Preface

Advanced Visual Quantum Mechanics is a systematic effort to investigate and to teach quantum mechanics with the aid of computer-generated animations. But despite its use of modern visualization techniques, it is a conventional textbook of (theoretical) quantum mechanics. You can read it without a computer, and you can learn quantum mechanics from it without ever using the accompanying CD-ROM. But, the animations will greatly enhance your understanding of quantum mechanics. They will help you to get the intuitive feeling for quantum processes that is so hard to obtain from the mathematical formulas alone.

A first book with the title *Visual Quantum Mechanics* ("Book One") appeared in the year 2000. The CD-ROM for Book One earned the European Academic Software Award (EASA 2000) for outstanding innovation in its field. The topics covered by Book One mainly concerned quantum mechanics in one and two space dimensions. *Advanced Visual Quantum Mechanics* ("Book Two") sets out to present three-dimensional systems, the hydrogen atom, particles with spin, and relativistic particles. It also contains a basic course of quantum information theory, introducing topics like quantum teleportation, the EPR paradox, and quantum computers. Together, the two volumes constitute a fairly complete course on quantum mechanics that puts an emphasis on ideas and concepts and satisfies some modest requirements of mathematical rigor. Nevertheless, Book Two is fairly self-contained. References to Book One are kept to a minimum so that anyone with a basic training in quantum mechanics should be able to read Book Two independently of Book One. Appendix A includes a short synopsis of quantum mechanics as far as it was presented in Book One.

The CD-ROM included with this book contains a large number of QuickTime movies presented in a multimedia-like environment. The movies illustrate the text, add color, a time-dimension, and a certain level of interactivity. The computer-generated animations will help you to explore quantum mechanics in a systematic way. The point-and-click interface gives you quick and easy access to all the movies and lots of background information. You need no special computer skills to use the software. In fact, it is no more difficult than surfing the Internet. You are not required to produce simulations by yourself. The general idea is that you should first think about quantum mechanics and not about computers. The movies provide some phenomenological background. They will train and enhance your intuition, and the desire to understand the movies should motivate you to learn the (sometimes nasty, sometimes elegant) theory.

Computer visualizations are particularly rewarding in quantum mechanics because they allow us to depict objects and events that cannot be seen by other means. However, one has to be aware of the fact that the animations depict the mathematical objects describing reality, not reality itself. Usually, one needs some explanation and interpretation to understand the visualizations. The visualization method used here makes extensive use of color. It displays all essential information about the quantum state in an intuitive way. Watching the numerous animations will thus create an intuitive feeling for the behavior of quantum systems—something that is hardly achieved just by solving the Schrödinger equation mathematically. I would even say that the movies allow us to see the whole subject in a new way. In any case, the "visual approach" had a great influence on the selection of topics as well as on the style and the level of the presentation. For example, *Visual Quantum Mechanics* puts an emphasis on quantum dynamics, because a movie adds a natural time-dimension to an illustration. Whereas other textbooks stop when the eigenfunctions of the Hamiltonian are obtained, this book will go on to discuss dynamical effects.

It depends on the situation, but also on the personality of the student or of the teacher, how the movies are used. In some cases, the movies are certainly useful to stimulate the student's interest in some phenomenon. The animation thus serves to motivate the development of the theory. In other cases, it is, perhaps, more appropriate to show a movie confirming the theory by an example. Personally, I present the movies by video projection as a supplement to an introductory course on quantum mechanics. I talk about the movies in a rather informal way, and soon the students start asking interesting questions that lead to fruitful discussions and deeper explanations. Often, the movies motivate students to study related topics on their own initiative.

One could argue that in advanced quantum mechanics, visualizations are not very useful because the student has to learn abstract notions and that he or she should think in terms of linear operators, Hilbert spaces, and so on. It is certainly true that a solid foundation of these subjects is indispensable for a deeper understanding, and you will have occasion to learn much about the mathematical theory from this text. But, I claim that despite a good training in the abstract theory, you can still gain a lot from the visualizations.

Talking about my own experience, I found that I learned much, even about simple systems, when I prepared the movies for *Visual Quantum Mechanics*. For example, having done research on the mathematical aspects of the Dirac equation for several years, I can claim to have a good background concerning the quantum mechanical abstractions in this field. But nevertheless, I was not able to predict how a wave packet performing a "Zitterbewegung" would appear until I started to do some visualizations of that phenomenon. Moreover, when one tries to understand the visualizations one often encounters phenomena, that one is able to explain with the theory, but that one simply hasn't thought of before. The main thing that you can gain from the visualizations is a good feeling for the behavior of solutions of the quantum mechanical equations.

Though the CD-ROM presents a few simple interactive simulations in the chapter about qubits, the overwhelming content consists of prefabricated movies. A true computer simulation, that is, a live computation of some process, would of course allow a higher degree of interactivity. The reader would have more flexibility in the choice of parameters and initial conditions. But in many cases, this approach is forbidden because of the insufficient speed of present-day computers. Moreover, in order to produce a useful visualization, one has to analyze the physical system very carefully. For every situation, one has to determine the scale of space and time and suitable ranges of the parameters where something interesting is going to happen. In quantum mechanics, the number of possibilities is very large, and if one chooses the wrong parameter values, it is very likely that nothing can be seen that is easily interpreted or that shows some effect in an interesting way. Therefore, I would not recommend to learn basic quantum mechanics by doing time-consuming computer simulations.

Producing simulations and designing visualizations can, however, bring enormous benefit to the advanced student who is already familiar with the foundations of quantum mechanics. Many of the animations on the CD-ROM were done with the help of Mathematica. With the exception of the Mathematica software, all the necessary tools for producing similar results are provided on the CD-ROM: The source code for all movies, Mathematica packages both for the numerical solution of the Schrödinger equation and for the graphical presentation of the results, and OpenGL-based software for the three-dimensional visualization of wave functions. My recommendation is to start with some small projects based on the examples provided by the CD-ROM. It should not be difficult to modify the existing Mathematica notebooks by slightly varying the parameters and initial conditions, and then watching and interpreting the results. You could then proceed to look for other examples of quantum systems that might be good for a physically or mathematically interesting visualization. When you produce a visualization, often some natural questions about the system will arise. This makes it necessary to learn more about the system (or about quantum mechanics), and by knowing the system better, you will produce better visualizations. When the visualization finally becomes useful, you will understand the system almost perfectly. This is "learning by doing", and it will certainly enhance your understanding of quantum mechanics, as the making of this book helped me to understand quantum mechanics better. Be warned, however, that personal computers are still too slow to perform simulations of realistic quantum mechanical processes within a reasonable time. Many of the movies provided with this book typically took several hours to generate.

Concerning the mathematical prerequisites, I tried to keep the two books on an introductory level. Hence, I tried to explain all the mathematical methods that go beyond basic courses in calculus and linear algebra. But, this does not mean that the content of the book is always elementary. It is clear that any text that sets out to explain quantum phenomena must have a certain level of mathematical sophistication. Here, this level is occasionally higher than in other introductions, because the text should provide the theoretical background for the movies. Doing visualizations is more than just obtaining numerical solutions. A surprising amount of mathematical know-how is in fact necessary to prepare an animation. Without presenting too many unnecessary details, I tried to include just what I thought was necessary to produce the movies. My approach to teaching quantum mechanics thus makes no attempt to trivialize this subject. The animations do not replace mathematical formulas. But in order to facilitate the approach for the beginner, I marked some of the more difficult sections as "special topics" and placed the symbol $\boxed{\Psi}$ in front of paragraphs intended for the mathematically interested reader. These parts may be skipped at first reading.

Though the book thus addresses students and scientists with some background in mathematics, the movies (together with the movies of Book One) can certainly be used in front of a wider audience. The success, of course, depends on the style of the presentation. I myself have had the occasion to use the movies in lectures for high-school students and for scientifically interested people without any training in higher mathematics. Based on this experience, I hope that the book together with CD-ROM will have broader applications than each could have if used alone.

According to its subtitle, Book Two can be divided roughly into three parts: atomic physics (Chapters 1–3), quantum information theory (Chapters 4–6), and relativistic quantum mechanics (Chapters 7, 8). This division, however, should not be taken too seriously. For example, Chapter 4 on qubits completes the discussion of spin-1/2 particles in Chapter 3 and serves at the same time as an introduction to quantum information theory. Chapter 5 discusses composite quantum systems by combining topics relevant for quantum information theory (for example, two-qubit systems) with topics relevant for atomic physics (for example, addition of angular momenta).

Together, Book One and Book Two cover a wide range of the standard quantum physics curriculum and supplement it with a series of advanced topics. For the sake of completeness, some important topics have been included in the form of several appendices: the perturbation theory of eigenvalues, the variational method, adiabatic time evolution, and formal scattering theory. Though most of these matters are very well suited for an approach using lots of visualizations and examples, I simply had neither time nor space (the CD-ROM is full) to elaborate on these topics as I would have liked to do. Therefore, these appendices are rather in the style of an ordinary textbook on advanced theoretical physics. I would be glad if this material could serve as a background for the reader's own ventures into the field of visualization. If there should ever be another volume of Visual Quantum Mechanics, it will probably center on these topics and on others like the Thomas-Fermi theory, periodic potentials, quantum chaos, and semiclassical quantum mechanics, just to name a few from my list of topics that appear to be suitable for a modernized approach in the style of Visual Quantum Mechanics.

This book has a home page on the internet with URL

`http://www.uni-graz.at/imawww/vqm/`

An occasional visit to this site will inform you about software upgrades, printing errors, additional animations, etc.

Acknowledgements

I would like to thank my son Wolfgang who quickly wrote the program "QuantumGL" when it turned out that the available software wouldn't serve my purposes. Thanks to Manfred Liebmann, Gerald Roth, and Reinhold Kainhofer for help with *Mathematica*-related questions. I am very grateful to Jerry Batzel who read large parts of the manuscript and gave me valuable hints to improve my English. This book owes a lot to Michael A. Morrison. He studied the manuscript very carefully, made a large number of helpful comments, asked lots of questions, and eliminated numerous errors. Most importantly, he kept me going with his enthusiasm. Thanks, Michael. Financial support from Steiermärkische Landesregierung, from the University of Graz, and from Springer-Verlag is gratefully acknowledged.

Graz, January 2004 *Bernd Thaller*

Springer

http://www.springer.com/978-0-387-20777-3

Advanced Visual Quantum Mechanics
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2005, XIV, 518 p. 103 illus., Hardcover
ISBN: 978-0-387-20777-3