PAUL HARRISON

# Quantum Wells, Wires and Dots

3rd Edition

Theoretical and Computational Physics of Semiconductor Nanostructures

WILEY

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## Theoretical and Computational Physics of Semiconductor Nanostructures

Third Edition

**Paul Harrison**
**The University of Leeds, UK**


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# QUANTUM WELLS, WIRES AND DOTS

*To Claire, Hannah and Joe*

# PREFACE

I have been working on theoretical and computational studies of the electronic, optical and magnetic properties of semiconductor heterostructures for well over a decade. During this time I have had to follow through various theoretical derivations from either books or research papers and frankly I've struggled time and time again. There never seems to be enough detail and what is commonly a couple of lines in a research paper can literally turn into many pages of precise mathematics.

With the advent of computers and their wide application to science, the emphasis of theoretical work has changed. Years ago, theoreticians aimed to produce short neat relationships, which summarised physical effects. The concentration dependency of the metal–insulator transition of Mott is an excellent example of a complex process summarised in a compact equation, which could then be evaluated by hand. The modern approach to the same problem would be to take a microscopic model of a semiconductor, calculate the bandstructure, and then vary the impurity concentration, thus deducing an empirical relationship from the numerics. The material system would then be changed and the process repeated. It would therefore appear that the old way was preferable, but in these times of materials modelling and device design, *quantitative results* are what we're paid for.

### What this book is not

This book is unusual in that what it doesn't contain is as important as what it does contain, and furthermore, without the omissions this book would not exist. This book is not a book about condensed matter, nor is it a book about the physical properties of

semiconductor heterostructures. It is not a book reporting the wealth of experimental measurements made on low–dimensional semiconductor systems, nor is it meant to be a general light reading book that you might cuddle up with in bed!

This book isn't even a review of all the methods that are available for calculating various properties. This book is merely an in-depth look at how quantities *can* be calculated. It is not meant to be the definitive guide; I'm sure there are better methods available than some of those presented here.

So all that remains is to say...

### What this book is

This book is aimed at providing *all* of the essential information, both theoretical and computational, in order that the reader can, starting from essentially nothing, understand how the electronic, optical and transport properties of semiconductor heterostructures are calculated. However, perhaps more importantly, starting from this low common denominator, this text is designed to lead the reader through a series of simple example theoretical and computational implementations, and slowly build from solid foundations, to a level where the reader can begin to initiate theoretical investigations or explanations of their own.

I believe that there are two aspects to theoretical work, with the first being to analyse and interpret experimental data, while the second is to advance new ideas. My hope is that this book will certainly facilitate the former and I believe that I will at least provide the knowledge and skills base from which quantified predictions can be developed from the beginnings of an idea.

I hope that this book will appeal to readers from outside the low dimensional semiconductor community. Some of the examples developed will certainly be relevant to the semiconductor community at large, while the microscopic calculations presented could be of interest to other areas of condensed matter, such as carbon nanostructures, high–temperature superconductors, etc.

I have attempted here to write a book almost in the style of a mathematics course text. In such books they often describe briefly why differential equations or integration are important and then move on to show the standard techniques for solution, followed by examples and perhaps the application to real problems. Sometimes the books just state 'This is a binomial expansion and here's what you do'. In some ways this book follows both those routes. I expect that many readers will look at this present book having already a great deal of appreciation for their own particular problem. I would think that they have already quantified it in terms of, e.g. 'I must calculate the exciton binding energy'. Then they'll find that this book shows them exactly how to carry this out, and indeed provides the computer codes for them to achieve their aim quickly. I wouldn't expect a reader to pick this work up knowing nothing about solid state physics—it is not aimed at that particular person—and as I've stated already, there are many excellent books available which describe in detail the electronic, optical, transport, and other properties of semiconductors and semiconductor heterostructures. It is not my aim here to compete with these in any way; indeed I hope this present work will complement the earlier works.

Therefore this book was written to fill a need, namely collecting and documenting together derivations. It is a chance to set the mathematics in stone. By incorporating

all of the steps in a derivation there is no possiblity of hiding away and 'glossing over' any point that is not fully understood. In many ways this means leaving oneself bare, for any mistakes or errors *will* be spotted, but this will give the opportunity for them to be corrected and hence allow the text to converge (perhaps through later editions) to a true record, which will be of use to future generations of students and researchers alike.

PAUL HARRISON

*The University of Leeds*

*June 1999*

The opportunity of correcting a dozen or so errors in the equations and one or two of the figures was taken for this, the first reprinting of this work. A list of these changes can be found on the book's web site.

PAUL HARRISON

*The University of Leeds*

*April 2001*

Perhaps the biggest change for this second edition has been brought about by the decision to drop the accompanying CD-ROM. This was done for a couple of reasons, the first one being that many of the people I met who had bought the book told me they only trusted their own codes and saw writing them as part of their own personal development. The second reason was that dropping the CD-ROM allowed the publisher to drop the price. With the introduction of a paperback version too, it is hoped that the book will be more accessible to students. To compensate for this the contents of the CD-ROM from the first edition will be published exactly as was on the book's website. Some of these codes have had updates already published so you'll need to consult with the relevant section, some of the codes will have been affected by the errata since discovered and some of the codes have basically been rewritten and improved, but you won't have access to them!

There is quite a bit of new material. In particular I've added sections on effects of magnetic fields on quantum wells, excited impurity levels, screening of the optical phonon interaction, acoustic and optical deformation potential scattering and spin-orbit coupling in the pseduopotential calculation. Perhaps more importantly, realising my own limitations I've commissioned contributions from some of my colleagues and this has resulted in new chapters on strained quantum wells and **k.p** theory. To keep the style of the book consistent I've edited these contributed works into my style.

PAUL HARRISON

*The University of Leeds*

*March 2005*

Again, in this third edition there is quite a bit of new material and again I've relied on the expertise of my colleagues. So, although I've expanded work on scattering rates

into a new chapter on electron transport, it is my colleagues who have added the bulk of the new material with new chapters on quantum dots, optical waveguides and optical properties of quantum wells. So there are about 100 pages of new material. Again, I've done the final edit to make sure the book keeps its continuity of style and I hope it remains as readable as before. Even as I write these final words I realize there's still more that could be added, such as Monte Carlo simulations of electron transport, more advanced pseudopotential calculations of nanostructures, more on non-linear optics and perhaps even nanophotonics...but we'll leave that for another year!

PAUL HARRISON

*The University of Leeds*

*June 2009*

# ACKNOWLEDGEMENTS

I am indebted to so many people with whom I've worked over the years that these acknowledgements have the potential for turning into a substantial work in themselves. Almost everybody with whom I've shared an office or a research project will look through this book and be able to say 'Ah yes, I helped him with that...'. I am truly grateful to everybody and it is such discussions that have in many ways motivated me to write this book.

In particular I would like to thank people such as John Davies, Winston Hagston and John Killingbeck who motivated me in my undergraduate days and spurred me on to my PhD work. At Newcastle I was lucky to be part of an excellent group with some truly great computational physicists. Perhaps the most important of these were Ian Morrison who in less than an hour really explained the bulk pseudopotential derivation to me and Jerry Hagon who put up with my endless computing questions. I must also include my tutors, Milan Jaros and David Herbert and, of course, my colleagues Andy Beavis and Richard Turton.

Without doubt the largest contribution to my knowledge base came during my formative years as a postdoctoral research assistant with Winston Hagston. Besides sparking my interest in quantum mechanics as an undergraduate and then luring me back to Hull, Winston showed the way in two of the major derivations that I document here. In particular, the first of the quantum confined impurity calculations I attempted, namely the spherically symmetric wave function, and together with Thomas Piorek, a substantial fraction of the electron–LO phonon scattering rate.

I am indebted to all of my research colleagues at Hull, particularly the theoreticians Tom Stirner, (the already mentioned) Thomas Piorek, Richard Roberts, Fei Long, and Jabar Fatah, all for humouring and implementing my ideas for heterostructure research.

Although I had already been working with electron–phonon scattering for a number of years and had implemented this on a computer, it was my colleague Paul Kinsler who showed me where the equations that I started with, actually came from. I believe this puts the phonon scattering rate work on a much surer footing and I am very grateful for his contribution.

I would also like to thank other colleagues at Leeds, in particular Bill Batty who on comparing the results of my implementation of the shooting technique for the solution of Schrödinger's equation, actually spotted an instance when a not insignificant error arose. This forced me to look again at the iterative equation for the case of a variable effective mass and to deduce the much more stable and accurate form presented in this work. Bill Batty also deserves a mention for proof reading of my manuscript along with Kate Donovan, Marco Califano and Byron Alderman.

For the second edition I am deeply indebted to my colleagues Zoran Ikonić and Vladimir Jovanović for contributing entirely new chapters. They are both helping to fill in gaps that this edition is certainly much better for. Some of my students have also pointed out some mistakes and opportunities for improvements in particular Jim McTavish, Nenad Vukmirović, Vladimir Jovanović, Ivana Savić and Craig Evans. Thanks guys the book is all the better for your hard work. Thanks also to all the people who contributed errata from the First Edition; these are all published on the book's website.

For this third edition I am very grateful to my colleagues Marco Califano, Craig Evans and Dragan Indjin, who have contributed entirely new chapters on their specialist areas of work. In turn, Dragan Indjin would like to thank Vitomir Milanović and Jelena Radovanović for their help. Again, I think the book is better for having contributions from specialists who can add more than I can on my own. They have all worked really hard to a tight deadline and I must thank them for putting up with me perpetually nagging them to finish their work. My interations with Alex Valavanis, Leon Lever and Will Freeman, in particular, have been very valuable. Thanks guys. Marie Barber and Zoran Ikonić deserve special mention for helping me in all aspects of my work and without them this new edition wouldn't exist.

Finally, I would like to express my gratitude to my employers, The University of Leeds and the School of Electronic and Electrical Engineering, for providing me in the first instance with a University Research Fellowship, which gave me an excellent platform on which to build a career in research. It was the flexibility of this scheme which allowed me the time to undertake the first edition. Since that time my employees have continued to support me and provide me with a position in which I can earn my living through research, teaching and administration, but still have enough time left over to work on the later editions.

P.H.

# ABOUT THE AUTHOR(S)

Paul Harrison is currently working in the Institute of Microwaves and Photonics (IMP), which is a research institute within the School of Electronic and Electrical Engineering at the University of Leeds in the United Kingdom. He can always be found on the web, at the time of writing, at:

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Paul is working on a wide variety of projects, most of which centre around exploiting quantum mechanics for the creation of novel opto-electronic devices, largely, but not exclusively, in semiconductor *Quantum Wells, Wires and Dots.* Up-to-date information can be found on his web page. He is always looking for exceptionally well-qualified and motivated students to study for a PhD degree with him—if interested, please don't hesitate to contact him.

Zoran Ikonić was a Professor at the University of Belgrade and is now also a researcher in the IMP. His research interests and experience include the full width of semiconductor physics and optoelectronic devices, in particular, band structure calculations, strain-layered systems, carrier scattering theory, non-linear optics, as well as conventional and quantum mechanical methods for device optimization.

Vladimir Jovanović completed his PhD at the IMP on physical models of quantum well infrared photodetectors and quantum cascade lasers in GaN- and GaAs-based materials for near-, mid- and far-infrared (terahertz) applications.

Marco Califano is a Royal Society University Research Fellow based in the IMP at Leeds whose main interests focus on atomistic pseudopotential modelling of the electronic and optical properties of semiconductor nanostructures of different materials for applications in photovoltaics

Craig A. Evans completed his PhD on the optical and thermal properties of quantum cascade lasers in the School of Electronic and Electrical Engineering, University of Leeds in 2008. He then worked as a Postdoctoral Research Assistant in the IMP working in the field of rare-earth doped fibre lasers and integrated photonic device modelling and has now joined the staff of the school.

Dragan Indjin is an Academic Research Fellow in the IMP and has research interests in semiconductor nanostructures, non-linear optics, quantum computing and spintronics.

# ABOUT THE BOOK

99.5% of this book was produced with 'open source' not-for-profit software. The text was prepared with LaTeX2$\epsilon$ using Wiley's own style (class) files. It was input by hand initially with the aid of the excellent 'VI Like Emacs' (vile) and then with the superb 'Vi IMproved' (vim/gvim). The schematic diagrams were prepared using 'xfig', the $x$-$y$ plots with 'xmgr/xmgrace' and three-dimensional molecular models with 'RasMol'. 'BibView' was used to maintain a BIBTEX database in the earlier editions. Manuscript preparation has been under all three of the most popular operating systems by now!

Further information about the book, including errata and the software from the first edition is available on the book's web page, which is currently:

`http://www.imp.leeds.ac.uk/qwwad/`

# INTRODUCTION

Since their discovery/invention by Esaki and Tsu in the 1970s, semiconductor quantum wells and superlattices have evolved from scientific curiosities to a means of probing the fundamentals of quantum mechanics, and more recently into wealth-creating semiconductor devices.

In this work, a brief resumé of quantum theory and solid state physics is given before launching into the main body of the book—the theoretical and computational framework of semiconductor heterostructures. The first chapter introduces the concepts of effective mass and envelope function approximations, which are two cornerstone theories, from a quite different perspective. Usually these two techniques are introduced from rigorous mathematics with some approximations—see, for example, the works by Bastard and Burt. The motivation behind this approach is to introduce these concepts from very simplistic intuitive, and at times, graphical arguments. The range of validity of such approximations is not being challenged; they are good theories and used many times in this book. This present approach is merely to reinforce these ideas in 'pictures rather than words'.

The aim of this book is to provide solid foundations in the theoretical methods necessary for calculating *some* of the basic electronic and optical properties of semiconductor quantum wells, wires and dots. Some background knowledge will be required; I often cite Ashcroft and Mermin [1] and Blakemore [2] for support material in solid state physics, and works such as Eisberg [3] and Weidner and Sells [4] for quantum theory. This present treatise should be considered to complement existing books in the field. I thoroughly recommend the books by Jaros [5], Davies and Long [6], Kelly [7], Turton [8], Ivchenko

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