dirac's delta-function
ϵ – dielectric constant of the medium; relative deformation
ϵ_0 – permittivity of free space
ε – energy
ϕ – electrostatic field potential
φ – azimuthal angle; chiral angle; phase difference
λ – wavelength; parameter in characteristic equation
λ_{Br} – de Broglie wavelength
μ – magnetic permeability; magnetic moment
μ_l – orbital magnetic moment
μ_B – Bohr magneton
$\nabla^2 = \dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2}$ – Laplace operator
ψ – stationary wavefunction
Ψ – time-dependent wavefunction
Ω – angular velocity of a particle
ω – frequency
ω_e – frequency of electron oscillations
ω_q – frequency of harmonic oscillator
ρ – three-dimensional density
$\boldsymbol{\tau}$ – torque
θ – polar angle