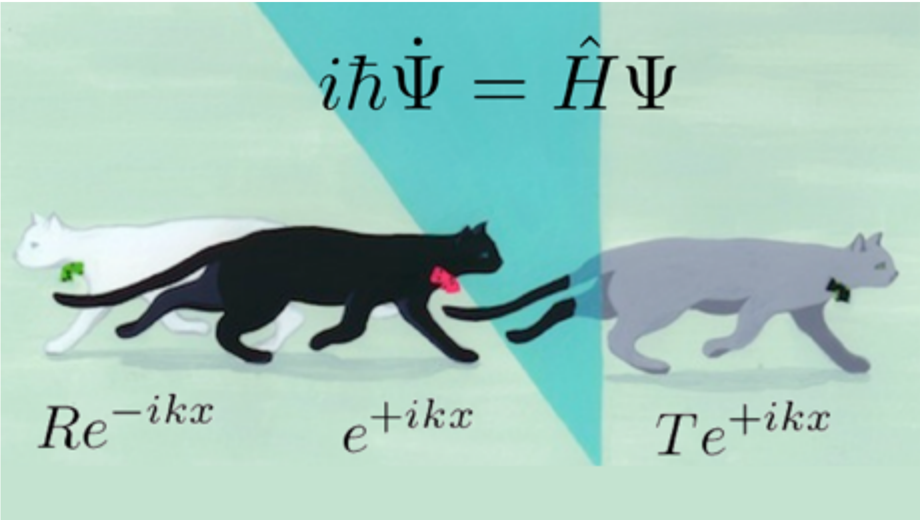
Exploring Quantum Physics

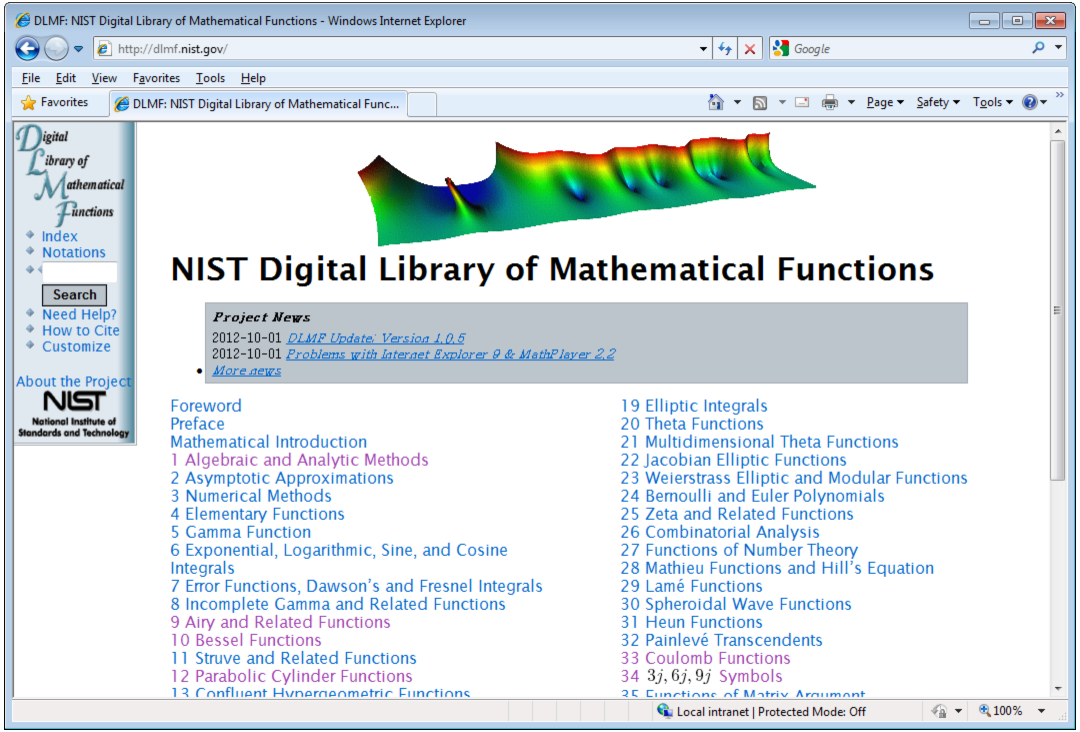
Coursera, Spring 2013 Instructors: Charles W. Clark and Victor Galitski

Solving the Schrödinger Equation

Part III. 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

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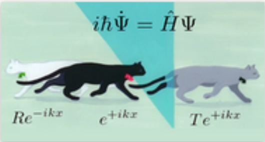
Solving the Schrödinger Equation

UNIVERSITY OF MARYLAND

Exploring Quantum Physics
by Dr. Charles Clark and Dr. Victor Galitski



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Additional Materials

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

Wikimedia Public Domain

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

$$V(x) = V_0$$
$$V(x) = V_0 + V_1 x$$
$$V(x) = V_0 + V_1 x + V_2 x^2$$

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

Erwin Schrödinger
1887-1961
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"for the discovery of new productive forms of atomic theory".

$$V(x) = V_0$$

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

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

$$V(x) = V_0$$

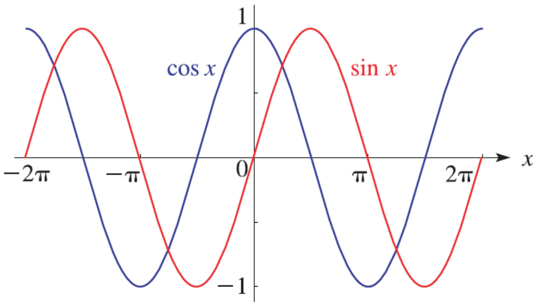
$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + V_0\right]\Psi(x) = E\Psi(x) \quad \rho = kx \quad \frac{\hbar^2 k^2}{2m} = \|E - V_0\| \quad \Psi(x) = \psi(kx)$$

$E > V_0$ **oscillatory**

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

$\sin(\rho)$

$\cos(\rho)$

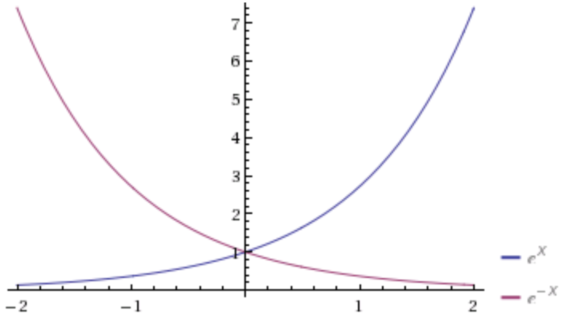


divergent $E < V_0$

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

$\exp(\rho)$

$\exp(-\rho)$



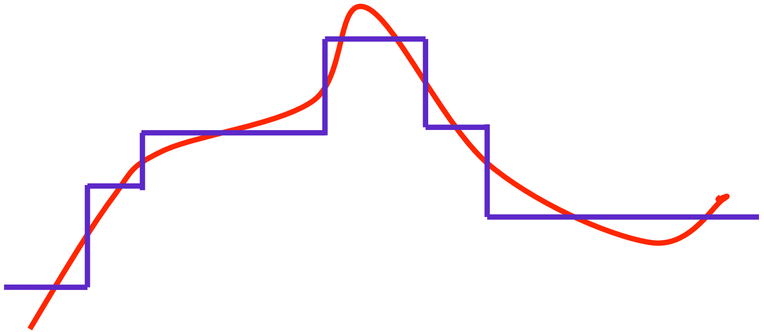
Solving the Schrödinger Equation

$$V(x) = V_0$$

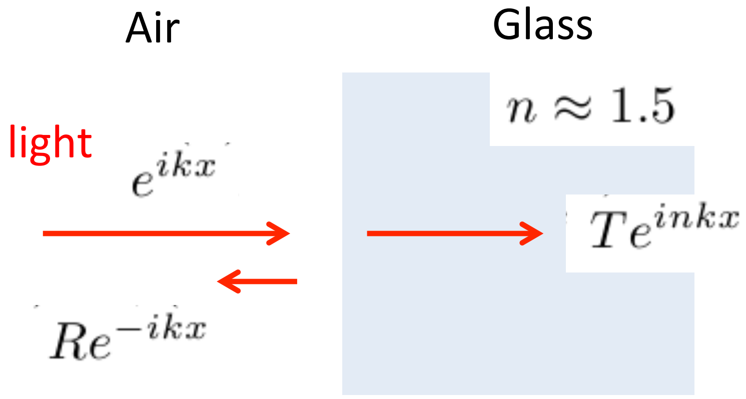
$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + V_0\right]\Psi(x) = E\Psi(x) \qquad x = k\rho \qquad \frac{\hbar^2 k^2}{2m} = \|E - V_0\|$$

Simulate general V(x) by constant segments

Solve exactly segment-by-segment



An example that you see every day



In-video quiz

This is a reasonable model of light coming from air $(x < 0)$ into glass $(x > 0)$. The index of refraction of this glass is $n = 1.5$.

\vspace {12 pt}

The Schr\"{o}dinger equation in the air region $(x < 0)$ can be cast in the form

\vspace {12 pt}

$\left[\frac{\partial^2}{\partial x^2} + k^2 \right] \psi (x) = 0$, and its solution there is given by

\vspace {12 pt}

$\psi(x) = e^{ikx} + R e^{-ikx}$

\vspace {12 pt}

The Schr\"{o}dinger equation in the glass region $(x > 0)$ can be cast in the form

\vspace {12 pt}

$\left[\frac{\partial^2}{\partial x^2} + n^2 k^2 \right] \psi (x) = 0$, and its solution there is given by

\vspace {12 pt}

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

\vspace {12 pt}

Find R by requiring that the wavefunction and its derivative be continuous at $x=0$. The fraction of the incident light reflected from the glass back into the air is given by $|R|^2$. Which of these is closest to its value, expressed as a percentage (i.e. $R = 1$ would be espressed as 100\%)?

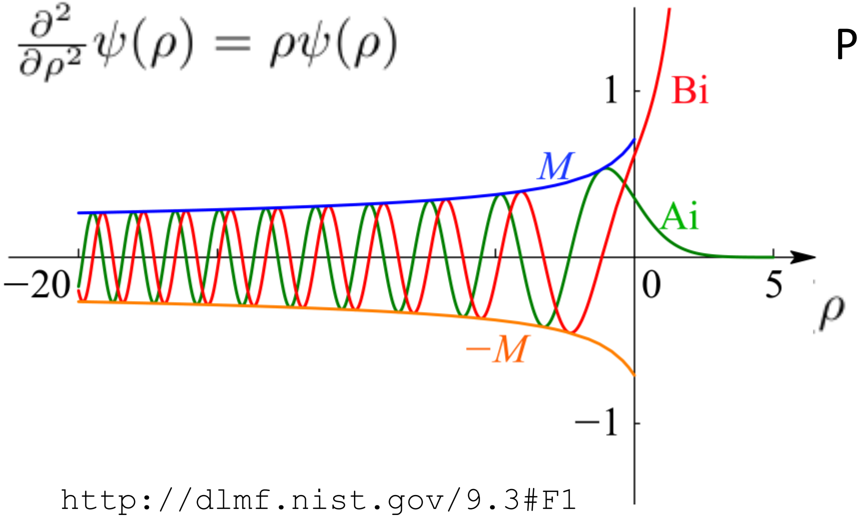
\vspace {12 pt}

Solving the Schrödinger Equation

$$V(x) = V_0 + V_1 x$$

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + V_0 + V_1 x\right]\Psi(x) = E\Psi(x) \qquad x = \frac{\alpha\rho + E - V_0}{V_1} \qquad \alpha = \left[\frac{\hbar^2 V_1^2}{2M}\right]^{1/3}$$

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



http://dlmf.nist.gov/9.3#F1

Pair of universal solutions: Airy functions

$$\mathrm{Ai}(\rho),\ \mathrm{Bi}(\rho)$$

Both oscillatory for $\rho < 0$

Ai: quantum bouncing ball

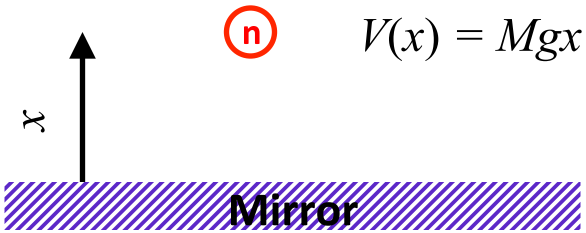
Bi: scanning tunneling microscope

Solving the Schrödinger Equation

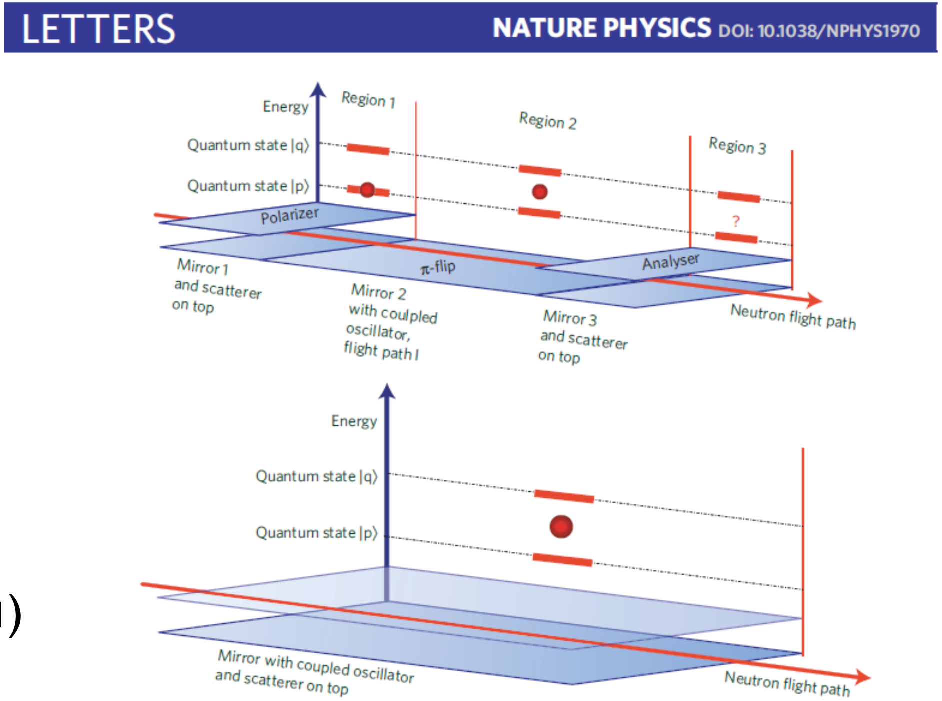
The quantum-mechanical bouncing ball

Measurement of energy levels of a neutron bouncing off a mirror in the Earth's gravitational field

$$V(x) = Mgx$$



"Realization of a gravity-resonance-spectroscopy technique," T. Jenke, *et al.*, *Nature Physics* **7**, 468 (2011)



Solving the Schrödinger Equation

$$V(x) = Mgx$$

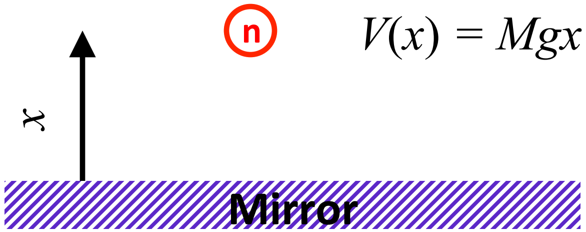
$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + Mgx\right]\Psi(x) = E\Psi(x) \qquad x = \frac{\alpha\rho + E}{Mg} \qquad \alpha = \left[\frac{\hbar^2 M g^2}{2}\right]^{1/3}$$

Energy levels of a neutron bouncing off a mirror in the Earth's gravitational field

g = acceleration due to Earth's gravity ≈ 9.8 m s^{-2}

M = mass of neutron = 1.67 x 10^{-27} kg

$\Psi(x)$ = 0 for $x = 0$, the surface of the mirror



In-video quiz

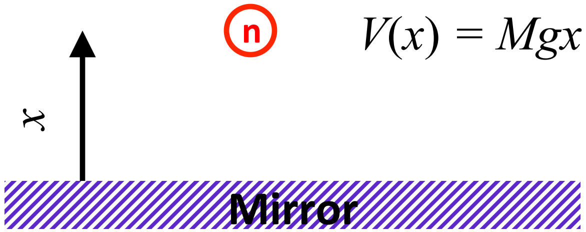
For a neutron bouncing off a mirror in the Earth's gravitational field, the Schr\"{o}dinger equation is
\vspace {5 mm}
$ \left[-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + Mgx\right]\Psi(x) = E \Psi(x)$
where M is the neutron mass and g the acceleration due to Earth's gravity. The wavefunction $\Psi(x)$ must vanish when x has the value corresponding to the surface of the mirror: $x=0$. In other words, the neutron is perfectly reflected by the mirror.
\vspace {5 mm}
In the transformation to the dimensionless variable, ρ, we found the relationship $x = \frac{\alpha \rho + E}{Mg}$. What are the units of α in terms of $\mathrm{mass} [\mathrm{M}], \mathrm{length} [\mathrm{L}],$ and time $[\mathrm{T}]$?
\vspace {5 mm}
$[\mathrm{M}][\mathrm{L}]^2[\mathrm{T}]^{-2}$ correct
\vspace {5 mm}
it is dimensionless
\vspace {5 mm}
$[\mathrm{M}][\mathrm{L}][\mathrm{T}]^{-1}$
\vspace {5 mm}
$[\mathrm{L}][\mathrm{T}]^{-2}$
\vspace {5 mm}

Solving the Schrödinger Equation

$$V(x) = Mgx$$

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + Mgx\right]\Psi(x) = E\Psi(x) \qquad x = \frac{\alpha\rho + E}{Mg} \qquad \alpha = \left[\frac{\hbar^2 M g^2}{2}\right]^{1/3}$$

Energy levels of a neutron bouncing off a mirror in the Earth's gravitational field



$V(x) = Mgx$

g = acceleration due to Earth's gravity ≈ 9.8 m s^{-2}

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$\Psi(x)$ = 0 for $x = 0$, the surface of the mirror

α must have units of energy

In-video quiz

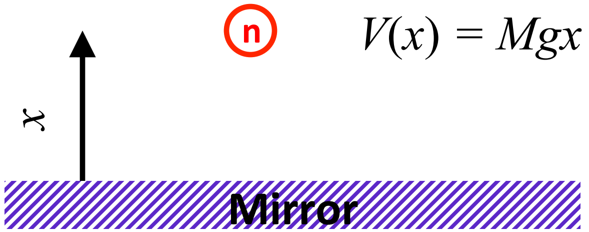
For a neutron bouncing off a mirror in the Earth's gravitational field, the Schr\"{o}dinger equation is
\vspace {5 mm}
$ \left[-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + Mgx\right]\Psi(x) = E \Psi(x)$
where M is the neutron mass and g the acceleration due to Earth's gravity. The wavefunction $ \Psi(x)$ must vanish when x has the value corresponding to the surface of the mirror: $x=0$. In other words, the neutron is perfectly reflected by the mirror.
\vspace {5 mm}
In the transformation to the dimensionless variable, ρ, we found the relationship $x = \frac{\alpha \rho + E}{Mg}$. In terms of the classical motion performed by a particle with the same mass, M, and energy$E$, what is the significance of the coordinate value $\rho = 0$?
\vspace {5 mm}
The kinetic energy is a maximum at $\rho = 0$
The surface of the mirror is at $\rho = 0$
The particle attains its maximum distance from the mirror at $\rho = 0$ correct
The point $\rho = 0$ is in the classically-forbidden region and is never reached by the classical particle.

Solving the Schrödinger Equation

$$V(x) = Mgx$$

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + Mgx\right]\Psi(x) = E\Psi(x) \qquad x = \frac{\alpha\rho + E}{Mg} \qquad \alpha = \left[\frac{\hbar^2 M g^2}{2}\right]^{1/3}$$

Energy levels of a neutron bouncing off a mirror in the Earth's gravitational field



g = acceleration due to Earth's gravity ≈ 9.8 m s^{-2}

M = mass of neutron = 1.67 x 10^{-27} kg

$\Psi(x)$ = 0 for $x = 0$, the surface of the mirror

α must have units of energy

ρ = 0 describes the "classical turning point", i.e. the place where the velocity changes sign.

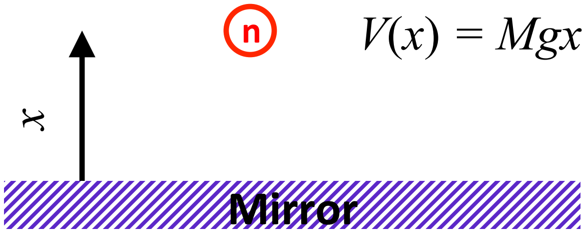
Solving the Schrödinger Equation

$$V(x) = Mgx$$

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + Mgx\right]\Psi(x) = E\Psi(x) \qquad x = \frac{\alpha\rho + E}{Mg} \qquad \alpha = \left[\frac{\hbar^2 M g^2}{2}\right]^{1/3}$$

$\mathrm{Ai}(\rho)$ is the relevant solution.

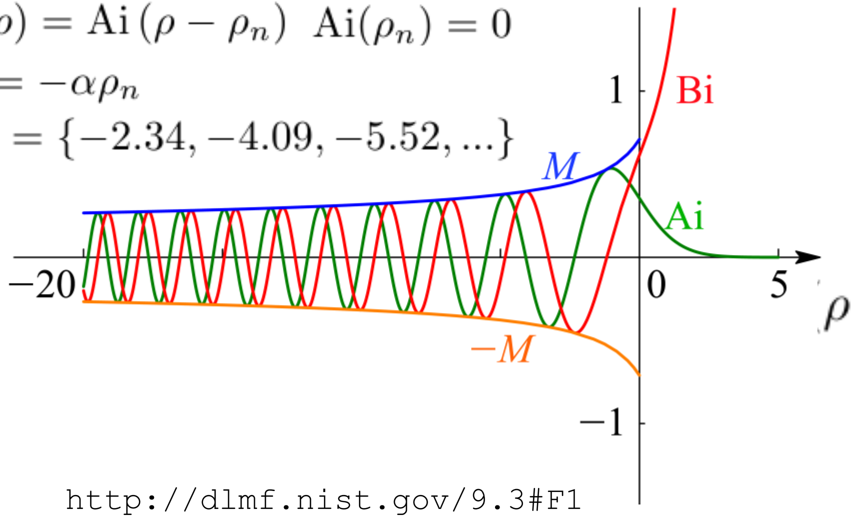
We position the mirror at its nodes to generate all of the eigenfunctions.



$$\phi_n(\rho) = \mathrm{Ai}(\rho - \rho_n) \quad \mathrm{Ai}(\rho_n) = 0$$

$$E_n = -\alpha\rho_n$$

$$\{\rho_n\} = \{-2.34, -4.09, -5.52, \ldots\}$$



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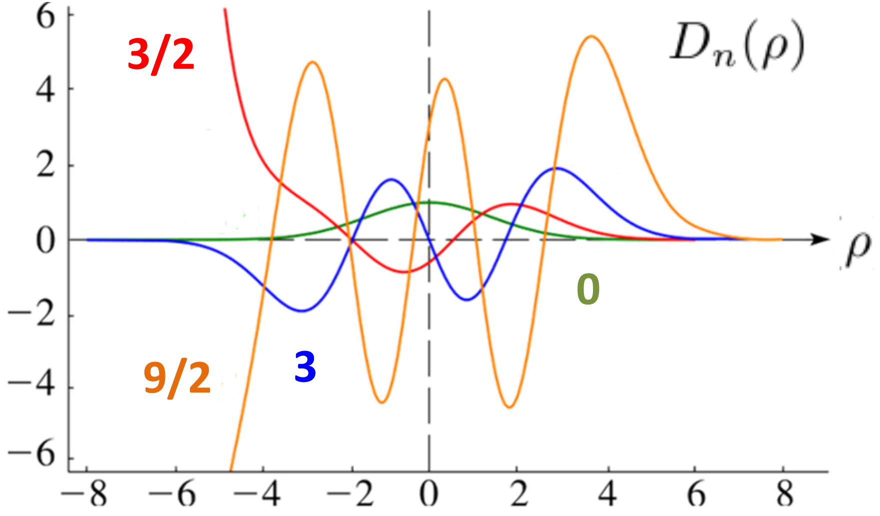
Solving the Schrödinger Equation

$$V(x) = V_0 + V_1 x + \frac{m\omega^2}{2} x^2$$

$$\rho = \frac{x - x_1}{d} \qquad d = \sqrt{\frac{\hbar}{m\omega}} \qquad x_1 = -\frac{V_1}{m\omega^2} \qquad E = \hbar\omega\left(n + \tfrac{1}{2}\right) + V_0 + \frac{V_1 x_1^2}{2}$$

$$\frac{\partial^2 \psi(\rho)}{\partial \rho^2} + \left(n + \tfrac{1}{2} - \tfrac{1}{4}\rho^2\right)\psi(\rho) = 0$$

Two solutions: the parabolic cylinder functions $D_n(\rho)$ and $D_n(-\rho)$. Both of these *diverge* unless *n* = integer.



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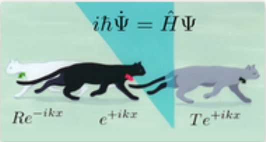

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