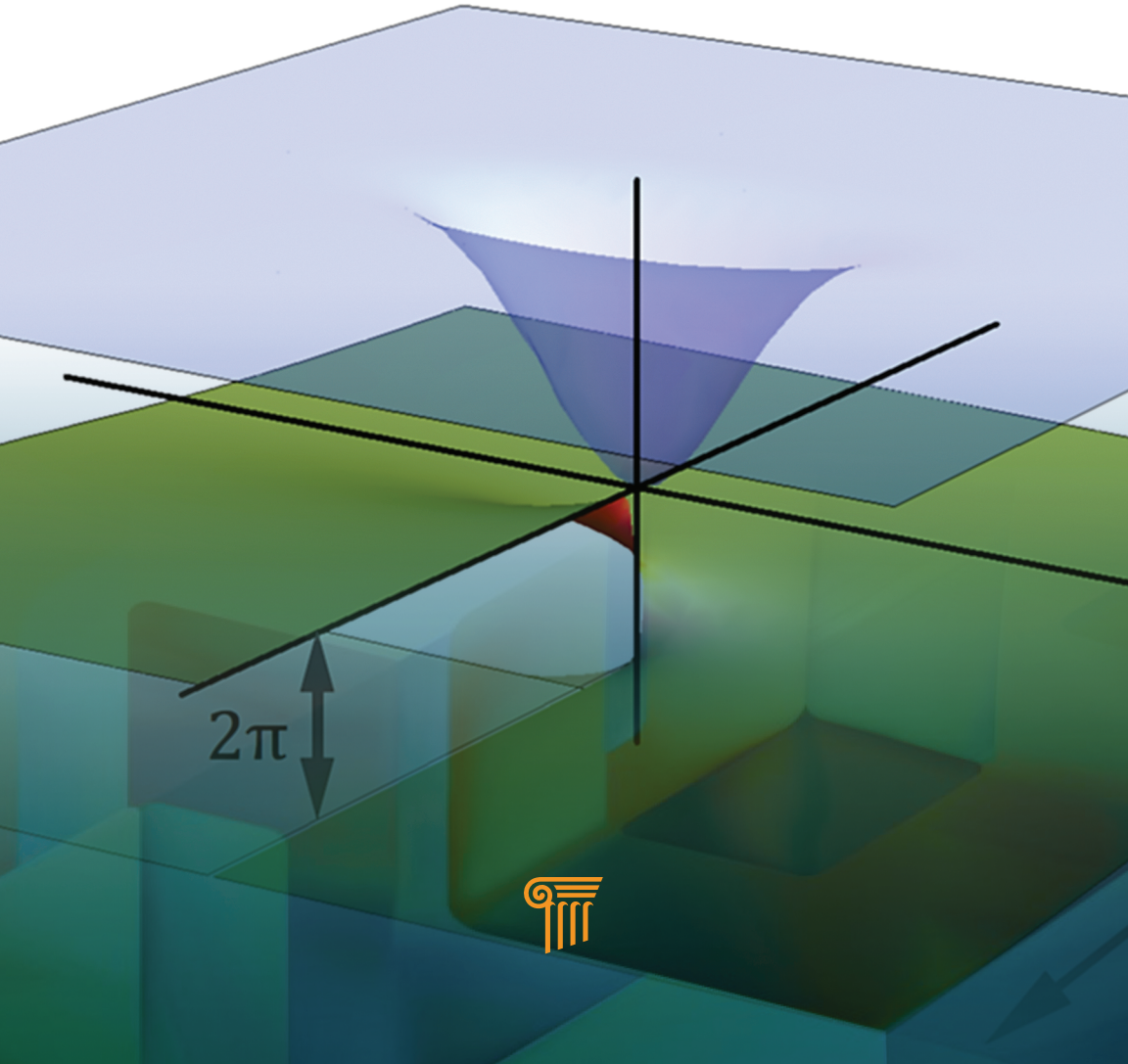
Dissipative Quantum Mechanics of Nanostructures

Electron Transport, Fluctuations, and Interactions

Andrei D. Zaikin | Dmitry S. Golubev



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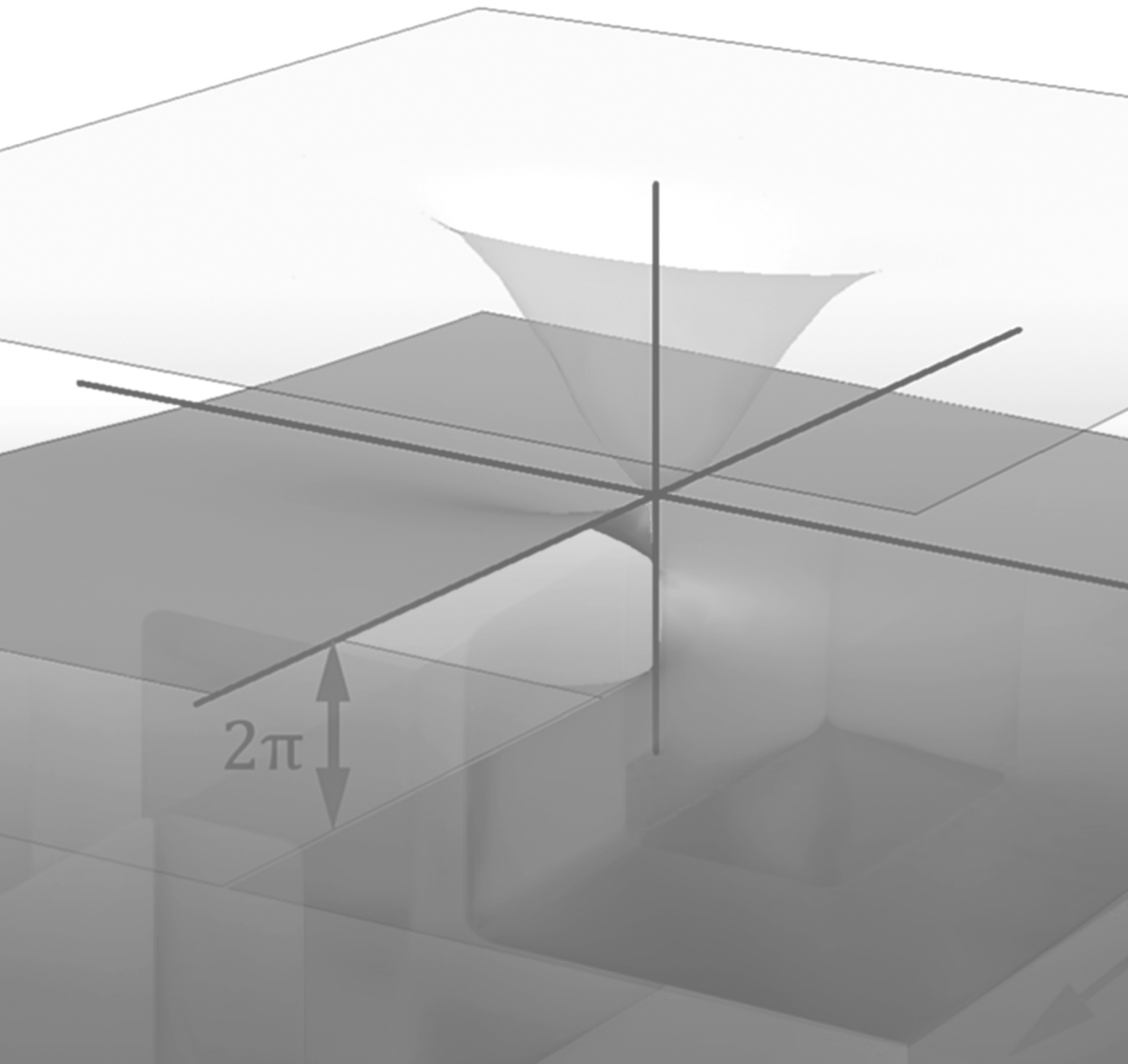

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To my father and teacher

—Andrei D. Zaikin

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Preface

This book is a largely extended and updated version of the lecture course that one of us (A. D. Z.) taught at I. E. Tamm Department of Theoretical Physics of P. N. Lebedev Physical Institute in Moscow in 2007–2008. The purpose of this book is to provide a systematic and comprehensive coverage of physical ideas, theoretical methods, and key results in a rapidly developing field of quantum transport and macroscopic quantum phenomena in a wealth of available nanoscale structures. Better understanding of the whole scope of such phenomena is extremely important both from fundamental point of view as well as for fabrication of high-quality nanodevices with controlled parameters involved in a variety of applications.

In nanostructures elementary charge carriers—electrons—are usually confined to a limited volume interacting both with each other and with lattice ions and simultaneously suffering multiple scattering events on impurities, barriers, surface imperfections, and other defects. Electron interaction with other degrees of freedom generally yields two major consequences—*quantum dissipation* and *quantum decoherence*. In other words, even at very low temperatures interacting electrons can lose both their energy and their ability to quantum interference. These two different (though not unrelated) processes are at the heart of all quantum phenomena discussed in this book.

A perturbative in the interaction approach—intuitively appealing due to its relative simplicity—often fails to adequately account for quantum dynamics of interacting many-body systems, particularly in the low energy limit. In such cases one has no choice but to employ nonperturbative techniques. Path integral formulation of quantum theory is particularly well suited for this purpose and it is intensively exploited throughout our book. Most conveniently, path

integral methods allow to implement the central idea of tracing out all the degrees of freedom of an interacting system on which no direct measurements are being performed and, at the same time, keeping complete information about the influence of those on the remaining variable(s) of interest to be measured. In this way we arrive at the concept of effective actions and Feynman-Vernon influence functionals. This approach is elaborated and employed for the analysis of quantum transport and fluctuations in mesoscopic and nanostructured conductors in the presence of interactions.

This book is useful for a possibly broader readership ranging from masters and PhD students to post docs and senior researchers. We assume that the reader has basic knowledge of quantum mechanics and statistical physics (within the frames of the standard university courses) and is also familiar with the Feynman path integrals on an introductory level. The book is divided into two parts. Its first part covers relatively more conventional materials and can also be used as a textbook at the master student level. The second part of the book deals with a number of topics which, although also quite well established by now, may be viewed by some readers as somewhat more advanced. At the same time, this is by no means "two books in one," all 20 chapters are united within the same general concept and, as the reader will observe, are intimately related to each other in many respects. In this sense, the book division into two parts can also be disregarded, if one so wishes.

We have made a substantial effort to make the book self-contained. In most cases we provide the reader with sufficient details and explanations for understanding the basic physics behind the result and learning how this result can technically be reproduced without digging into a lot of extra literature. It is by no means our goal here to present an extensive coverage of the experiment; only in a few exceptional cases we give a brief account of the experimental situation in the corresponding sub-field. At the same time, we provide sufficiently rich bibliography that allows to overview all topics touched upon in this book. While selecting these topics we were merely guided by our research interests and experience. Some other topics are inevitably left behind, which does not necessarily reflect their secondary importance for the field.

In this book we express our views on the field which have been formed in the course of our own research and—not to a lesser extent—as a result of our continuous collaborations and valuable discussions with our many colleagues and friends who shared their interest on this beautiful piece of physics. It is a pleasure to thank all of them for the numerous fruitful interactions we had with them over decades of our research.

Andrei D. Zaikin
Dmitry S. Golubev
Spring 2019

Introduction

Quantum physics of nanostructures is a rich and rapidly developing field. Most of the fundamental problems of modern condensed matter physics involve various aspects of quantum transport and fluctuation phenomena at the nanoscale. In addition, continuing miniaturization of devices, gadgets, and electronic schemes, together with quickly growing number of nanotechnological applications, also demand a profound understanding of the underlying physics.

What are the main specific features of nanostructures? On one hand, these systems are *low-dimensional* by definition. As physics in reduced dimension may differ quite substantially from that in the bulk, theoretical tools should be adjusted accordingly in order to properly respond to the above challenges. On the other hand, the number of relevant degrees of freedom, such as electrons and magnetic impurities. still remains *macroscopically large* despite the small system size. In this situation it is essential to properly account for quantum many-body effects which occur in the presence of interactions. Hence, one generally needs to simultaneously describe both quantum mechanical and quantum statistical evolution of the system. In other words, in order to determine the behavior of relevant observables it is necessary not only to perform the corresponding quantum averages but also to determine the quantum state with respect to which these averages are being performed.

General and elegant ways to deal with this situation were proposed in sixties in two seminal papers by Keldysh [220] and by Feynman and Vernon [119]. Approaching the problem from somewhat different prospectives these authors formulated the central idea to describe quantum evolution of an interacting

many-body system in terms of a single particle density matrix. As quantum dynamics of the latter is determined by the product of the two corresponding matrix elements one naturally arrives at the concept of real-time evolution along the so-called *Keldysh contour* which consists of forward and backward time branches. Interactions generally mix up quantum variables defined on each of these branches making it impossible to consider one of them independently of the other. This idea allowed Keldysh to formulate the diagram technique fully describing quantum dynamics of non-equilibrium interacting many-body systems.

Feynman and Vernon took a somewhat different route. They proposed to trace out all "non-interesting" degrees of freedom already at the very beginning of the calculation and then to deal with the reduced density matrix which only accounts for the observable(s) of interest. Technically this approach is most conveniently implemented with the aid of Feynman path integrals and yields the concept of *Feynman–Vernon influence functional,* which in general contains complete information about the influence of the averaged out degrees of freedom on the variable(s) of interest. The equivalence of Keldysh and Feynman–Vernon techniques is verified by expanding the reduced density matrix derived within the latter approach in powers of the corresponding influence functional. In this way one formally recovers the full diagrammatic series of the Keldysh technique.

This book deals with a broad scope of applications of the influence functional technique in condensed matter physics. It consists of 20 chapters and is divided into two parts. The first part (Chapters 1 to 7) describes the basics of the influence functional theory and several most well-known applications of this powerful technique. In Chapter 1 we introduce Feynman–Vernon influence functionals and discuss the Caldeira–Leggett effective action approach to quantum dissipation. This approach yields Gaussian influence functional which captures a number of generic features of quantum dissipative environments and, at the same time, remains simple enough to deal with practical calculations. We also illustrate the relation between the Feynman–Vernon-Caldeira–Leggett path integral technique and several other methods, such as quasiclassical Langevin equation, quantum mechanical time depen-

dent perturbation theory, and Keldysh technique. In Chapter 2 we extend Feynman–Vernon idea of the influence functional, applying it to junctions between two bulk normal metals or superconductors. Of primary importance here is the case of tunnel (Josephson) junctions. Starting from the microscopic Hamiltonian for such systems we trace out all electron degrees of freedom (playing the role of an effective quantum dissipative bath) and derive the so-called Ambegaokar–Eckern–Schön (AES) effective action formulated in terms of a single collective variable—the Josephson phase—which accounts for quantum dissipative dynamics of the system. We also demonstrate how to extend this microscopic approach to metallic junctions with arbitrary transmissions of their conducting channels and to spatially extended metallic conductors. We emphasize a direct link between these results and the phenomenological Caldeira–Leggett effective action derived in Chapter 1.

In Chapters 3–7 we discuss several important examples illustrating key advantages of the influence functional technique developed in Chapters 1 and 2. In Chapter 3 we analyze real-time dynamics of a quantum particle interacting with a dissipative Caldeira–Leggett bath and introduce one of the most fundamental concepts in quantum theory—quantum decoherence. Provided this particle is moving in the absence of any external potential (or in a parabolic potential) one can obtain an exact solution of the problem which also allows to address the issue of quantum decoherence without employing any approximation. In many physical situations, however, nonlinear effects can also play a substantial role. In those cases no exact solution is anymore possible, and one should reside to various approximations. One example of that kind—a dissipative quantum particle on a ring described by the action equivalent to that of AES—is addressed in Chapter 3.

In Chapter 4 we consider another important physical example—quantum dissipative decay of a metastable state. Yet another example, quantum dynamics of a damped particle in a double-well potential, is discussed in Chapter 5. Both these problems are of a special interest in connection with fundamentally important experiments on macroscopic quantum tunneling (MQT) and macroscopic quantum coherence (MQC) demonstrating macroscopic quantum behavior of Josephson junctions, as also indicated in Chapter 2.

The situation of "tunneling into continuum" addressed in Chapter 4 essentially implies incoherent decay since the probability for a quantum particle to return back to its initial state is negligibly small due to both the potential profile and the effect of dissipation. On the contrary, in the case of a double-well potential with (almost) degenerate minima considered in Chapter 5 the quantum particle can tunnel back and forth between these minima gradually losing its coherence in the presence of weak dissipation. Obviously such process cannot anymore be described in terms of incoherent decay and the probability to find the particle in one of the wells exhibits damped coherent oscillations in time. In practice this situation can be realized, e.g., in a Josephson junction embedded in a superconducting loop in which case coherent oscillations of the magnetic flux inside the loop can be observed. Such systems can also be used for practical implementation of superconducting qubits.

Chapter 6 continues our analysis of macroscopic quantum dynamics of ultrasmall Josephson junctions. Provided the bias current is weak, many minima of the Josephson potential in the phase space have almost the same energy and quantum dynamics of the phase variable gets substantially modified as compared to that studied in Chapter 5. According to quantum mechanics, in this case the wave function of a "Josephson particle" describes Bloch states. Dissipation can significantly alter this picture. In Chapter 6 we demonstrate that nontrivial interplay between quantum coherence, dissipation and Coulomb effects yields a rich variety of properties which can be accessed not only by means of the Josephson phase variable but also through the canonically conjugate quantum variable of the junction charge. In the presence of linear Ohmic dissipation these two variables turn out to be strictly dual to each other. This remarkable property allows one to proceed much further in understanding of this problem.

It is rather obvious that quantum fluctuations, dissipation and Coulomb effects should persist not only in superconducting but also in normal tunnel junctions provided their size remains sufficiently small. In Chapter 7 we specifically address quantum behavior of tunnel nanojunctions between two normal metallic electrodes. Transport properties of such structures turn out to be rather complicated provided Coulomb interaction between electrons is

taken into account. Coulomb interaction tends to block the process of electron tunneling between metallic electrodes and, hence, to reduce the current flowing through a tunnel barrier. On the other hand, electron tunneling gives rise to charge fluctuations which in turn tend to diminish Coulomb blockade effects. This nontrivial trade-off in small size tunnel junctions is analyzed in details in Chapter 7.

In the second part of this book we further develop the idea of the influence functional applying it to a number of advanced problems of modern condensed matter theory. With this analysis we in general go quite far both from the simple Caldeira–Leggett model of Chapter 1 and from the AES approach of Chapter 2. Following this route we discover plenty of new physics not contained within the Caldeira–Leggett type of models.

Chapters 8 and 9 deal with the problem of a quantum particle propagating in a diffusive electron gas. Provided this particle (e.g., a muon) is distinguishable from electrons in a disordered metal the corresponding influence functional can be constructed relatively easily just by taking into account the effect of quantum electromagnetic fields produced by fluctuating electrons forming an effective environment. In Chapter 8 we implement this program and arrive at a non-Gaussian influence functional for a quantum particle, which is then employed to describe equilibrium properties of this particle in the presence of interactions and disorder. In particular, addressing the effect of persistent currents we again approach the problem of interaction-induced quantum decoherence at low temperatures. In contrast to Chapter 3, however, we do not anymore restrict our analysis to the phenomenological Caldeira–Leggett model but rather employ a microscopically derived influence functional for a diffusive electron gas.

Turning now to the problem of a degenerate interacting electron gas one immediately observes a conceptual problem: Direct application of the same influence functional formalism as in Chapter 8 fails in this case simply because electrons are indistinguishable. Each electron could simultaneously be a particle of interest and a part of an effective environment for this particle. Hence, in order to apply the Feynman–Vernon strategy to interacting Fermi systems it is necessary to keep track of the Pauli principle. This task is

accomplished in Chapter 9. The key step here is to derive a formally exact equation for the density matrix of a single electron propagating in the environment formed by quantum electromagnetic fields produced by fluctuating electrons. This equation depends on the electron distribution function and, hence, explicitly accounts for the Pauli principle. Afterward one can integrate out the electromagnetic fields and construct the influence functional for interacting electrons in disordered metallic conductors, which includes Fermi statistics. We also consider several applications of this influence functional technique, including quantum kinetic equation approach, Keldysh technique for interacting fermions, and quasiclassical Langevin equation.

The path integral technique worked out in Chapter 9 usually allows for a straightforward non-perturbative treatment of the problem with disorder and interactions, provided one is able to properly identify relevant quasiclassical electron paths. Technically this is possible, e.g., for weakly disordered spatially extended conductors. On the other hand, for spatially restricted and strongly non-uniform structures, such as quantum dots and granular metals the description in terms of quasiclassical electron trajectories may fail. In such cases electron scattering on disorder should be treated on more general footing without employing any quasiclassics. A proper tool for that is the scattering matrix formalism. The main idea here is to "marry" this formalism with a non-perturbative description of electron–electron interactions. Following this route one can quite generally model a disordered conductor by an array of (metallic) quantum dots connected via junctions (scatterers). A clear advantage of this model is that it allows one to treat weakly and strongly disordered conductors in both spatially restricted and spatially extended geometries within the same theoretical framework. Detailed implementation of these ideas is contained in Chapters 10–13 of this book.

In Chapter 10 we introduce the concept of the scattering matrix and derive the influence functional for short coherent conductors which accounts for the effect of electron–electron interactions. In Chapter 11 we apply this formalism to the problem of (weak) Coulomb blockade in metallic conductors. In particular, we establish a fundamental relation between shot noise and interaction effects in

electron transport, extend these ideas further to higher correlators and also address non-perturbative interaction effects. We further extend our scattering matrix analysis of charging effects applying it to single metallic quantum dots (Chapter 12) and their arrays (Chapter 13), eventually building a bridge to describe interaction effects in disordered metallic wires.

Chapters 14 and 15 are devoted to the analysis of weak localization and interaction-induced quantum dephasing of electrons in disordered conductors at low temperatures. While in Chapters 3, 5, and 8 quantum decoherence in (or close to) the ground state of an interacting system is addressed without including Fermi statistics, in Chapters 14 and 15 the Pauli principle is fully accounted for. In Chapter 14 we apply the influence functional formalism developed in Chapter 9 for weakly disordered conductors where quantum dynamics of electrons can be described in terms of their semiclassical trajectories. This formalism is well suited in order to proceed non-perturbatively to all orders in the interaction and also to establish direct links with models considered in Chapters 3 and 8 as well as with the $P(E)$-theory elaborated in Chapter 7. In Chapter 15 we address the same problem employing the combination of the scattering matrix formalism and the path integral influence functional technique of Chapters 10–13. This approach allows to extend our non-perturbative analysis of interaction-induced dephasing of electrons, e.g., to quantum dots and strongly disordered metals and to construct a unified description of this fundamentally important phenomenon embracing a broad range of disordered conductors.

In the last five chapters of this book we develop some of the above ideas further applying them to various superconducting structures. In Chapter 16 we consider hybrid metallic structures composed of normal and superconducting electrodes. Low-energy electron transport in such system is due to the mechanism of Andreev reflection which involves conversion of an incident electron into a Cooper pair and a hole propagating in the opposite direction. As a result, twice the electron charge is being transferred in the course of such electron-hole reflection. In Chapter 16 we analyze various aspects of this charge transport and fluctuation effects in normal-superconducting metallic hybrids and generalize

fundamental relation between these effects and electron–electron interactions already established in Chapters 10 and 11 for normal junctions. Remarkably, it turns out that the relation between shot noise and Coulomb interaction effects in such hybrid structures can also be extended to non-local phenomena, such as crossed Andreev reflection.

Chapter 17 is devoted to the analysis of Coulomb effects and fluctuations in superconducting weak links not containing any tunnel barrier, such as superconducting quantum point contacts or superconductor-normal-metal-superconductor junctions. Unlike in the first part of this book (Chapters 2 and 4–6), in Chapter 17 we employ the influence functional technique in order to examine a nontrivial interplay between fluctuation and charging effects in superconducting contacts beyond the tunneling limit. In such systems quasiparticles with energies below the superconducting gap are confined inside the weak link forming a discrete set of Andreev levels that essentially contribute to the supercurrent. At the same time, under certain conditions these low- energy bound states can be viewed as an effective quantum dissipative environment which may become particularly important at higher barrier transmissions.

In Chapter 18 we elaborate a detailed microscopic derivation of the effective action for spatially extended superconductors. We again follow the basic idea of the Feynman–Vernon influence functional technique and integrate out the electron degrees of freedom. This task is now by far more complicated than in the case of various superconducting junctions treated in Chapters 2, 16, and 17. It is not anymore possible to express the effective action in terms of only one quantum variable because (*a*) the superconducting phase is now a quantum field rather than just one degree of freedom, (*b*) fluctuations of the absolute value of the order parameter both in space and in time are important, (*c*) fluctuating electromagnetic potentials cannot in general be integrated out and (*d*) superconducting fluctuations and other dynamical processes may drive the quasiparticle distribution function far from equilibrium. The key idea here is to make use of the Ward identities which help to construct a manifestly gauge invariant effective action for a superconductor. The real-time Keldysh version of this action allows

to account for diverse dynamical and fluctuation effects and under certain conditions reduces to a set of Langevin equations which provide a full description within the Gaussian approximation for the fluctuating fields.

An important application of the above general theory concerns quantum dynamical effects in ultrathin superconducting wires. Provided the thickness of such wires enters the range below $\sim$100 nm non-Gaussian fluctuations of the superconducting order parameter—the so-called thermal and quantum phase slips (TAPS and QPS)—start playing an important role. For example, proliferation of QPS in superconducting nanowires drives such systems into a resistive state which may even turn insulating in the zero temperature limit. A detailed theory of this and other TAPS- and QPS-related phenomena in superconducting nanowires is developed in Chapter 19. Chapter 20—the last one in this book—is devoted to quantum effects in superconducting nanorings. In this chapter we analyze the effect of quantum phase slips on the ground properties of these nanorings, such as persistent currents and related phenomena. We also apply our path integral formalism in order to address the superconducting parity effect and its impact on persistent currents in superconducting nanorings with various types of weak links.

In this book an effort is made to maintain a subtle balance between describing theoretical methods and techniques and displaying a rich landscape of physical phenomena accessed by these methods. On one hand, seemingly very different problems and ideas can be united and conveniently compared to each other if analyzed within the same general theoretical approach. On the other hand, the approach itself demonstrates its enormous power if successfully applied in rather different sub-fields of condensed matter physics and beyond. A nice illustration for that is provided by the material covered in this book.