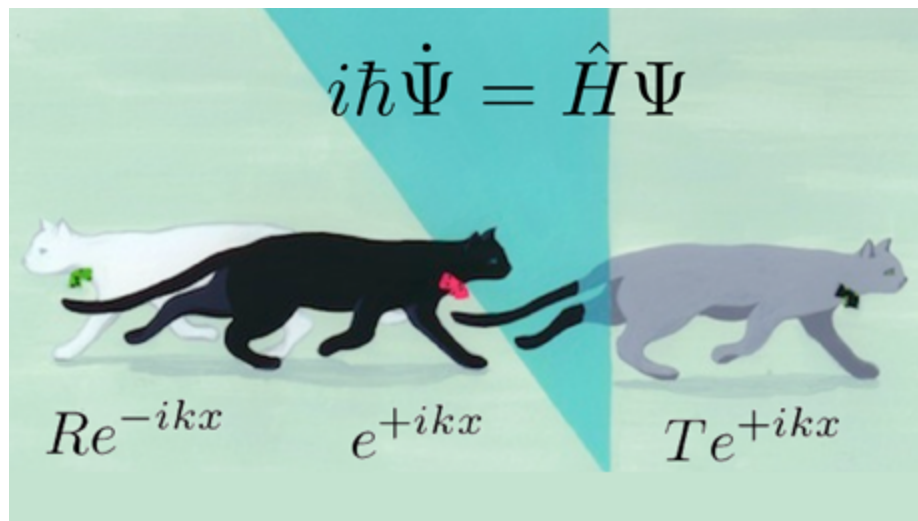
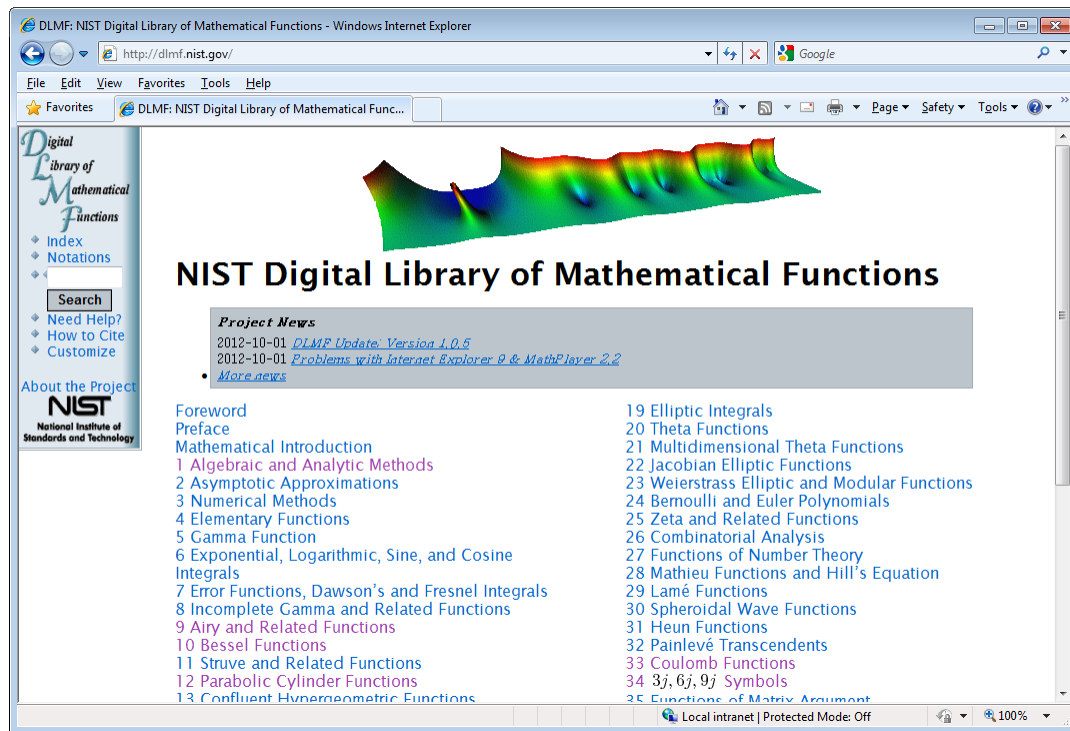


Solving the Schrödinger Equation

Part V. Use of Special Functions



Solving the Schrödinger Equation



<http://dlmf.nist.gov>

Primary reference for:

- Definitions
- Function properties
- Graphics
- TeX encoding
- MathML encoding
- Semantic search

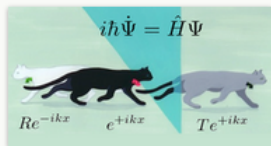
Free access worldwide

Solving the Schrödinger Equation



Exploring Quantum Physics

by Dr. Charles Clark and Dr. Victor Galitski



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Mathematical References

For those who may want to brush up on their mathematics before or during the courses, we present [a short crash course on the mathematics of Quantum Mechanics](#).

[Solution of frequently-encountered Schrödinger equations in terms of special functions](#) - a one-page reference chart of known solutions

Demonstration of numerical solution of the Schrödinger equation - we provide [a spreadsheet](#) that demonstrates a simple numerical technique for solving the Schrödinger equation. This is a Microsoft Excel .xls document, which has also been tested with the freely-available [Google Sheets](#). A brief description of the method is contained [in this document](#)

Our notation for and definition of special functions of mathematics (e.g. Bessel, Legendre, Laguerre, etc.) is taken from [The NIST Digital Library of Mathematical Functions](#) (DLMF). The DLMF is a free online digital library that gives extensive mathematical reference information on these functions and guidance to their applications

In examples and exercises in which numerical values of physical constants are called for, we use the values given in [The CODATA Internationally Recommended Values of the Fundamental Physical Constants](#) .

In examples and exercises that use atomic data, we use the values given in [The Handbook of Basic Atomic Spectroscopic Data](#) .

We use a standard periodic table of the elements in the lectures and exercises. A high-resolution version is available as a free download at [Atomic Properties of the Elements](#) .

Original scientific literature

Some lectures draw on material from original scientific literature, which we provide here for the convenience of students.

Solving the Schrödinger Equation

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Erwin Schrödinger
1887-1961

1933 Nobel Prize in Physics
"for the discovery of new
productive forms of atomic
theory".

Who was first to solve the Schrödinger equation using special functions?

Schrödinger's first papers on wave mechanics used special functions to solve the equations for the harmonic oscillator and hydrogen atom.

He mapped those equations onto standard existing, well-studied equations of mathematical physics.

We shall take the same approach here.

Solving the Schrödinger Equation

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Three one-dimensional examples

$$V(x) = V_0$$

$$V(x) = V_0 + V_1x$$

$$V(x) = V_0 + V_1x + V_2x^2$$

These map on to exponential, Airy and parabolic cylinder functions respectively and illustrate general principles that are important in the *numerical* solution of one-dimensional Schrödinger equations.

Solving the Schrödinger Equation

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$$V(x) = V_0$$

$$\left[-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + V_0 \right] \Psi(x) = E \Psi(x)$$

Need solutions *for all* E so that we can find those that will satisfy particular boundary equations.

Transform the Schrödinger equation into the standard form

$$\frac{\partial^2}{\partial \rho^2} \psi(\rho) \pm \psi(\rho) = 0$$

that defines the exponential function

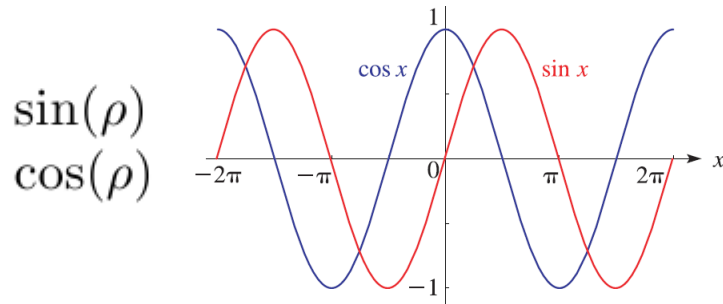
Solving the Schrödinger Equation

$$V(x) = V_0$$

$$\left[-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + V_0 \right] \Psi(x) = E \Psi(x) \quad \rho = kx \quad \frac{\hbar^2 k^2}{2m} = \|E - V_0\| \quad \Psi(x) = \psi(kx)$$

$E > V_0$ **oscillatory**

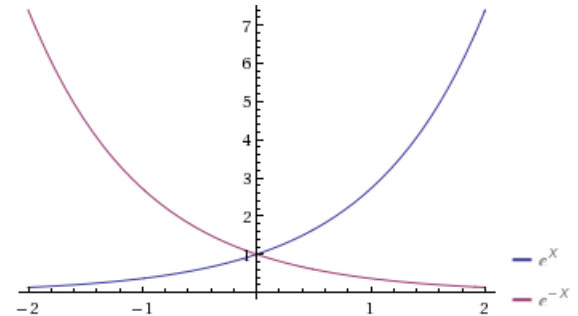
$$\frac{\partial^2}{\partial \rho^2} \psi(\rho) + \psi(\rho) = 0 ;$$



divergent $E < V_0$

$$\frac{\partial^2}{\partial \rho^2} \psi(\rho) - \psi(\rho) = 0$$

$\exp(\rho)$
 $\exp(-\rho)$

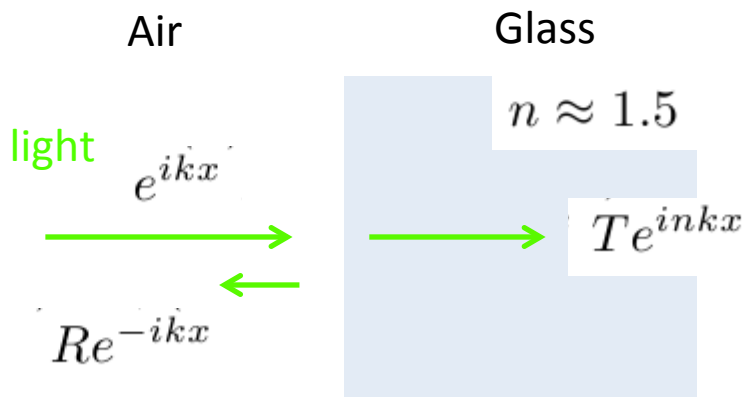


Solving the Schrödinger Equation

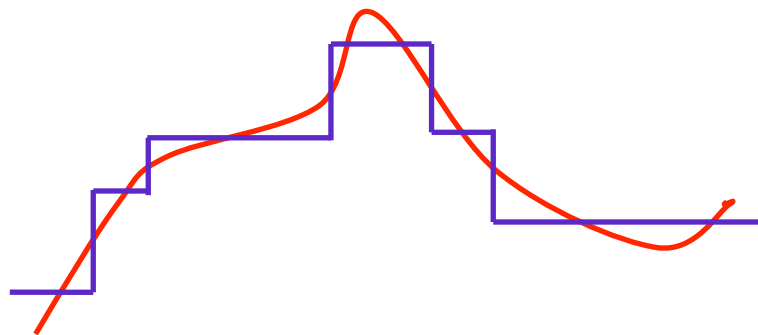
$$V(x) = V_0$$

$$\left[-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + V_0 \right] \Psi(x) = E \Psi(x) \quad x = k\rho \quad \frac{\hbar^2 k^2}{2m} = \|E - V_0\|$$

An example that you see every day



Simulate general **V(x)** by **constant segments**
Solve exactly segment-by-segment

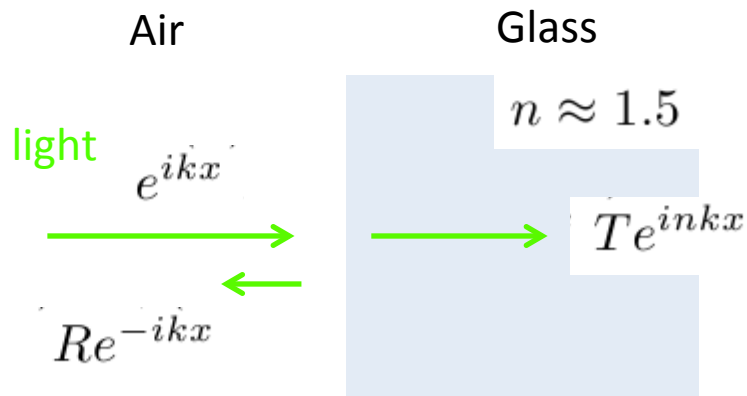


Solving the Schrödinger Equation

$$V(x) = V_0$$

$$\left[-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + V_0 \right] \Psi(x) = E \Psi(x) \quad x = k\rho \quad \frac{\hbar^2 k^2}{2m} = \|E - V_0\|$$

An example that you see every day



$$\Psi(x) = e^{ikx} + Re^{-ikx}$$

$$\Psi(x) = Te^{inkx}$$

$$\Psi(0) = 1 + R$$

$$\frac{d\Psi(0)}{dx} = ik(1 - R)$$

$$\frac{1 - R}{1 + R} = n$$

$$R = \frac{1 - n}{1 + n} = -\frac{0.5}{2.5}$$

