

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.

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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 *nanostuctures* 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.

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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}_{gr} – gravitational force
- \mathbf{F}_L – Lorentz force
- \mathbf{F}_m – magnetic force
- \mathbf{F}_e – electric force
- g – acceleration due to gravity; density of states
- \mathbf{H} – magnetic field intensity
- H_n – Hermite polynomials
- \mathcal{H} – Hamiltonian operator
- h – Planck’s constant
- \hbar – reduced Planck constant

- I – current
- I_T – tunneling current
- $\mathbf{i}, \mathbf{j}, \mathbf{k}$ – unit coordinate vectors
- K – kinetic energy; superlattice wavenumber
- k – spring constant; wavenumber
- \mathbf{k} – wavevector
- k_B – Boltzmann’s constant
- $k_e = 1/(4\pi\epsilon_0)$ – coefficient in SI system
- l – orbital quantum number
- \mathbf{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
- \mathbf{P} – Poynting vector
- \mathcal{P} – pressure
- P – probability
- \mathbf{p} – momentum
- \mathbf{q} – wavevector
- Q – charge
- q – charge of a particle
- R – universal gas constant
- r – magnitude of radius vector
- r_1 – first Bohr radius
- \mathbf{r} – coordinate vector
- R_∞ – Rydberg’s constant
- \mathbf{R}_c – radius vector of center of mass
- \mathbf{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
- $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ – 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
- τ – torque
- θ – polar angle