Visual Quantum Mechanics

Selected Topics with Computer-Generated Animations of Quantum-Mechanical Phenomena

Bernd Thaller

CD-ROM INCLUDED

Bernd Thaller

Visual Quantum Mechanics

Selected Topics with Computer-Generated Animations of Quantum-Mechanical Phenomena

CD-ROM
INCLUDED

Springer TELOS® THE ELECTRONIC LIBRARY OF SCIENCE

Bernd Thaller
Institute for Mathematics
University of Graz
A-8010 Graz
Austria
bernd.thaller@kfunigraz.ac.at

Library of Congress Cataloging-in-Publication Data
Visual quantum mechanics : selected topics with computer-generated animations of quantum-mechanical phenomena / Bernd Thaller.
p. cm.
Includes bibliographical references and index.
ISBN 0-387-98929-3 (hc. : alk. paper)
1. Quantum theory. 2. Quantum theory—Computer simulation.
I. Title.
QC174.12.T45 2000
530.12'0113—dc21 99-42455

Printed on acid-free paper.

Production managed by Steven Pisano; manufacturing supervised by Jacqui Ashri.
Photocomposed pages prepared from the author's LaTeX files.
Printed and bound by Hamilton Printing Co., Rensselaer, NY.
Printed in the United States of America.

9 8 7 6 5 4 3 2 1

ISBN 0-387-98929-3 Springer-Verlag New York Berlin Heidelberg SPIN 10743163

Visual Quantum Mechanics

Preface

In the strange world of quantum mechanics the application of visualization techniques is particularly rewarding, for it allows us to depict phenomena that cannot be seen by any other means. *Visual Quantum Mechanics* relies heavily on visualization as a tool for mediating knowledge. The book comes with a CD-ROM containing about 320 digital movies in QuickTime™ format, which can be watched on every multimedia-capable computer. These computer-generated animations are used to introduce, motivate, and illustrate the concepts of quantum mechanics that are explained in the book. If a picture is worth a thousand words, then my hope is that each short animation (consisting of about a hundred frames) will be worth a hundred thousand words.

The collection of films on the CD-ROM is presented in an interactive environment that has been developed with the help of Macromedia Director™. This multimedia presentation can be used like an adventure game without special computer skills. I hope that this presentation format will attract the interest of a wider audience to the beautiful theory of quantum mechanics.

Usually, in my own courses, I first show a movie that clearly depicts some phenomenon and then I explain step-by-step what can be learned from the animation. The theory is further impressed on the students' memory by watching and discussing several related movies. Concepts presented in a visually appealing way are easier to remember. Moreover, the visualization should trigger the students' interest and provide some motivation for the effort to understand the theory behind it. By "watching" the solutions of the Schrödinger equation the student will hopefully develop a feeling for the behavior of quantum-mechanical systems that cannot be gained by conventional means.

The book itself is self-contained and can be read without using the software. This, however, is not recommended, because the phenomenological background for the theory is provided mainly by the movies, rather than the more traditional approach to motivating the theory using experimental results. The text is on an introductory level and requires little previous knowledge, but it is not elementary. When I considered how to provide the theoretical background for the animations, I found that only a more mathematical approach would lead the reader quickly to the level necessary to understand the more intricate details of the movies. So I took the opportunity to combine a vivid discussion of the basic principles with a more advanced presentation of some mathematical aspects of the formalism. Therefore, the book will certainly serve best as a companion in a theoretical physics course, while the material on the CD-ROM will be useful for a more general audience of science students.

The choice of topics and the organization of the text is in part due to purely practical considerations. The development of software parallel to writing a text is a time-consuming process. In order to speed up the publication I decided to split the text into two parts (hereafter called Book One and Book Two), with this first book containing selected topics. This enables me to adapt to the technological evolution that has taken place since this project started, and helps provide the individual volumes at an affordable price. The arrangement of the topics allows us to proceed from simple to more and more complicated animations. Book One mainly deals with spinless particles in one and two dimensions, with a special emphasis on exactly solvable problems. Several topics that are usually considered to belong to a basic course in quantum mechanics are postponed until Book Two. Book Two will include chapters about spherical symmetry in three dimensions, the hydrogen atom, scattering theory and resonances, periodic potentials, particles with spin, and relativistic problems (the Dirac equation).

Let me add a few remarks concerning the contents of Book One. The first two chapters serve as a preparation for different aspects of the course. The ideas behind the methods of visualizing wave functions are fully explained in Chapter 1. We describe a special color map of the complex plane that is implemented by *Mathematica* packages for plotting complex-valued functions. These packages have been created especially for this book. They are included on the CD-ROM and will, hopefully, be useful for the reader who is interested in advanced graphics programming using *Mathematica*.

Chapter 2 introduces some mathematical concepts needed for quantum mechanics. Fourier analysis is an essential tool for solving the Schrödinger equation and for extracting physical information from the wave functions. This chapter also presents concepts such as Hilbert spaces, linear operators, and distributions, which are all basic to the mathematical apparatus of quantum mechanics. In this way, the methods for solving the Schrödinger equation are already available when it is introduced in Chapter 3 and the student is better prepared to concentrate on conceptual problems. Certain more abstract topics have been included mainly for the sake of completeness. Initially, a beginner does not need to know all this "abstract nonsense," and the corresponding sections (marked as "special topics") may be skipped at first reading. Moreover, the symbol $\boxed{\Psi}$ has been used to designate some paragraphs intended for the mathematically interested reader.

Quantum mechanics starts with Chapter 3. We describe the free motion of approximately localized wave packets and put some emphasis on the statistical interpretation and the measurement process. The Schrödinger equation for particles in external fields is given in Chapter 4. This chapter on states and observables describes the heuristic rules for obtaining the correct quantum observables when performing the transition from classical to quantum mechanics. We proceed with the motion under the influence of boundary conditions (impenetrable walls) in Chapter 5. The particle in a box serves to illustrate the importance of eigenfunctions of the Hamiltonian and of the eigenfunction expansion. Once again we come back to interpretational difficulties in our discussion of the double-slit experiment.

Further mathematical results about unitary groups, canonical commutation relations, and symmetry transformations are provided in Chapter 6 which focuses on linear operators. Among the mathematically more sophisticated topics that usually do not appear in textbooks are the questions related to the domains of linear operators. I included these topics for several reasons. For example, solutions that are not in the domain of the Hamiltonian have strange temporal behavior and produce interesting effects when visualized in a movie. Some of these often surprising phenomena are perhaps not widely known even among professional scientists. Among these I would like to mention the strange behavior of the unit function in a Dirichlet box shown in the movie CD 4.11 (Chapter 5).

The remaining chapters deal with subjects of immediate physical importance: the harmonic oscillator in Chapter 7, constant electric and magnetic fields in Chapter 8, and some elements of scattering theory in Chapter 9. The exactly solvable quantum systems serve to underpin the theory by examples for which all results can be obtained explicitly. Therefore, these systems play a special role in this course although they are an exception in nature.

Many of the animations on the CD-ROM show wave packets in two dimensions. Hence the text pays more attention than usual to two-dimensional problems, and problems that can be reduced to two dimensions by exploiting their symmetry. For example, Chapter 8 presents the angular-momentum decomposition in two dimensions. The investigation of two-dimensional systems is not merely an exercise. Very good approximations to such systems do occur in nature. A good example is the surface states of electrons which can be depicted by a scanning tunneling microscope.

The experienced reader will notice that the emphasis in the treatment of exactly solvable systems has been shifted from a mere calculation of eigenvalues to an investigation of the dynamics of the system. The treatment of the harmonic oscillator or the constant magnetic field makes it very clear that in order to understand the motion of wave packets, much more is needed than just a derivation of the energy spectrum. Our presentation includes advanced topics such as coherent states, completeness of eigenfunctions, and Mehler's integral kernel of the time evolution. Some of these results certainly go beyond the scope of a basic course, but in view of the overwhelming number of elementary books on quantum mechanics the inclusion of these subjects is warranted. Indeed, a new book must also contain interesting topics which cannot easily be found elsewhere. Despite the presentation of advanced results, an effort has been made to keep the explanations on a level that can be understood by anyone with a little background in elementary calculus. Therefore I hope that the text will fill a gap between the classical texts (e.g., [39], [48], [49], [68]) and the mathematically advanced presentations (e.g., [4], [17], [62], [76]). For those who like a more intuitive approach it is recommended that first a book be read that tries to avoid technicalities as long as possible (e.g., [19] or [40]).

Most of the films on the CD-ROM were generated with the help of the computer algebra system *Mathematica*. While *Mathematica* has played an important role in the creation of this book, the reader is not required to have any knowledge of a computer algebra system. Alternate approaches which use symbolic mathematics packages on a computer to teach quantum mechanics can be found, for example, in the books [18] and [36], which are warmly recommended to readers familiar with both quantum mechanics and *Mathematica* or Maple. However, no interactive computer session can replace an hour of thinking just with the help of a pencil and a sheet of paper. Therefore, this text describes the mathematical and physical ideas of quantum mechanics in the conventional form. It puts no special emphasis on symbolic computation or computational physics. The computer is mainly used to provide quick and easy access to a large collection of animated illustrations, interactive pictures, and lots of supplementary material. The book teaches the concepts, and the CD-ROM engages the imagination. It is hoped that this combination will foster a deeper understanding of quantum mechanics than is usually achieved with more conventional methods.

While knowledge of *Mathematica* is not necessary to learn quantum mechanics with this text, there is a lot to find here for readers with some experience in *Mathematica*. The supplementary material on the CD-ROM includes many *Mathematica* notebooks which may be used for the reader's own computer experiments.

In many cases it is not possible to obtain explicit solutions of the Schrödinger equation. For the numerical treatment we used external C++ routines linked to *Mathematica* using the MathLink interface. This has been done to enhance computation speed. The simulations are very large and need a lot of computational power, but all of them can be managed on a modern personal computer. On the CD-ROM will be found all the necessary information as well as the software needed for the student to produce similar films on his/her own. The exploration of quantum-mechanical systems usually requires more than just a variation of initial conditions and/or potentials (although this is sometimes very instructive). The student will soon notice that a very detailed understanding of the system is needed in order to produce a useful film illustrating its typical behavior.

This book has a home page on the internet with URL

`http://www.kfunigraz.ac.at/imawww/vqm/`

As this site evolves, the reader will find more supplementary material, exercises and solutions, additional animations, links to other sites with quantum-mechanical visualizations, etc.

Acknowledgments

During the preparation of both the book and the software I have profited from many suggestions offered by students and colleagues. My thanks to M. Liebmann for his contributions to the software, and to K. Unterkofler for his critical remarks and for his hospitality in Millstatt, where part of this work was completed. This book would not have been written without my wife Sigrid, who not only showed patience and understanding when I spent 150% of my time with the book and only -50% with my family, but who also read the entire manuscript carefully, correcting many errors and misprints. My son Wolfgang deserves special thanks. Despite numerous projects of his own, he helped me a lot with his unparalleled computer skills. I am grateful to the people at Springer-Verlag, in particular to Steven Pisano for his professional guidance through the production process. Finally, a project preparation grant from Springer-Verlag is gratefully acknowledged.

Bernd Thaller

Contents

Chapter 1

Visualization of Wave Functions

Chapter summary: Although nobody can tell how a quantum-mechanical particle looks like, we can nevertheless visualize the complex-valued function (wavefunction) that describes the state of the particle. In this book complex-valued functions are visualized with the help of colors. By looking at Color Plate 3 and browsing through the section "Visualization" on the accompanying CD-ROM, you will quickly develop the necessary feeling for the relation between phases and colors. You need to study this chapter only if you want to understand the ideas behind this method of visualization in more detail and if you want to increase your familiarity with complex-valued functions. Here we derive the mathematical formulas describing the color map that associates a unique color to every complex number. This color map is defined with the help of the HLS color system (hue-lightness-saturation): The phase of a complex number is given by the hue and the absolute value is described by the lightness of the color (the saturation is always maximal). On the CD-ROM you will find the *Mathematica* packages `ArgColorPlot.m` and `ComplexPlot.m` which implement this color map on a computer. These packages have been used to create most of the color plates in this book and most of the movies on the CD-ROM. In this chapter you will also find a comparison of various other methods for visualizing complex-valued functions in one and more dimensions. Finally, we describe some ideas for a graphical representation of spinor wave functions.

1.1. Introduction

Many quantum-mechanical processes can be described by the Schrödinger equation, which is the basic dynamic law of nonrelativistic quantum mechanics. The solutions of the Schrödinger equation are called *wave functions* because of their oscillatory behavior in space and time. The accompanying CD-ROM contains many pictures and movies of wave functions.

Unfortunately, it is not at all straightforward to understand and interpret a graphical representation of a quantum phenomenon. Wave functions, like other objects of quantum theory, are idealized concepts from which statements about the physical reality can only be derived by means of certain interpretation rules. Therefore a picture of a wave function does not show the quantum system as it really looks like. In fact, the whole concept of "looking like something" cannot be used in the strange world of quantum mechanics. Most phenomena take place on length scales much smaller than the wavelength of light.

With the help of some mathematical procedures, a wave function allows us to determine the probability distributions of physical observables (like position, momentum, or spin). Thus, the wave function gives high-dimensional data at each point of space and time and it is a difficult task to visualize such an amount of information. Usually, it is not possible to show all that information in a single graph. One has to concentrate on particular aspects and to apply special techniques in order to display the information in a form that can be understood.

Mathematically speaking, a wave function is a complex-valued function of space and time; a spinor wave function even consists of several components. In this first chapter I describe some methods of visualizing such an object. In the following chapters you will learn how to extract the physically relevant information from the visualization.

For the visualization of high-dimensional data a color code can be very useful. Because the set of all colors forms a three-dimensional manifold (see Sect. 1.2.2), it is possible—at least in principle—to represent triples of data values using a color code. Unfortunately, the human visual system is not able to recognize colors with quantitative precision. But at least we can expect that an appropriately chosen color code helps to visualize the most important qualitative features of the data.

1.2. Visualization of Complex Numbers

As a first step, I want to discuss some possibilities to visualize complex values. It is my goal to associate a unique color to each complex number. You will learn about the various color systems in some detail because this subject is relevant for the actual implementation on a computer.

CD 1.1 and Color Plate 3 show an example of such a color map, designed mainly for on-screen use. Here the phase of the complex number determines the hue of the color, and the absolute value is represented by the lightness of the color. This color map will be now described in more detail.

1.2.1. The two-dimensional manifold of complex numbers

Any complex number z is of the form

$$z = x + \mathrm{i}y, \qquad x = \operatorname{Re} z, \quad y = \operatorname{Im} z. \tag{1.1}$$

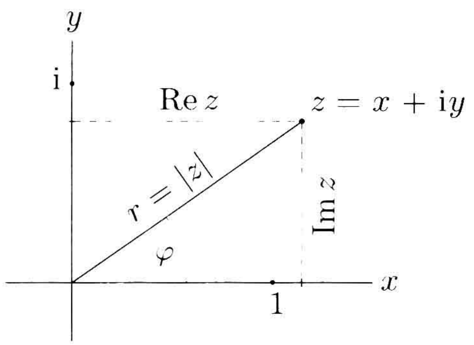

FIGURE 1.1. Graphical representation of a complex number z in Cartesian and in polar coordinates.

Here i is the complex unit which is defined by the property $\mathrm{i}^2 = -1$. The values x and y are real numbers which are called the *real part* and the *imaginary part* of z, respectively. The field of all complex numbers is denoted by $\mathbb{C}$.

Thus, complex numbers $z \in \mathbb{C}$ can be represented by pairs (x, y) of real numbers and visualized as points in the two-dimensional complex plane.

Using polar coordinates (r, φ) in the complex plane gives another representation, the *polar form* of a complex number (see Fig. 1.1)

$$z = r\cos\varphi + \mathrm{i}\, r\sin\varphi = r\,\mathrm{e}^{\mathrm{i}\varphi}, \qquad r = |z|, \quad \varphi = \arg z. \tag{1.2}$$

Here we have used Euler's formula

$$\mathrm{e}^{\mathrm{i}\varphi} = \cos\varphi + \mathrm{i}\sin\varphi. \tag{1.3}$$

The non-negative real number r is the *modulus* or *absolute value* of z and the angle ϕ is called the *phase* or *argument* of z.

For $z = r\,\mathrm{e}^{\mathrm{i}\varphi} = x + \mathrm{i}y$ the *conjugate complex number* is $\overline{z} = r\,\mathrm{e}^{-\mathrm{i}\varphi} = x - \mathrm{i}y$.

One often adds the *complex infinity* ∞ to the complex numbers. This can be explained easily with the help of a stereographic projection.

The stereographic projection: You can interpret the complex plane as the xy-plane in the three-dimensional space $\mathbb{R}^3$. Consider a sphere of radius R centered at the origin in $\mathbb{R}^3$. Draw the straight line which contains the point $(x, y, 0)$ (corresponding to the complex number $z = x + \mathrm{i}y$) and the north pole $(0, 0, R)$ of the sphere. Then the *stereographic projection* of z is the intersection of that line with the surface of the sphere. Obviously, this gives a unique point on the sphere for each complex number z. Using polar coordinates $(\theta,\ \varphi)$ on the sphere, it is clear that the azimuthal angle φ is

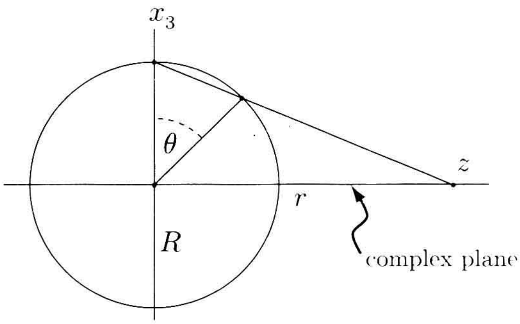

FIGURE 1.2. Stereographic projection of a complex number z with $|z| = r$.

just the phase of $z = r\,\exp(\mathrm{i}\varphi)$,

$$\varphi = \arg z. \tag{1.4}$$

A little trigonometric exercise (see Fig. 1.2) shows that the polar angle θ is given by

$$\theta = \pi - 2\arctan\frac{r}{R}, \qquad r = |z|. \tag{1.5}$$

In that way the circle with radius R in $\mathbb{C}$ is mapped onto the equator of the sphere. A complex number $z = r\exp(\mathrm{i}\varphi)$ is mapped to the northern hemisphere if $r > R$, and to the southern hemisphere if $r < R$. The origin $z = 0$ is mapped onto the south pole of the sphere, $\theta = \pi$. Every point of the sphere—except the north pole—is the image of some complex number under the stereographic projection, and the correspondence is one-to-one. The north pole $\theta = 0$ of the sphere is interpreted as the image of a new element, called *complex infinity* and denoted by ∞. The complex infinity has an infinite absolute value and an undefined phase (like $z = 0$). Obviously, ∞ can be used to represent $\lim_{n\to\infty} z_n$ for all sequences (z_n) that have no finite accumulation point.

With a stereographic projection, the whole set of complex numbers together with complex infinity can be mapped smoothly and in a one-to-one fashion onto a sphere. Because the sphere is a compact two-dimensional surface we can regard the set $\overline{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$ as a compact two-dimensional manifold. It is called the *compactified complex plane*.

EXERCISE 1.1. *Check your familiarity with complex numbers. Express* $|z|$ *and* $\arg z$ *in terms of* $\operatorname{Re} z$ *and* $\operatorname{Im} z$, *and vice versa.*

EXERCISE 1.2.. *Given two complex numbers* z_1 *and* z_2 *in polar form describe the absolute values and the phases of* $z_1 z_2$, z_1/z_2 *and* $z_1 + z_2$.

EXERCISE 1.3. *The stereographic projection is one-to-one and onto. Determine the inverse mapping from the sphere of radius R onto the compactified complex plane $\overline{\mathbb{C}}$.*

1.2.2. The three-dimensional color manifold

For the purpose of visualization we want to associate a color to each complex number. Before doing so, let's have a short look at various methods of describing colors mathematically.

The set of all colors that can be represented in a computer is a compact, three-dimensional manifold. It can be described in many different ways. Perhaps the most common description is given by the RGB model (CD 1.2).

The RGB color system: In the RGB system the color manifold is defined as the three-dimensional unit cube $[0,1] \times [0,1] \times [0,1]$. The points in the cube have coordinates (R, G, B) which describe the intensities of the primary colors red, green, and blue. The corners $(1,0,0)$, $(0,1,0)$, and $(0,0,1)$ (= red, green, and blue at maximal intensity) are regarded as basis elements from which all other colors (R, G, B) can be obtained as linear combinations (additive mixing of colors). Of special importance are the complementary colors "yellow" $(1,1,0)$ (=red+green), "magenta" $(1,0,1)$, and "cyan" $(0,1,1)$, which are also corner points of the color cube. The two remaining corners are "black" $(0,0,0)$ and "white" $(1,1,1)$. All shades of gray are on the main diagonal from black to white. In *Mathematica*, the RGB colors are implemented by the color directive `RGBColor`.

In order to visualize a complex number by a color, we have to define a mapping from the two-dimensional complex plane into the three-dimensional color manifold. This can be done, of course, in an infinite number of ways. For our purposes we will define a mapping which is best described by another set of coordinates on the color manifold.

The HSB and HLS color systems: A measure for the distance between any two colors $C^{(1)} = (R^{(1)}, G^{(1)}, B^{(1)})$ and $C^{(2)} = (R^{(2)}, G^{(2)}, B^{(2)})$ in the color cube is given by the maximum metric

$$d(C^{(1)}, C^{(2)}) = \max\{|R^{(1)} - R^{(2)}|, |G^{(1)} - G^{(2)}|, |B^{(1)} - B^{(2)}|\}. \qquad (1.6)$$

The distance of a color $C = (R, G, B)$ from the black origin $O = (0,0,0)$ is called the *brightness* b of C,

$$b(C) = d(C, O) = \max\{R, G, B\}. \qquad (1.7)$$

The *saturation* $s(C)$ is defined as the distance of C from the gray point on the main diagonal which has the same brightness. Hence

$$s(C) = \max\{R, G, B\} - \min\{R, G, B\}. \qquad (1.8)$$