Quantum Processes in Semiconductors

FIFTH EDITION

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B. K. RIDLEY

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Preface to the Fifth Edition

Semiconductor physics is of fundamental importance in understanding the behaviour of semiconductor devices and for improving their performance. Among the more recent devices are those exploiting the properties of III–V nitrides, and others that explore the technical possibilities of manipulating the spin of the electron. The III–V nitrides, which have the hexagonal structure of wurtzite (ZnO), have properties that are distinct from those like GaAs and InP, which have the cubic structure of zinc blende (ZnS). Moreover, AlN and GaN have large band gaps, which make it possible to study electron transport at very high electric fields without producing breakdown. This property, combined with an engineered large electron population, makes GaN an excellent candidate for high-power applications. In such situations the role of hot phonons and their coupling with plasmon modes cannot be ignored. This has triggered a number of recent studies concerning the lifetime of hot phonons, leading to the discovery of new physics. An account of hot-phonon effects, the topic of the first of the new chapters, seemed to be timely.

In the new study of spintronics, a vital factor is the rate at which an out-of-equilibrium spin population relaxes. The spin of the electron scarcely enters the subject matter of previous editions of this book other than in relation to the density of states, so an account of spin processes has been overdue, hence the second of the new chapters in this edition. The rate of spin relaxation is intimately linked to details of the band structure, and in describing this relationship I have taken the opportunity to describe the band structure of wurtzite and the corresponding eigenfunctions of the bands, from which the cubic results are deduced. There are several processes that relax spin in bulk material, and these are described.

The properties of semiconductors extend beyond the bulk. All semiconductors have surfaces and, when incorporated into devices, they have interfaces with other materials. The physics of metal–semiconductor interfaces has been studied ever since the discovery of rectifying properties in the early part of the 20th century. More recently, the advent of so-called low-dimensional devices has highlighted problems connected with the physics of interfaces between different semiconductors, so an account of the properties of surfaces and interfaces was, it seemed to me, no longer timely, but long overdue. Hence, the third new chapter.

This new edition is therefore designed to expand (rather than replace) the physics of bulk semiconductors found in the previous edition. The

expansion has been motivated by the subject matter of my own research and that of colleagues at the Universities of Essex and Cornell. I am particularly indebted to Dr Angela Dyson for her insightful collaboration in these studies.

Thorpe-le-Soken, 2013 B.K.R.

Preface to the Fourth Edition

This new edition contains three new chapters concerned with material that is meant to provide a deeper foundation for the quantum processes described previously, and to provide a statistical bridge to phenomena involving charge transport. The recent theoretical and experimental interest in fundamental quantum behaviour involving mixed and entangled states and the possible exploitation in quantum computation meant that some account of this should be included. A comprehensive treatment of this important topic involving many-particle theory would be beyond the scope of the book, and I have settled on an account that is based on the single-particle density matrix. A remarkably successful bridge between single-particle behaviour and the behaviour of populations is the Boltzmann equation, and the inclusion of an account of this and some of its solutions for hot electrons was long overdue. If the Boltzmann equation embodied the important step from quantum statistical to semi-classical statistical behaviour, the drift-diffusion model completes the trend to fully phenomenological description of transport. Since many excellent texts already cover this area I have chosen to describe only some of the more exciting transport phenomena in semiconductor physics such as those involving a differential negative resistance, or involving acoustoelectric effects, or even both, and something of their history.

A new edition affords the opportunity to correct errors and omissions in the old. No longer being a very assiduous reader of my own writings, I rely on others, probably more than I should, to bring errors and omissions to my attention. I have been lucky, therefore, to work with someone as knowledgeable as Dr N.A. Zakhleniuk who has suggested an update of the discussion of cascade capture, and has noted that the expressions for the screened Bloch–Gruneisen regime were for 2-D systems and not for bulk material. The update and corrections have been made, and I am very grateful for his comments.

My writing practically always takes place at home and it tends to involve a mild autism that is not altogether sociable, to say the least. Nevertheless, my wife has put up with this once again with remarkable good humour and I would like to express my appreciation for her support.

Thorpe-le-Soken, 1999 B.K.R.

Preface to the Third Edition

One of the topics conspicuously absent in the previous editions of this book was the scattering of phonons. In a large number of cases phonons can be regarded as an essentially passive gas firmly anchored to the lattice temperature, but in recent years the importance to transport of the role of out-of-equilibrium phonons, particularly optical phonons, has become appreciated, and a chapter on the principal quantum processes involved is now included. The only other change, apart from a few corrections to the original text (and I am very grateful to those readers who have taken the trouble to point out errors) is the inclusion of a brief subsection on exciton annihilation, which replaces the account of recombination involving an excitonic component. Once again, only processes taking place in bulk material are considered.

Thorpe-le-Soken B.K.R.
December 1992

Preface to the Second Edition

This second edition contains three new chapters—'Quantum processes in a magnetic field', 'Scattering in a degenerate gas', and 'Dynamic screening'—which I hope will enhance the usefulness of the book. Following the ethos of the first edition I have tried to make the rather heavy mathematical content of these new topics as straightforward and accessible as possible. I have also taken the opportunity to make some corrections and additions to the original material—a brief account of alloy scattering is now included—and I have completely rewritten the section on impact ionization. An appendix on the average separation of impurities has been added, and the term 'third-body exclusion' has become 'statistical screening', but otherwise the material in the first edition remains substantially unchanged.

Thorpe-le-Soken 1988 B.K.R.

Preface to the First Edition

It is a curious fact that in spite of, or perhaps because of, their overwhelming technological significance, semiconductors receive comparatively modest attention in books devoted to solid state physics. A student of semiconductor physics will find the background theory common to all solids well described, but somehow all the details, the applications, and the examples—just those minutiae which reveal so vividly the conceptual cast of mind which clarifies a problem—are all devoted to metals or insulators or, more recently, to amorphous or even liquid matter. Nor have texts devoted exclusively to semiconductors, excellent though they are, fully solved the student's problem, for they have either attempted global coverage of all aspects of semiconductor physics or concentrated on the description of the inhomogeneous semiconducting structures which are used in devices, and in both cases they have tended to confine their discussion of basic physical processes to bare essentials in order to accommodate breadth of coverage in the one and emphasis on application in the other. Of course, there are distinguished exceptions to these generalizations, texts which have specialized on topics within semiconductor physics, such as statistics and band structure to take two examples, but anyone who has attempted to teach the subject to postgraduates will, I believe, agree that something of a vacuum exists, and that filling it means resorting to research monographs and specialist review articles, many of which presuppose a certain familiarity with the field.

Another facet to this complex and fascinating structure of creating, assimilating, and transmitting knowledge is that theory, understandably enough, tends to be written by theoreticians. Such is today's specialization that the latter tend to become removed from direct involvement in the empirical basis of their subject to a degree that makes communication with the experimentalist fraught with mutual incomprehension. Sometimes the difficulty is founded on a simple confusion between the disparate aims of mathematics and physics—an axiomatic formulation of a theory may make good mathematical sense but poor physical sense—or it may be founded on a real subtlety of physical behaviour perceived by one and incomprehended by the other, or more usually it may be founded on ignorance of each other's techniques, of the detailed analytic and numerical approximations propping up a theory on the one hand, and of the detailed method and machinery propping up an experimental result on the other. Certainly, experimentalists cannot avoid being theoreticians from time to time, and they have to be aware of the basic theoretical structure of their subject. As students of physics operating in an area where physical intuition is more

important than logical deduction they are not likely to appreciate a formalistic account of that basic structure even though it may possess elegance. Intuition functions on rough approximation rather than rigour, but too few accounts of theory take that as a guide.

This book, then, is written primarily for the postgraduate student and the experimentalist. It attempts to set out the theory of those basic quantum-mechanical processes in homogeneous semiconductors which are most relevant to applied semiconductor physics. Therefore the subject matter is concentrated almost exclusively on electronic processes. Thus no mention is made of phonon–phonon interactions, nor is the optical absorption by lattice modes discussed. Also, because I had mainstream semiconductors like silicon and gallium arsenide in mind, the emphasis is on crystalline materials in which the electrons and holes in the bands obey non-degenerate statistics, and little mention is made of amorphous and narrow-gap semiconductors. Only the basic quantum mechanics is discussed; no attempt is made to follow detailed applications of the basic theory in fields such as hot electrons, negative-differential resistance, acousto-electric effects, etc. To do that would more than triple the size of the book. The theoretical level is at elementary first- and second-order perturbation theory, with not a Green's function in sight; this is inevitable, given that the author is an experimentalist with a taste for doing his own theoretical work. Nevertheless, those elementary conceptions which appear in the book are, I believe, the basic ones in the field which most of us employ in everyday discussions, and since there is no existing book to my knowledge which contains a description of all these basic processes I hope that this one will make a useful reference source for anyone engaged in semiconductor research and device development.

Finally, a word of caution for the reader. A number of treatments in the book are my own and are not line-by-line reproductions of standard theory. Principally, this came about because the latter did not exist in a form consistent with the approach of the book. One or two new expressions have emerged as a by-product, although most of the final results are the accepted ones. Where the treatment is mine, the text makes this explicit.

Colchester 1981 B.K.R

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Band structure of semiconductors

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1.1. The crystal Hamiltonian

For an assembly of atoms the classical energy is the sum of the following:

(a) the kinetic energy of the nuclei;
(b) the potential energy of the nuclei in one another's electrostatic field;
(c) the kinetic energy of the electrons;
(d) the potential energy of the electrons in the field of the nuclei;
(e) the potential energy of the electrons in one another's field;
(f) the magnetic energy associated with the spin and the orbit.

Dividing the electrons into core and valence electrons and leaving out magnetic effects leads to the following expression for the crystal Hamiltonian:

$$H = \sum_l \frac{\mathbf{p}_l^2}{2M_l} + \sum_{l,m} U(\mathbf{R}_l - \mathbf{R}_m) + \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i,l} V(\mathbf{r}_i - \mathbf{R}_l) + \sum_{i,j} \frac{e^2/4\pi\epsilon_0}{|\mathbf{r}_i - \mathbf{r}_j|} \tag{1.1}$$

where l and m label the ions, i and j label the electrons, $\mathbf{p}$ is the momentum, M is the ionic mass, m is the mass of the electron, $U(\mathbf{R}_l - \mathbf{R}_m)$ is the interionic potential, and $V(\mathbf{r}_i - \mathbf{R}_l)$ is the valence–electron–ion potential.

The Schrödinger equation determines the time-independent energies of the system:

$$H\Xi = E\Xi \tag{1.2}$$

where H is now the Hamiltonian operator.

1.2. Adiabatic approximation

The mass of an ion is at least a factor of 1.8×10^3 greater than that of an electron, and for most semiconductors the factor is well over 10^4. For comparable energies and perturbations ions therefore move some 10^2 times slower than do electrons, and the latter can be regarded as