2D Infinite Square Well Example

Units: energy is in eV, distance is in nm, and ct is in nm

\( h\bar{c} = 197 \) Planck's constant times c in eV nanometers

\( mc^2 = 511000 \) Electron rest energy in eV

\( a = 0.05 \) Radius of the well in nm

Example plots of Bessel functions:

Bessel Function of 1st Kind: \( J_0(x) \)

Bessel Function of 1st Kind: \( J_1(x) \)

Bessel Function of 1st Kind: \( J_2(x) \)
M := 10  Number of different Bessel functions to consider
N := 8   How many values of wave number to calculate (# of zeros of each Bessel Function)

Program to search for the first N zeroes of each of the Bessel functions, to find the allowed
values of the radial wave number. MathCad does not have a built in function to do this.

\[
\begin{align*}
k &:= \left\{ \begin{array}{l}
\text{for } m \in 0..M \\
x \leftarrow 0.2 \\
y \leftarrow J_n(m, x) \\
n \leftarrow 0 \\
\text{while } n < N \\
x \leftarrow x + 0.1 \\
\text{if } J_n(m, x) \cdot y < 0 \\
n \leftarrow n + 1 \\
\text{trace}^{m,n}(x, y) \\
z_{m,n} \leftarrow \text{root}(J_n(m, x), x, x - 0.1, x) \\
y \leftarrow J_n(m, x)
\end{array} \right.
\end{align*}
\]

\[
\begin{align*}
m &:= 0..M \\
n &:= 1..N
\end{align*}
\]

\[
\omega_{m,n} := \frac{\hbar \cdot c \cdot m}{2 \cdot mc^2} \quad \text{Angular frequencies (divided by c)}
\]

Calculate normalization factors:

\[
\begin{align*}
N_{m,n} &:= \frac{1}{\int_0^a \left( \left| J_n(m, r) \right|^2 \cdot r \cdot dr \right)^{1/2}} \int_0^a \left( \left| J_n(m, r) \right|^2 \cdot r \cdot dr \right)^{1/2} \cdot r \cdot dr \\
\end{align*}
\]

Normalized radial wave functions:

\[
\begin{align*}
\Psi_{m,n,r} &:= \frac{1}{\sqrt{2\pi}} \cdot R_{m,n,r} \cdot e^{-i \cdot m \phi} \\
\end{align*}
\]

Stationary state eigenfunctions

\[
\begin{align*}
\Psi(m,n,r,\phi,ct) &:= \Psi_{m,n,r,\phi} \cdot e^{-i \cdot \omega_{m,n} \cdot ct} \quad \text{Solutions to the full time-dependent S.E.}
\end{align*}
\]
The form of these wave functions was obtained by separation of variables of the 2D Schrödinger equation in polar coordinates. See the related problem in Homework #5.

\[ ct := \text{FRAME} \cdot 4 \]

Time (times c) at which to evaluate the wave function. \( ct \) is in units of nm. The FRAME variable is zero by default but is used to increment the time when making animations (see below).

**Probability densities to plot. First, some of the stationary states:**

\[ f_0(x, y) := \left( \left| \Psi \left( 0, 1, \sqrt{x^2 + y^2}, \text{atan2}(x, y), ct \right) \right| \right)^2 \]

Ground State Probability Density

Note: in these plots I set the grid such that the function is never evaluated at the origin, so that I don't run into a problem with the atan2 function not being defined. To see the settings, double click on the plot and then click on the tab "Quick Plot Data".
\[ f_1(x, y) := \left| \Psi(1, 1, \sqrt{x^2 + y^2}, \text{atan2}(x, y), ct) \right|^2 \]

1st Excited State Probability Density

\[ f_2(x, y) := \left| \Psi(0, 2, \sqrt{x^2 + y^2}, \text{atan2}(x, y), ct) \right|^2 \]

2nd Excited State Probability Density
Now plot a mixture of two stationary states of different energy:

\[
f(x, y) := \left( |\Psi(0, 1, \sqrt{x^2 + y^2}, \text{atan}2(x, y), ct) + \Psi(1, 1, \sqrt{x^2 + y^2}, \text{atan}2(x, y), ct)| \right)^2
\]

This is a mixture of stationary states of different energy, so this probability density will evolve with time. Also, even though the individual probability densities of the stationary states are all phi symmetric, in a mixture that is not the case, as illustrated here.

The time dependent plots can be animated. From the Tools menu select Animation-Record. Enter the range for the FRAME variable (e.g. 0 to 100), select the plot with the rubber-band cursor, and then click Animate.
Expand an initial phi-symmetric state in terms of these eigenfunctions. In this case only \( m=0 \) is needed.

\[
\sigma := \frac{a}{5} = 0.01 \quad \text{Width in radius of the initial Gaussian packet}
\]

\[
\psi_0(r) := \frac{1}{\sqrt{2\pi \sigma^2}} e^{-\frac{r^2}{4\sigma^2}} \quad \text{Initial, normalized wave function (Gaussian in radius)}
\]

\[
c_n := \left( \int_0^a R(0,n,r) \, \psi_0(r) \, r \, dr \right) \quad \text{Expansion coefficients, determined by numerical integration}
\]

\[
f(r) := \sum_n \left( c_n \cdot R(0,n,r) \right) \quad \text{Truncated series expansion of the initial wave function}
\]

\[
2\pi \left[ \int_0^a \left( |f(r)|^2 \right) \cdot r \, dr \right] = 1 \quad \text{Check the normalization of the truncated series}
\]

**Initial radial wave function**

This is a check that the truncated series matches well the initial wave function.

\[
\Psi_g(r, \phi, ct) := \sum_n \left( c_n \cdot R(0,n,r) \cdot e^{i\omega_0 n c t} \right) \quad \text{Full time-dependent wave function}
\]
\[ f_g(x, y) := \left( |\Psi_g(x^2 + y^2, \text{atan}(x, y), ct) | \right)^2 \] Probability density in Cartesian coordinates

\[ \Phi \text{-Symmetric Wave Packet} \]

Another example: make the wave packet propagate in the x direction:

\[ k_0 := \frac{2}{a} \quad \sigma = 0.01 \quad k_0 \text{ is the wave number for the } x \text{-motion} \]

\[ \psi_1(r, \phi) := \frac{1}{\sqrt{2\pi\sigma^2}} \cdot e^{-\frac{r^2}{4\sigma^2}} \cdot e^{ik_0 r \cos(\phi)} \] Initial state, with an \( \exp(ikx) \) factor

\[ \int_0^{2\pi} \int_0^a \left( |\psi_1(r, \phi)| \right)^2 \cdot r \, dr \, d\phi = 1 \] Check the normalization of the initial state

\[ d_{m, n} := \int_0^{2\pi} \int_0^a \psi_1(r, \phi) \cdot \psi_1(r, \phi) \cdot r \, dr \, d\phi \] Expansion coefficients

\[ \Psi_p(r, \phi, ct) := \sum_m \sum_n \left( d_{m, n} \cdot \Psi(m, n, r, \phi, ct) \right) \] Full time-dependent wave function
\[
\int_0^{2\pi} \int_0^a \left( |\Psi_p(r, \phi, 0)| \right)^2 r \, dr \, d\phi = 0.929
\]

Note that the normalization is a bit off, due to numerical inaccuracies in the coefficients and the truncation of the series.

\[
f_p(x, y) := \left( \Psi_p \left( \sqrt{x^2 + y^2, \text{atan2}(x, y), ct} \right) \right)^2
\]

Probability density in cartesian coordinates

Wave Packet Moving in x Direction

Another example: make the wave packet go in circles:

\[
k_\phi := \frac{1}{2\pi} \quad \sigma := \frac{a}{5}
\]

k0 is the wave number for the x-motion

\[
\Psi_2(r, \phi) := \frac{1}{\sqrt{2\pi \sigma^2}} e^{-\frac{r^2}{4\sigma^2}} e^{ik_\phi \phi}
\]

Initial state

\[
\int_0^{2\pi} \int_0^a \left( |\Psi_2(r, \phi)| \right)^2 r \, dr \, d\phi = 0.999
\]

Check the normalization of the initial state
Expansion coefficients

\[ d_{m,n} := \int_0^{2\pi} \int_0^a \psi(m,n,r,\phi) \cdot \psi_2(r,\phi) \cdot r \, dr \, d\phi \]

Full time-dependent wave function

\[ \Psi_t(r,\phi,ct) := \sum_m \sum_n \left( d_{m,n} \cdot \Psi(m,n,r,\phi,ct) \right) \]

Note that the normalization is way off, due to numerical inaccuracies in the coefficients and the truncation of the series.

\[ \int_0^{2\pi} \int_0^a \left( |\Psi_t(r,\phi,0)| \right)^2 \cdot r \, dr \, d\phi = 0.876 \]

Probability density in cartesian coordinates

\[ f_t(x,y) := \left( \left| \Psi_t(\sqrt{x^2 + y^2}, \text{atan2}(x,y),ct) \right| \right)^2 \]