

Preface

The vigorous developments in nanoscience and nanotechnology in such areas as materials science, nanoelectronics and nanodevices, microfluidics, photonics, nano-optoelectronics, plasmonics, phononics, quantum computing, new phases of matter, and quantum information clearly require fundamental knowledge across all areas of physics, aside from familiarity with other established disciplines such as chemistry and microbiology. For physicists and engineers engaged in the analyses of experimental results, physical modeling, and large-scale numerical simulation of active nanodevices and nonequilibrium properties of nanostructures or open nanosystems, there is a need for a broad knowledge of the theoretical foundation of relevant quantum physics. It is the aim of this book to try to fill this need for computational scientists and engineers, as well as for people from other disciplines who felt the need to ‘cross the isle’.

This book provides a comprehensive introduction to two significant and pertinent theoretical developments, namely, (a) quantum superfield theory of nonequilibrium quantum physics in real time, and (b) discrete phase-space quantum mechanics. These two formalisms combine to form the foundation of computational nanoscience of *functional* nanomaterials and nanotechnology. Although the formulation of discrete phase space quantum mechanics was originally motivated to describe energy-band quantum dynamics of charge-carriers in crystalline solid,¹ it now occupies the central idea in the dynamics of qubit or two-state system in quantum computing.

The field of mesoscopic physics experienced a growth surge in the nineteen eighties. These studies involve the linear approximation of quantum transport in mesoscopic systems, basically serving as a departure from the statistical character of the well-known Kubo formula for the conductivity of condensed matter. On the other hand, the field of nanoelectronics requires the full power of nonequilibrium quantum physics to characterize the highly nonlinear and ultrafast characteristics of quantum nanodevices, where the quantum distribution function inside a nanodevice is

¹There, the number of lattice points is odd by virtue of the crystal inversion symmetry. The use of multiplicative inverse assumes that the number of lattice points is a prime number, primality is required for the nonzero elements to have multiplicative inverses.

required to match with the classical distribution function at the connecting leads, possessing a much larger number of degrees of freedom.

The purpose of this book is to give a broad analytical tool for attacking problems in quantized nonequilibrium dynamics of particles and fields in open systems, especially when openness is due to boundary interface and current-lead contacts (serving as particle and/or energy source and sink in nanodevices). Thus, a more complete background on quantum mechanical techniques is given in the first part of the book. It is intended to make the book self-contained for studying nonequilibrium quantum physics, to help graduate students and entering researchers pursue independent research on the challenging area of highly nonequilibrium nanoscience and nanotechnology. A deeper understanding of discrete quantum mechanics also requires us to give a brief overview of quantum computing and quantum information from a new point of view, which serves as an introduction to this intriguing area of research by itself. A strong emphasis on the principal role of generalized canonical variables in quantum physics, Hermitian and non-Hermitian, discrete and continuum, is the recurring theme that occupies most of the theoretical discussions in this book.

This book consists of eight parts. In Part 1 the foundation and methodology in quantum mechanics of particles and fields is given. Part 2 contains discussions of mesoscopic physics, centered on the Landauer and Landauer-Büttiker quantum conductance formulas. In Part 3 a number of quantum semiconductor quantum devices illustrate some of the novel devices that characterized the developments in nanoelectronics, including a more detailed discussion of the device physics of resonant tunneling nanodevices. A generalized quantum superfield theoretical formulation of nonequilibrium quantum physics in real time is discussed in Part 4. In Part 5 the operator Hilbert-space methods and quantum tomography based on mutually-unbiased bases are given in preparation for Part 6. In Part 6 the phase space formulation of discrete Wigner function on finite field and discrete phase-space quantum tomography is given. In Part 7 the phenomenological treatment of open quantum systems in terms of generalized measurements and evolution superoperator is given to supplement Part 4, to help clarify the various nonequilibrium correlation functions used in quantum superfield theoretical technique. For example, the dissipation, noise and mass kernels are discussed in more detail. An overview of quantum computing and quantum information, explicitly from the discrete phase-space point of view, is found in Part 8.

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