Physics of Nanostructured Solid State Devices

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Dedicated to the memory of my father

Preface

This textbook is intended to introduce a first year graduate student of electrical engineering and/or applied physics to concepts that are critical to understanding the behavior of charge carriers (electrons and holes) in modern nanostructured solid state devices. The student is assumed to have undergraduate background in solid state physics, solid state devices, and quantum mechanics. Many of the topics discussed here are specific to ultrasmall (nanostructured) devices, but some are more general and apply to any solid. This material is the result of the author's teaching a graduate level introductory course on electron theory of solids in three US universities over a period spanning nearly 25 years. It has been his experience that once students are able to grasp the concepts presented here and become comfortable with them, they are able to handle more difficult and specialized topics quite easily.

This book is organized into nine chapters. The first chapter reviews the steady-state "drift–diffusion model" of charge transport in solids that electrical engineers typically learn in their first undergraduate solid state device course. Physics undergraduates are less exposed to this topic, but should be able to grasp the concept easily. This chapter introduces the basic drift–diffusion model, starting with two important assumptions about the nature of charge conduction in solids, and emphasizes the notion that this model is valid only as long as nonlocal transport effects are absent. It ends with an introduction to the so-called "equations of state" (also known as drift–diffusion equations) that are used to compute the carrier concentration and current density in a solid state device self-consistently. Only steady-state transport is considered.

Chapter 2 discusses a more sophisticated charge transport model based on the Boltzmann Transport Equation (BTE). It derives this equation from conservation principles, and then uses it to deduce the generalized moment equation (or the hydrodynamic balance equation) which governs charge transport in the presence of both local and nonlocal effects. The steady-state drift–diffusion equations of Chap. 1 are shown to be special cases of the last equation. Two methods of solving the BTE—the relaxation time approximation and the Monte Carlo (MC) simulation method—are discussed and some analytical results are obtained from the relaxation time approximation. This chapter also discusses linear response transport or ohmic conduction and finds an expression for the linear response conductivity. It then distinguishes chemical potential from electrostatic potential inside a device and discusses a few important thermodynamic concepts pertinent to charge transport. Overall, the purpose of this chapter is to provide a sound basis for understanding both linear and nonlinear (or hot-carrier) transport in solids.

Chapter 3 reviews basic concepts in quantum mechanics, operators and their applications, energy quantization in quantum-confined systems (i.e., nanostructures) such as quantum wells, wires and dots, and ends with a description of time-independent and time-dependent perturbation theory. The purpose is to present the essential tools needed to understand and appreciate the quantum foundations of nanostructured solid state devices. As an example of applying quantum mechanics to a solid state device, time-independent perturbation theory is employed to elucidate the operation of an electro-optic modulator based on the quantum-confined Stark effect. Performance metrics of this device are calculated using perturbation theory, thereby exemplifying how quantum mechanics plays a critical role in device operation.

Chapter 4 presents methods of calculating the bandstructure (energy versus wavevector relation) of a crystalline solid based on time-independent perturbation theory. Since bandstructure plays a vital role in the operation of many devices, particularly optical devices, it is included in this book. More importantly, it is one more application of time-independent perturbation theory to an actual problem. We discuss four different bandstructure calculation methods—the nearly-free electron method, the orthogonalized plane wave (OPW) expansion method, the tight-binding approximation (TBA) and the $\vec{k} \cdot \vec{p}$ theory—three of which invoke time-independent perturbation theory. Band structure results are then applied to calculate the density of states of electrons and holes as a function of particle energy in bulk (three-dimensional systems) and nanostructured systems such as quantum wells (quasi two-dimensional) and wires (quasi one-dimensional). Based on the density of states, analytical expression are derived for equilibrium carrier concentrations in three-, two- and one-dimensional structures. This chapter ends with a derivation of the phonon and photon density of states in a crystal.

Chapter 5 illustrates the application of time-dependent perturbation theory to transport physics. It uses this theory to derive Fermi's Golden Rule which provides a useful prescription to calculate the rate with which an electron scatters as it travels through a solid and interacts with various entities such as impurities and phonons. These rates appear in the BTE and are first mentioned in Chap. 2, but derived here. In order to make the student comfortable in applying Fermi's Golden Rule to various problems, the scattering rate of an electron interacting with nonpolar acoustic phonons is derived in three-, two-, and one-dimensional systems as a function of the electron's kinetic energy. Such exercises are extremely instructive and reveal important physics associated with carrier interactions with the environment in both bulk- and quantum-confined systems. Once students master the technique of calculating the scattering rate due to any one type of interaction, they should be able to calculate the rate associated with any other type of interaction since the basic principle is the same. A few advanced topics such as phonon confinement and phonon bottleneck effects are also discussed.

Chapter 6 discusses electron–photon interactions and their impact on the optical properties of solids, while addressing the general concepts of absorption, spontaneous emission, and stimulated emission of light. Fermi's Golden Rule is utilized to calculate absorption and luminescence intensities as a function of photon energy in three-, two and one-dimensional systems. The basic physics behind the operation of some solid state optical devices, such as light emitting diodes (LED) and lasers, is also discussed. This chapter also discusses excitons since they impact optical properties of solids, and could produce nonlinear optical effects. Finally, some special topics of current interest in nanophotonics, such as polariton lasers, photonic crystals, and negative refraction are discussed. This is the only chapter that deals with "optical properties" of nanostructured solids; the rest are mainly focused on "transport properties."

Chapter 7 discusses the behavior of an electron in a magnetic field. It first introduces the Dirac equation and the Pauli equation to account for an electron's spin explicitly and then focuses on the "spinless" electron in order to discuss effects unrelated to the spin. The important concepts of magnetic vector potential and "gauge" are introduced, and the Schrödinger equation is solved in two- and one-dimensional systems to find the wavefunctions and energy eigenstates. Solution of the Schrödinger equation in a two-dimensional system leads to the idea of Landau level quantization, as well as its observable effects such as Shubnikov–deHaas conductance oscillations. In the context of one-dimensional systems, the concept of edge states is introduced along with hybrid magneto-electric states. A device application of the physics, namely the operation of a magneto-optical device based on quantum-confined Lorentz effect (QCLE) (a magnetic analog of the quantum-confined Stark effect) is discussed. This chapter concludes with a few basic remarks regarding the integer and fractional quantum Hall effect (FQHE).

Chapter 8 introduces some popular quantum transport formalisms such as the scattering matrix formalism, the Landau–Vlasov equation (which can be viewed as a quantum-mechanical equivalent of the collisionless BTE), the nonequilibrium Green's function approach, the Wigner distribution function, the Tsu–Esaki formalism, and the Landauer–Büttiker approach for linear response transport. Applications of these formalisms are presented in Chap. 9.

In Chap. 9, some of the quantum transport formalisms developed in Chap. 8 are applied to actual quantum devices. The Tsu–Esaki formula is used to calculate the tunneling current in resonant tunneling devices and numerous mesoscopic devices and phenomena are treated with the Landauer–Büttiker formalism. This chapter is intended to show how quantum mechanics impacts the operation of nanostructured devices.

The author is grateful to his numerous graduate students who had this course and often made valuable contributions to developing the course material. There are too

many of them to name here. He is also indebted to an anonymous reviewer who made helpful comments while reviewing the draft.

As always, in spite of the author's best efforts at proof reading, it is possible that some typographical errors have eluded detection. The author will be immensely grateful if they are brought to his notice by e-mailing him at sbandy@vcu.edu.

Welcome to the world of electron physics in nanostructured devices!

Table of Constants

Table 1 Table of universal constants

Free electron mass (m_0)	9.1×10^{-31} Kg.
Dielectric constant of free space (ϵ_0)	8.854×10^{-12} Farads/meter
Electronic charge (e)	1.61×10^{-19} Coulombs
Reduced Planck constant ($\hbar$)	1.05×10^{-34} Joules-sec
Bohr radius of ground state in H atom (a_0)	0.529 Å= 5.29×10^{-11} meters
Bohr magneton (μ_B)	9.27×10^{-24} Joules/Tesla

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