# Preface

This book is an introduction to a rapidly developing field of modern theoretical physics—the theory of quantum transport at nanoscale. The theoretical methods considered in the book are in the basis of our understanding of charge, spin, and heat transport in nanostructures and nanostructured materials and are widely used in nanoelectronics, molecular electronics, spin-dependent electronics (spintronics), and bioelectronics. Although some of these methods are already 20–25 years old, it is not so easy to find their systematic and consecutive description in one place. The main theoretical models and methods are distributed among many original publications, often written in different style and with different notations. During my research and teaching activities I had to overcome many obstacles to find required information. The results of my search I now present to your attention in more or less ordered form together with some original investigations.

The book is based on the lecture notes I used in the courses for graduate and postgraduate students at the University of Regensburg and Technische Universität Dresden (TU Dresden). Some base knowledge of theoretical physics, especially quantum mechanics, is assumed. But otherwise I have tried to make the text self-consistent and to derive all formulas. In some cases I have given the references for additional reading.

As this book grew up from the lecture notes, I hope it will serve as an advanced-level textbook for Master and Ph.D. students, and it can also be interesting to the experts working in the fields of quantum transport theory and nanoscience. To this end I have tried to combine modern theoretical results with the pedagogical level of explanations. This book will help to cover, to some extent, the gap between undergraduate-level textbooks and present day theoretical papers and reviews.

The book includes the Introduction and two parts. The first part is devoted to the basic concepts of quantum transport: Landauer–Büttiker method and matrix Green function formalism for coherent transport, Tunneling (Transfer) Hamiltonian and master equation methods for tunneling, Coulomb blockade, vibrons and polarons. The results in this part are obtained as possible without sophisticated techniques,

such as nonequilibrium Green functions, which are considered, in detail, in the second part. We give a general introduction to the nonequilibrium Green function theory. We describe in detail the approach based on the equation-of-motion technique, as well as a more sophisticated one based on the Dyson–Keldysh diagrammatic technique. The attention is mainly paid to the theoretical methods able to describe the nonequilibrium (at finite voltage) electron transport through interacting nanosystems, specifically the correlation effects due to electron-electron and electron-vibron interactions. We consider different levels of theoretical treatment, starting from a few-level model approach, such as the single-level electron-vibron (polaron) model and the Hubbard–Anderson model for Coulomb interaction. The general formalism for multilevel systems is considered, and some important approximations are derived.

The book is focused on the ideas and techniques of quantum transport theory in discrete-level systems, as it is discussed in detail in the Introduction. But we do not consider here explicitly particular applications of the theory to semiconductor devices or the molecular transport theory based on atomistic methods, in particular density functional theory (DFT).

The Introduction includes a comprehensive literature review, but for sure not complete. In the main text I did not try to cite all relevant publications, because it is more a textbook than a review. Nevertheless, I want to apologize for possibly missing important references.

Despite large efforts and time spent to improve the manuscript and to check it for misprints, the book definitely contains some mistakes, misprints, something is missed and should be added, as well as something would be better removed. I will greatly appreciate any comments and suggestions for improvement.

Dresden, Germany Dmitry A. Ryndyk

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