Interactive Quantum Mechanics

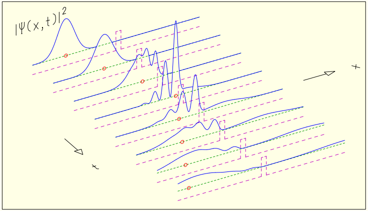
Siegmund Brandt
Physics Department
Siegen University

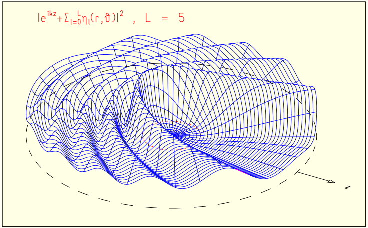
Abstract

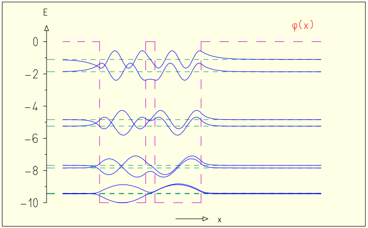
Together with Hans Dahmen and Tilo Stroh an interactive program was developed to demonstrate features of nonrelativistic quantum mechanics. Its usage is intended to supplement to lectures and exercises for students first exposed to quantum mechanics. The program has a Java interface, allows for the input of various parameters and produces as output two- and three-dimensional graphics and videos. Following a short introduction the talk concentrates on the presentation of examples, such as: harmonic waves and wave packets; free particles, bound states and scattering in various potentials in 1 and 3 dimensions; two-particle systems; distinguishable and indistinguishable particles; coherent and squeezed states in time-dependent motion; Kepler motion in quantum mechanics.

The Aim: Visualization of Nonrelativistic QM

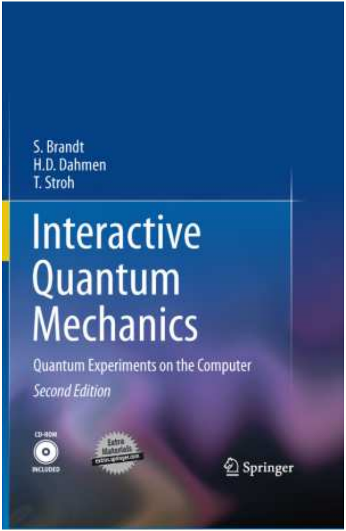
- Use computer to solve Schrödinger equation and present result graphically
- Students are hoped to develop a “feeling” for quantum mechanics by using the program INTERQUANTA as a laboratory





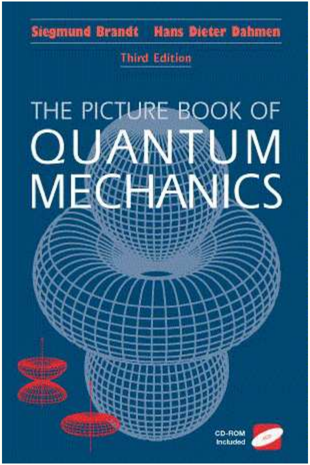


The Program INTERQUANTA (IQ)

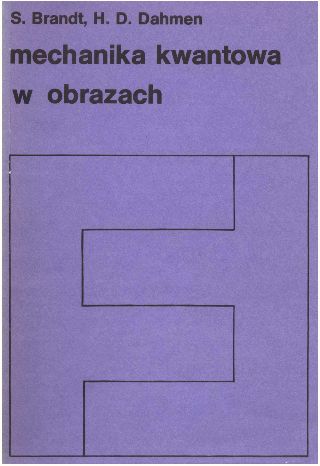


Springer, New York 2011

Prehistory I: The Picture Book of Quantum Mechanics



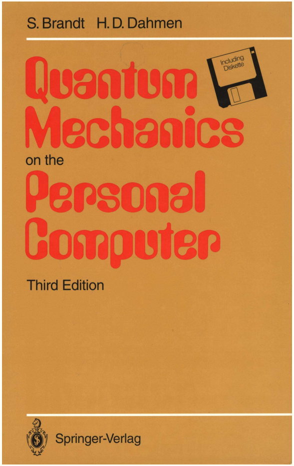
Wiley 1985; Springer 1995, 2001



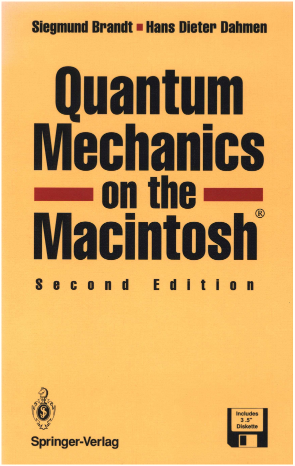
PWN 1989. *Translated by Tomasz Hofmokl*

Has appeared also in Japanese, Chinese, Luthuanian, Romanian, Slovak

Prehistory II: Quantum Mechanics on the PC (Mac)



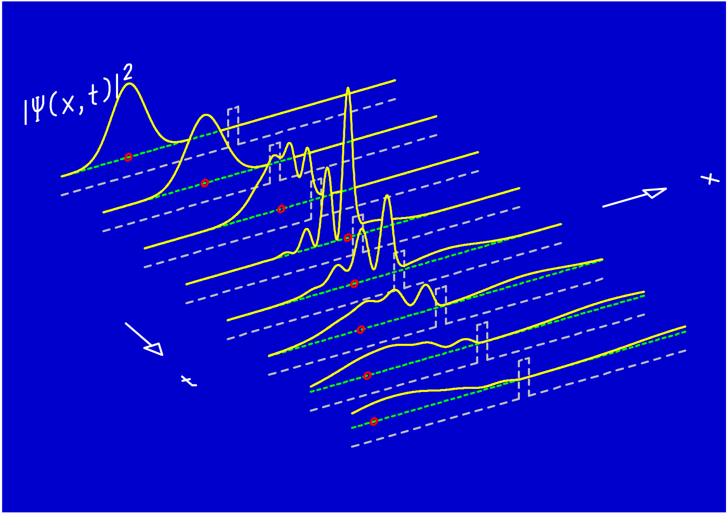
Springer 1989, 1992, 1994



Springer 1991, 1995

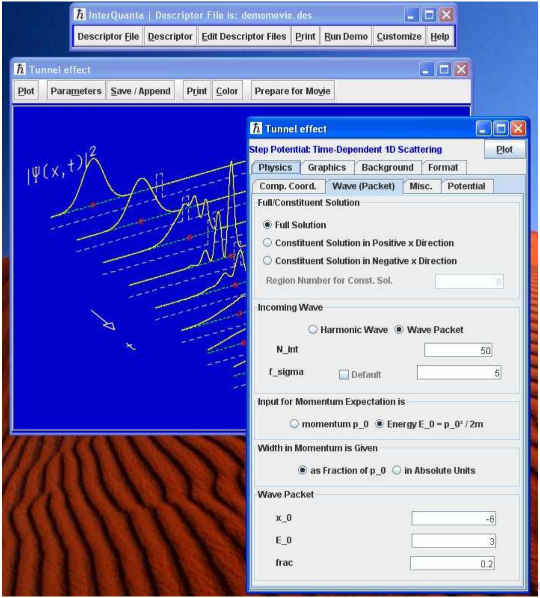
Has appeared also in German, Japanese, Iranian

A First Session



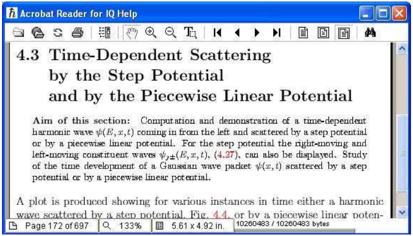
Structure of IQ

- Computing in FORTRAN
- Each Simulation completely defined by parameter set called *descriptor*
- Sets of descriptors grouped in *descriptor files*
- User Interface in Java operates on descriptor and presents graphics
- Object-oriented structure of Java allows for indefinite number of graphics and parameter panels on the screen. Useful for experimenting.
- Runs under Windows, Mac OS X, Linux; 32 and 64 bit
- No programming knowledge rquired of user



Help Facilities

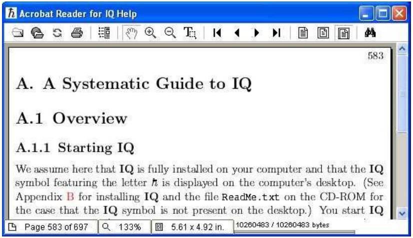
- Tool-tip texts
- Context-sensitive help
- Systematic Guide
- Full text of book



4.3 Time-Dependent Scattering by the Step Potential and by the Piecewise Linear Potential

Aim of this section: Computation and demonstration of a time-dependent harmonic wave $\psi(E,x,t)$ coming in from the left and scattered by a step potential or by a piecewise linear potential. For the step potential the right-moving and left-moving constituent waves $\psi_{\rightarrow,\pm}(E,x,t)$, (4.27), can also be displayed. Study of the time development of a Gaussian wave packet $\psi(x,t)$ scattered by a step potential or by a piecewise linear potential.

A plot is produced showing for various instances in time either a harmonic wave scattered by a step potential, Fig. 4.4, or by a piecewise linear poten-



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A. A Systematic Guide to IQ

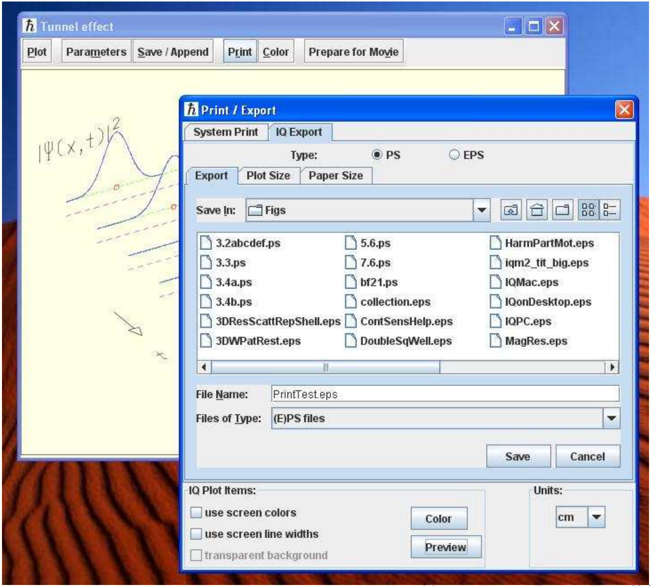
A.1 Overview

A.1.1 Starting IQ

We assume here that **IQ** is fully installed on your computer and that the **IQ** symbol featuring the letter $\hbar$ is displayed on the computer's desktop. (See Appendix B for installing **IQ** and the file `ReadMe.txt` on the CD-ROM for the case that the **IQ** symbol is not present on the desktop.) You start **IQ**

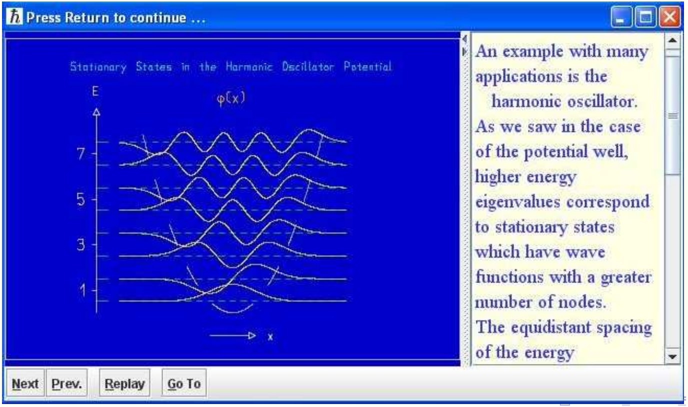
Printing

- Directly on system printer
- As ps or eps file
- Free choice of colors, line widths, format, paper size, etc.

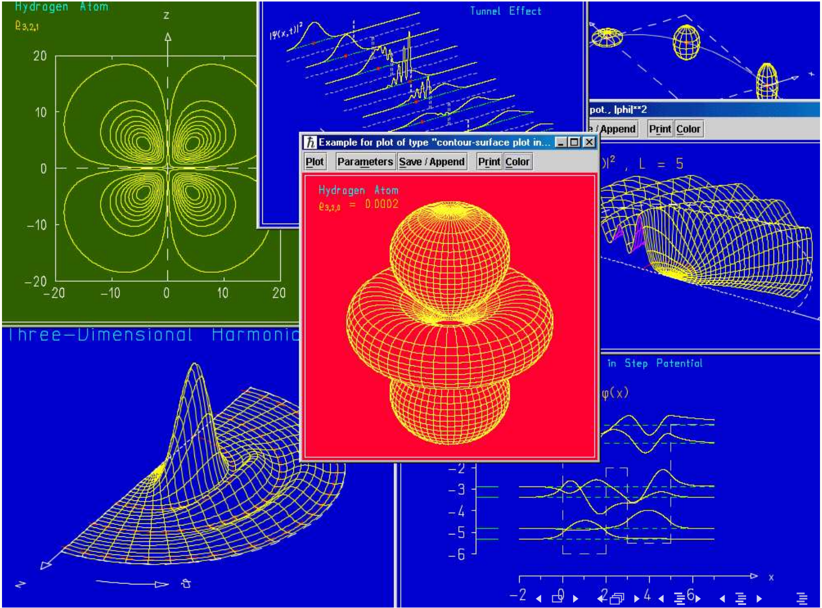


Running a Demo

- A demo consists of text and/or sound, directly produced IQ graphics, other graphics, movies
- Demos are available – as introductory lectures – on all 10 physics topics
- There are also demos introducing the user to IQ and to the creation of movies
- User can easily compose new demos



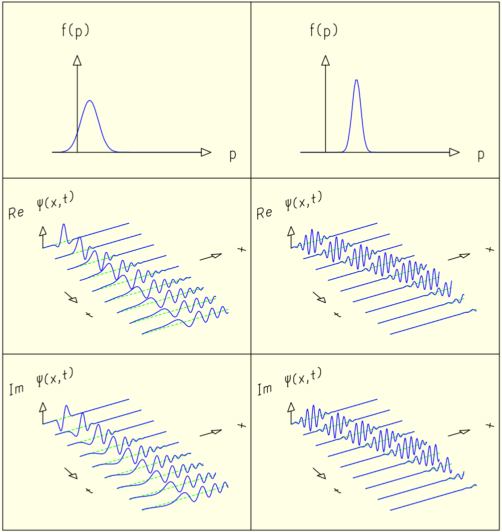
Physics Topics



Free Particle Motion in One Dimension

- Free Quantum-Mechanical Gaussian Wave Packet
- Free Optical Gaussian Wave Packet
- Quantile Trajectories
- Spectral Function of a Gaussian Wave Packet
- Wave Packet as a Sum of Harmonic Waves
- Phase-Space Distribution of Classical Mechanics
- Classical Phase-Space Distribution: Covariance Ellipse

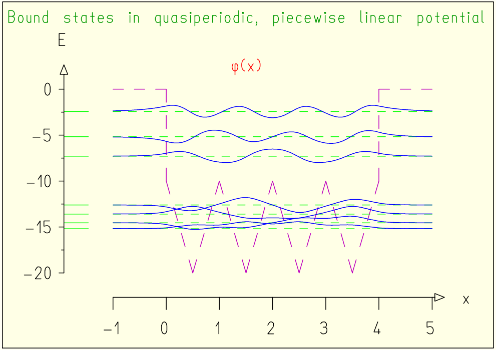
[Descriptors 1, 10, 14]



Bound States in One Dimension

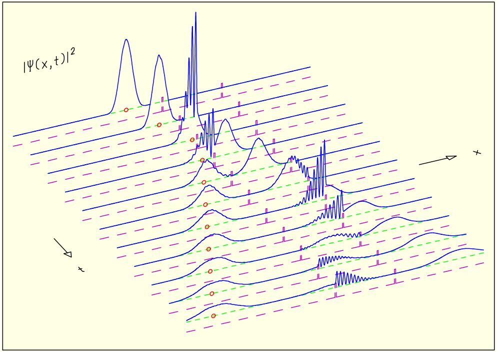
- Eigenstates in Deep Square Well
- Eigenstates in Harmonic Oscillator
- Eigenstates in Piecewise Constant Potential
- Eigenstates in Piecewise Linear Potential
- Harmonic Particle Motion
- Harmonic Motion of Classical Phase-Space Distribution
- Particle Motion in Deep Square Well

[Descriptors 1 – 8] Movie: Motion in deep sq. well



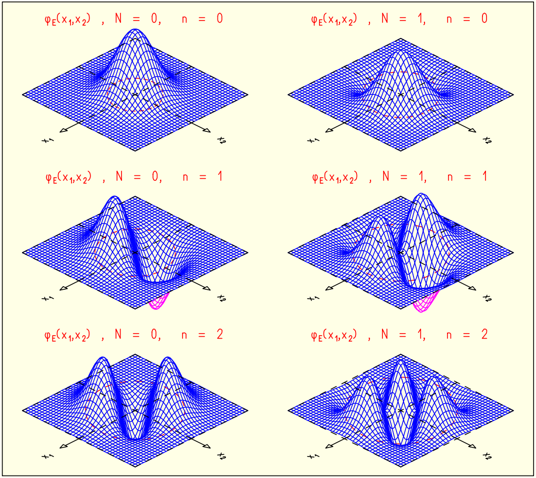
Scattering in One Dimension

- Stationary Scattering States
- Time-Dependent Scattering
- Transmission and Reflection. The Argand Diagram
- Optical Analoga



A Two-Particle System: Coupled Harmonic Oscillators

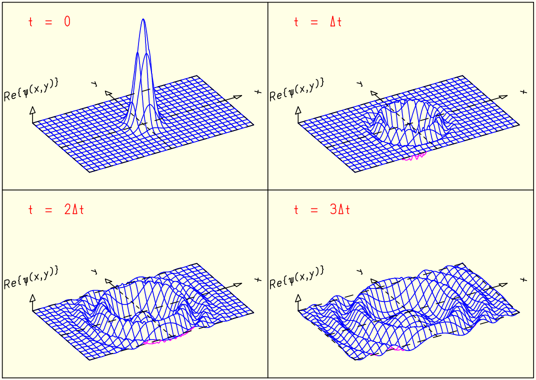
- Distinguishable and Indistinguishable Particles
- Stationary States
- Time Dependence of Global Variables
- Joint Probability Densities
- Marginal Distributions



[Help file for formulae
Descriptors 1, 2, 3]

Free Particle Motion in Three Dimensions

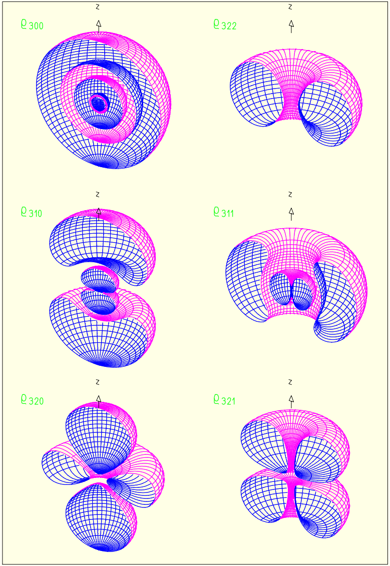
- 3D Harmonic Plane Wave
- Plane Wave Decomposed into Spherical Waves
- 3D Gaussian Wave Packet
- Probability Ellipsoid
- Angular-Momentum Decomposition of a Wave Packet



[Plane waves and 3D wave packet: Descriptors 1, 2, 5; Spherical waves and 3D wave packet: Descriptors 6, 7, 33]

Bound States in Three Dimensions

- Radial Wave Functions in Simple Potentials
- Radial Wave Functions in the Step Potential
- Probability Densities
- Contour Lines of the Probability Density
- Contour Surface of the Probability Density
- Harmonic Particle Motion



Schrödinger Eq. for Spherically Symmetric Potential

Stationary Schrödinger equation $\left(-\frac{\hbar^2}{2M}\Delta + V(r)\right)\varphi_E(\vec{r}) = E\varphi_E(\vec{r})$

Wave funtions factorize $\varphi_{E\ell m}(\vec{r}) = R_{E\ell}(r)\, Y_{\ell m}(\vartheta,\varphi)$; $\varrho_{n\ell m}(\vec{r}) = |\varphi_{n\ell m}(\vec{r})|^2$

Effective potential $V_\ell^{\mathrm{eff}}(r) = \frac{\hbar^2}{2M}\frac{\ell(\ell+1)}{r^2} + V(r)$

Radial Schrödinger equation $\left(-\frac{\hbar^2}{2M}\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}r + V_\ell^{\mathrm{eff}}(r)\right)R_{E\ell}(r) = ER_{E\ell}(r)$

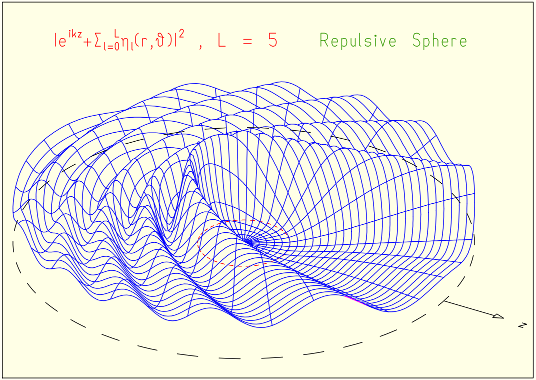
Radial wave functions depend on potential. In region q of a step potential

$$R_{\ell q}(k_q, r) = A_{\ell q} j_\ell(k_q r) + B_{\ell q} n_\ell(k_q r); \quad k_q = \left|\sqrt{2M(E - V_q)}/\hbar\right|; \quad q = 1, 2, \ldots, N$$

[Descriptors 5, 9, 13, 17, 18]

Scattering in Three Dimensions

- Radial Wave Functions in Step Potential
- Stationary Wave Functions and Scattered Waves
- Differential Cross Sections
- Scattering Amplitude. Phase Shift. Partial and Total Cross Sections
- Coulomb Scattering: Radial Wave Function
- Coulomb Scattering: 3D Wave Function



Scattering of plane wave by repulsive sphere

Plane Wave Scattered by Spher. Symm. Potential

Incident plane wave $\quad \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}} = \sum_{\ell=0}^{\infty}(2\ell+1)\mathrm{i}^{\ell} j_\ell(kr) P_\ell(\cos\vartheta)$

Stationary wave $\quad \varphi(\vec{k},\vec{r}) = \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}} + \eta(\vec{k},\vec{r})$

Partial stationary and scattered waves $\quad \varphi(\vec{k},\vec{r}) = \sum_{\ell=0}^{\infty}\varphi_\ell(\vec{k},\vec{r}); \quad \eta(\vec{k},\vec{r}) = \sum_{\ell=0}^{\infty}\eta_\ell(\vec{k},\vec{r})$

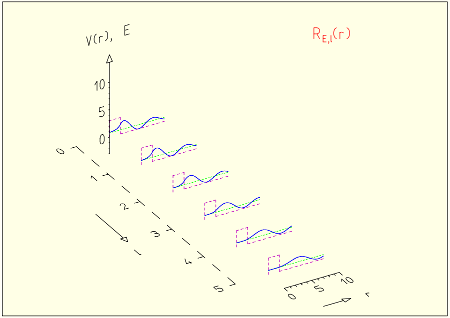
With R_ℓ properly normalized for inc. wave $\quad \eta_\ell(\vec{k},\vec{r}) = (2\ell+1)\mathrm{i}^{\ell}[R_\ell(k,r) - j_\ell(kr)]P_\ell(\cos\vartheta)$

Far outside ($kr \gg 1$): $\quad \eta(\vec{k},\vec{r}) \approx f(k,\vartheta)\frac{\mathrm{e}^{ikr}}{r}$

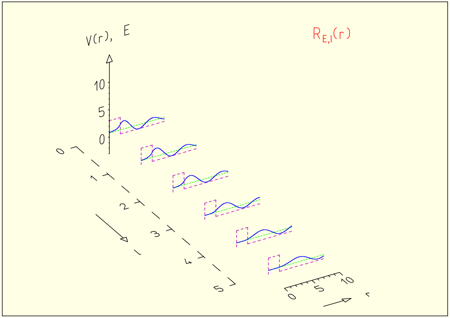
Scatt. amplitude and phase $\quad f(k,\vartheta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)f_\ell(k)P_\ell(\cos\vartheta); \quad f_\ell(k) = \mathrm{e}^{\mathrm{i}\delta_\ell}\sin\delta_\ell$

Cross sections $\quad \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(k,\vartheta)|^2; \quad \sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)|f_\ell(k)|^2; \quad \sigma_{\mathrm{tot}} = \sum_{\ell=0}^{\infty}\sigma_\ell$

Scatt. by Repulsive Sphere: Radial Wave Function

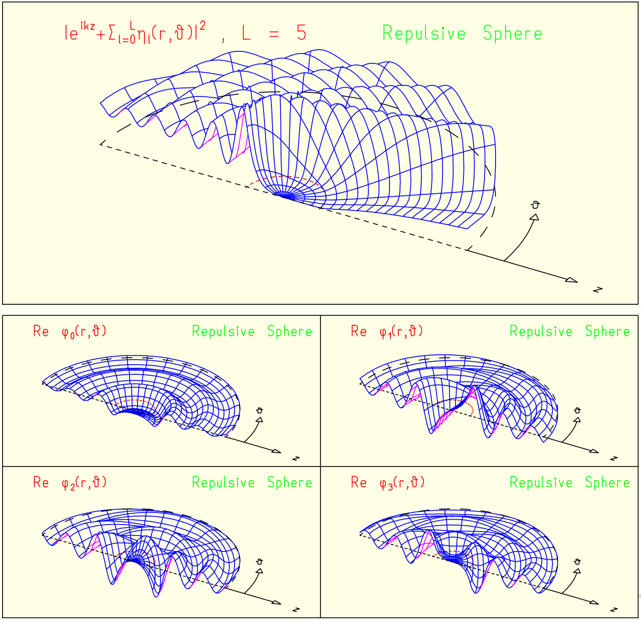


E fixed, ℓ runs

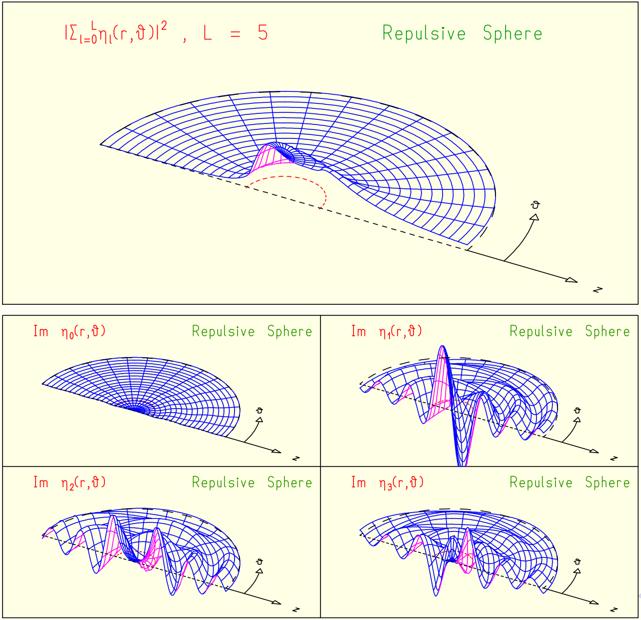


ℓ fixed, E runs

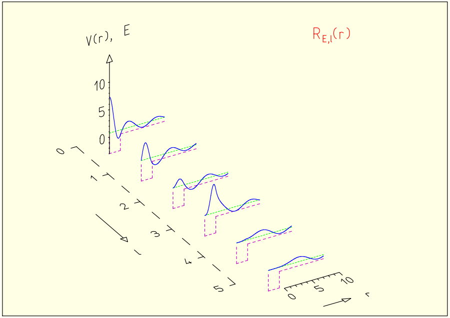
Scatt. by Repulsive Sphere: Stationary Wave



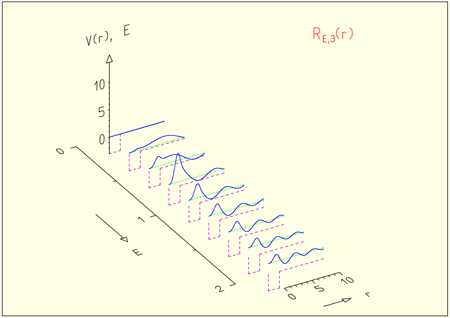
Scatt. by Repulsive Sphere: Scattered Wave



Scatt. by Attractive Sphere: Radial Wave Function

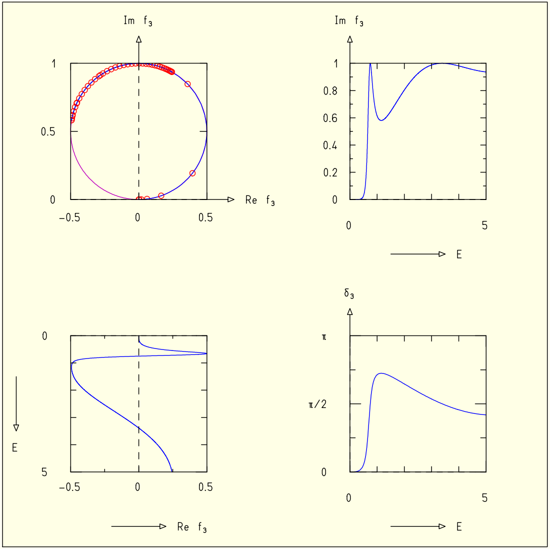


E fixed, ℓ runs

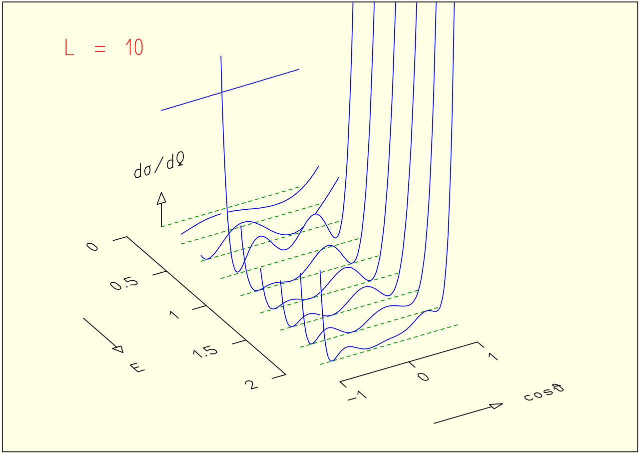


ℓ fixed, E runs

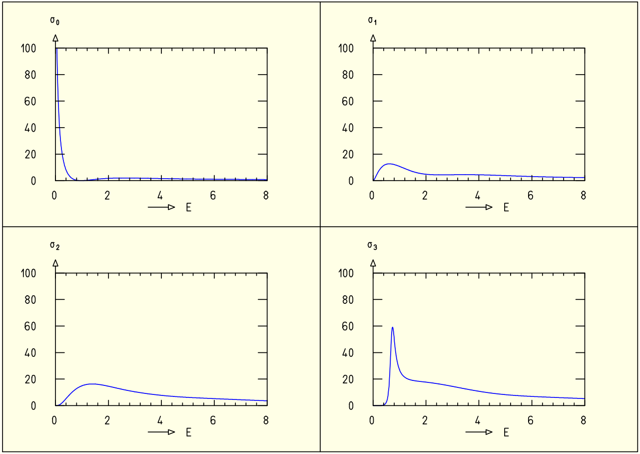
Scatt. by Attractive Sphere: Partial Scatt. Ampl.



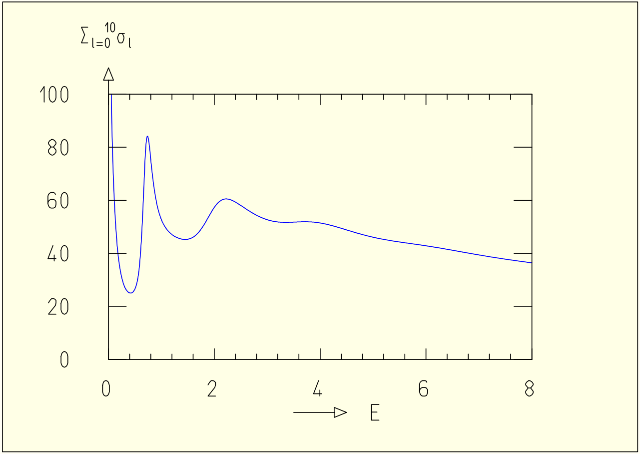
Scatt. by Attractive Sphere: Diff. Cross Section



Scatt. by Attractive Sphere: Partial Cross Sections

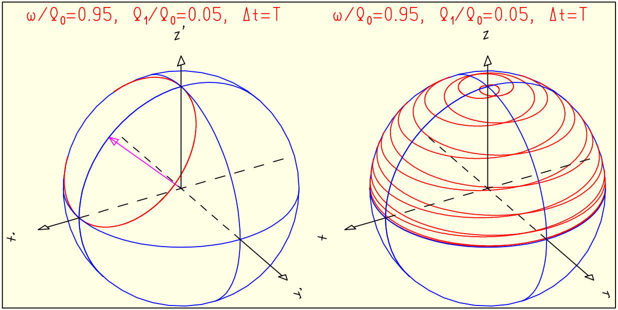


Scatt. by Attractive Sphere: Total Cross Sections



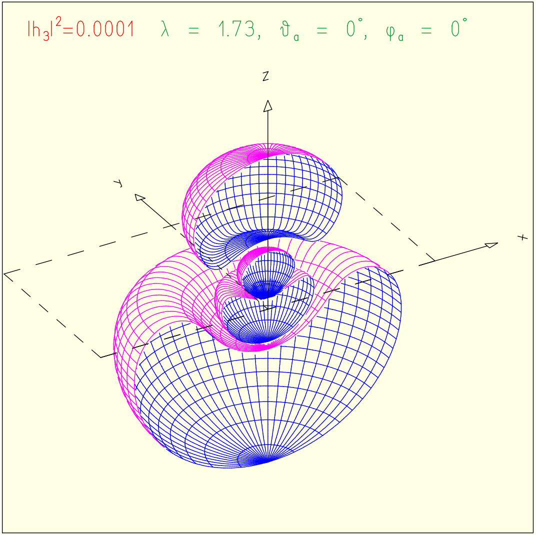
Magnetic Resonance

- The Spin-Expectation Vector near and at Resonance
- Resonance Form of the Rabi Amplitude



Hybridization

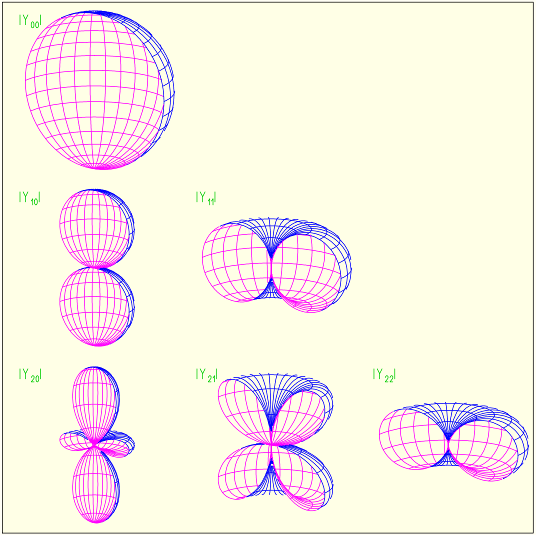
- Hybrid Wave Functions and Probability Densities
- Contour Lines of Hybrid Wave Functions and Probability Densities
- Contour Surfaces of Hybrid Probability Densities



Probability density of sp^3 hybrid for $n = 3$ shown as contour-surface plot in half-space $y > 0$

Functions of Mathematical Physics

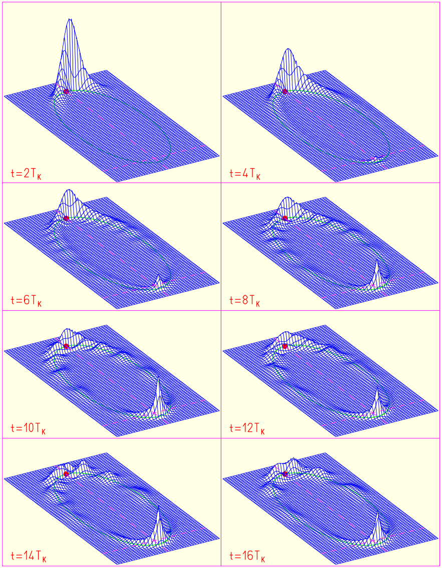
- Hermite Polynomials and Related Functions
- Legendre Polynomials and Related Functions
- Spherical Harmonics
- Bessel Functions and Related Functions
- Airy Functions
- Laguerre Polynomials
- Gaussian Distribution and Error Function
- Bivariate Gaussian Distribution
- Binomial and Poisson Distributions
- Simple Functions of a Complex Variable



Spherical Harmonics: 3D polar plots

An Extra: Kepler Motion in Quantum Mechanics

- Details in:
  S. D. Boris, S. B., H. D. Dahmen,
  T. Stroh, and M. L. Larsen,
  Phys. Rev. A 48 (1993) 2527
- Elliptic Orbits
  5 classical revolution periods
  108 classical revolution periods
- Hyperbolic Orbits
  Wide packet in attractive potential
  Narrow packet in attractive potential
  Wide packet in repulsive potential
  Narrow packet in repulsive potential



Quantum numbers of wave packet $n = 320 \pm 10$, $\ell = 140 \pm 10$

A Collection of Movies on the Web

http://www.tp1.physik.uni-siegen.de/ brandt/books/index.php?ID=IQM