Part II: Basic one-dimensional problems and More Quantum Mechanics

- Several essential QM 1D problems
- Build up quantum sense
- Pick up more QM through examples (general statements may be too abstract)
- Practice what we discussed in previous chapters

These problems are easy but sometimes tricky

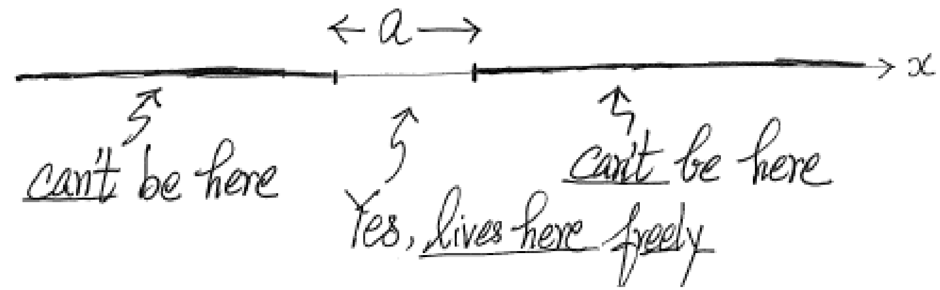
V. One-Dimensional Particle-in-a-box and Related Problems

- Easier to handle and to visualize
- Bring out very rich physics
- Understanding these simple problems gives you
  - many QM concepts and good quantum sense
  - a way to understand qualitatively
    - atoms, molecules, nuclei
    - much nanoscience

A. Particle in a One-Dimensional "box" or Infinite square well

Defining the problem: A particle of mass m living in 1D, confined to be in a range of length a but otherwise lives freely

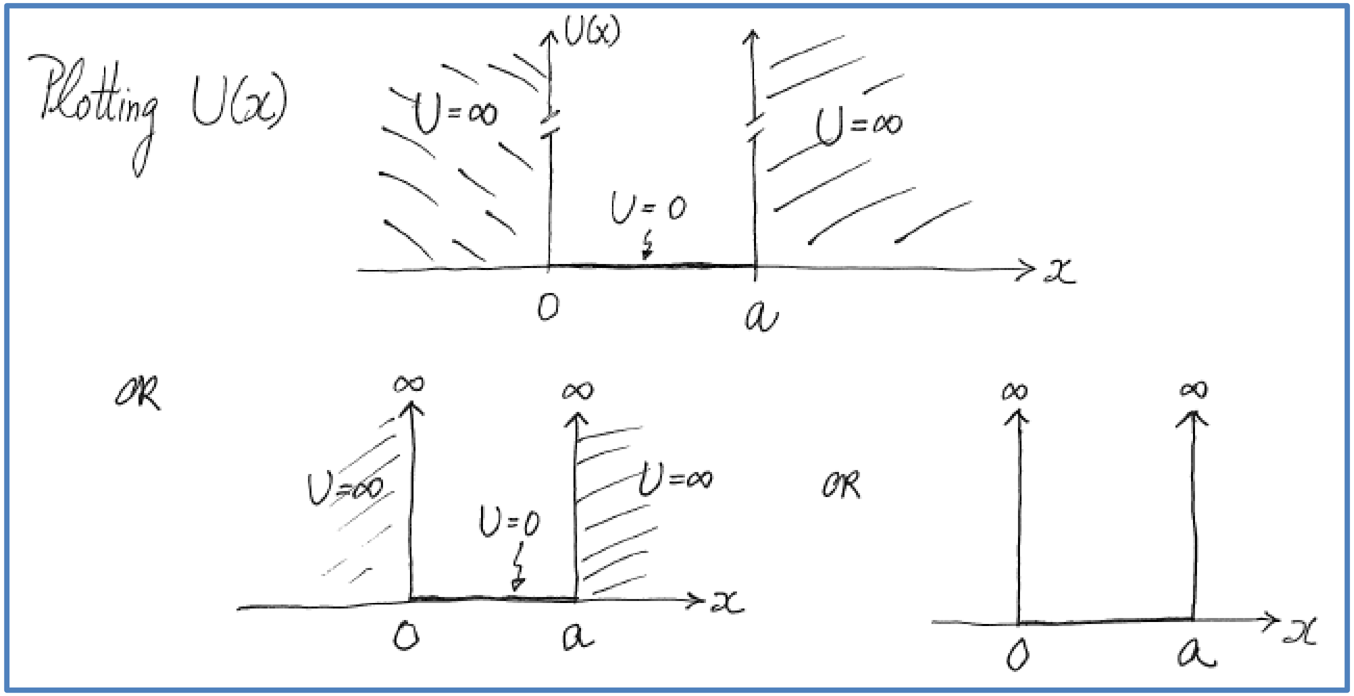
Meaning:



- 1D problem (everything happens in *x* only)
- Where to place the range is your choice (does it really matter?)
- What is *U(x)* that goes into TISE & TDSE?

One choice is

$$U(x) = \begin{cases} \infty & \text{for } x \leq 0 \text{ and } x \geq a \\ 0 & \text{for } 0 < x < a \end{cases}$$

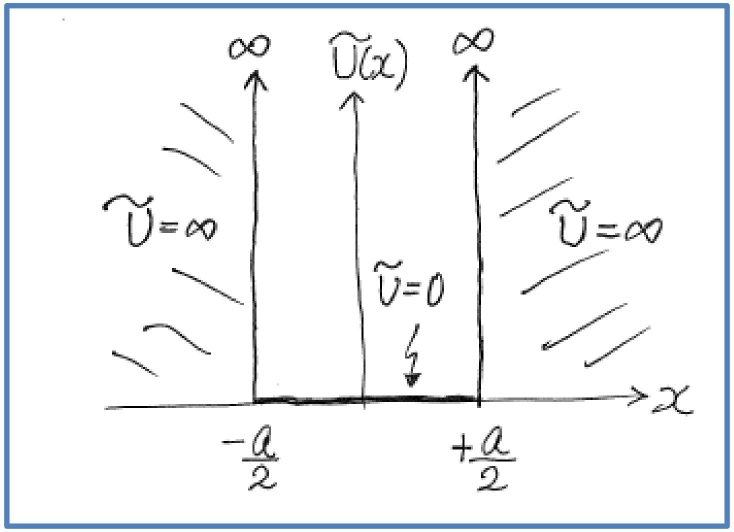


The important point is that you should know the meaning behind *U(x)* and the different ways it is being shown

Recall: It is a 1D problem. Plotting $U(x)$, of course, is a 2D plot. But the particle lives in $0 < x < a$. This is a trivial point but it has led to confusion among students.

Another choice could be

$$\tilde{U}(x) = \begin{cases} \infty & \text{for } x \leq -\frac{a}{2} \text{ and } x \geq +\frac{a}{2} \\ 0 & \text{for } -\frac{a}{2} < x < +\frac{a}{2} \end{cases}$$



Question: Think as we go along with solving TISE with *U(x)*. Will the different ways of placing the well/box change the physics? What will be changed, if not the physics?

(a) Solving TISE: Essential (Baby) Version Plus+

- Why? Solutions to TISE allow us to answer many QM questions

- $$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U(x)\,\psi(x) = E\,\psi(x) \qquad \left(\text{Many } \psi_E(x) \leftrightarrow E \text{ pairs}\right)$$

  - $U(x)$ is defined over whole range of x
  - Need to solve for $\psi(x)$ over all x (formally) [not only in $0<x<a$]

+ You might have done this before. But let's do it again and pay attention to some (obvious) details.

- Since $\underline{U=\infty}$ in $x \leq 0$ and $x \geq a$ (outside the well/box),
  $\psi(x) = 0$ for $x \leq 0$ and $x \geq a$.

$$\boxed{\text{TISE:} \quad \frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2}\left[U(x) - E\right]\psi(x)}$$

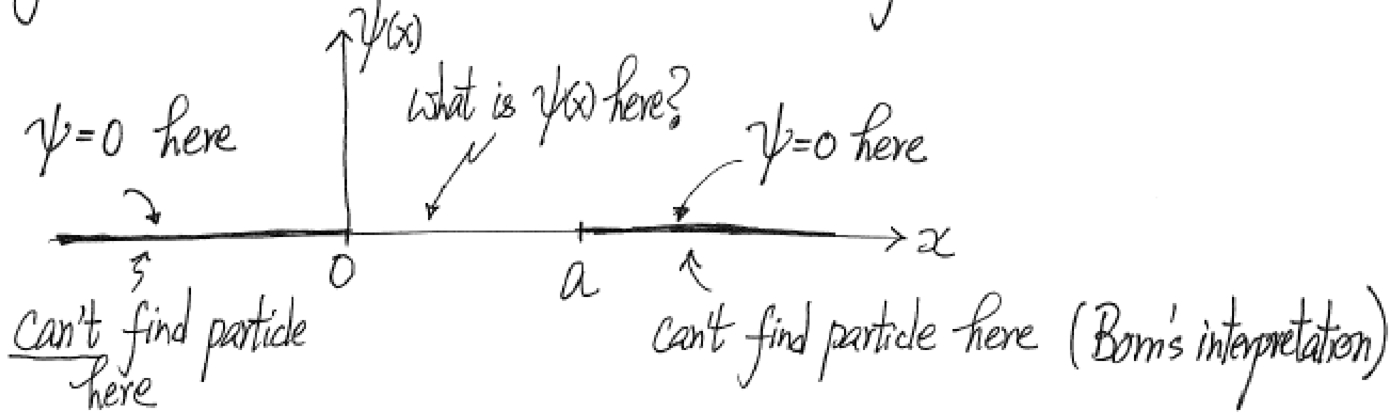
Recall: $\infty \cdot 0$ can be finite, but $\infty \cdot (\text{finite}) = \text{infinite}$

- When $U = \infty$ (outside well), only $\psi(x) = 0$ (<u>outside</u> well) can give a well-defined $\frac{d^2\psi}{dx^2}$ ("rate of change of slope")

$\therefore$ $\psi(x) = 0$ for $x \leq 0$ and $x \geq a$

[Remark: We will make this argument mathematical later, stay tuned]

Plotting $\psi(x)$ vs x (what we know too far)



Need to Solve for $\psi(x)$ for $0<x<a$

$U(x)=0$ (insider well/box) TISE: $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\,\psi(x)$

$$\text{or} \quad \frac{d^2}{dx^2}\psi(x) = -\frac{2mE}{\hbar^2}\psi(x)$$

[Some ψ with 2^{nd} derivative being "$-$itself", times a constant]

[Even without Math, sine and cosine work!]

• $\sin kx$ and $\cos kx$ work to solve $\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$

E hidden inside

$$\therefore \boxed{\psi(x) = A\sin kx + B\cos kx \quad \text{for } 0<x<a} \quad (*)$$

[This is what mathematics can tell. We are done with mathematics!]

But physics is more than Mathematics!

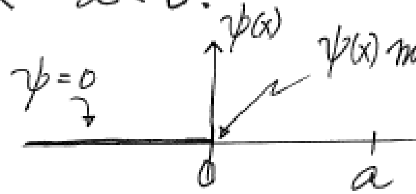
Physics: $\psi(x)$ must be well behaved!

What is important here is $\psi(x)$ must be continuous in the whole range of x $(-\infty < x < +\infty)$

Technically, we are considering boundary conditions. But don't worry about the name.

We know $\psi(x) = 0$ for $x \le 0$.

$\therefore \psi(0) = 0$



$\psi(x)$ must connect to $\psi(0) = 0$.

Apply (*) at $x=0$ (or $x \to 0$ if you like):

$$\psi(0) = \underbrace{0}_{\overset{\shortparallel}{\sin 0}} + B \cdot \underbrace{1}_{\overset{\shortparallel}{\cos 0}} = \underbrace{B = 0}_{\text{conclusion (killed cosine term)}}$$

continuity of ψ at $x=0$

Up to here:

$$\boxed{\psi(x) = A \sin kx \quad \text{for } 0 < x < a \qquad \text{E (eigenvalue) hidden in } k} \qquad (**)$$

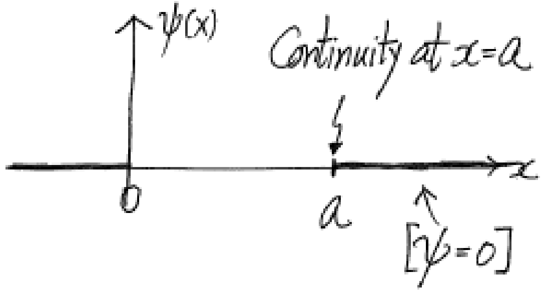
Continuous in $x \le 0$ and $x = 0$ and $0 < x < (a - \delta)$

a bit

But we also have $\psi(x) = 0$ for $x \geq a$, $\therefore \psi(a) = 0$

We must make sure the whole $\psi(x)$ is <u>continuous at $x = a$.</u>

Apply (**) at $x = a$:



$$\psi(a) \overset{\text{continuity}}{=} \underbrace{0 = A\sin(ka)}$$

> Must understand: Physics comes in to say...
> "<u>Not</u> all k (thus E) are legal"
> "Only specific values of k (thus E) give physically acceptable $\psi(x)$"

$$A \sin ka = 0 \Rightarrow \sin ka = 0 \Rightarrow \underbrace{ka = n\pi}_{\text{physics selects specific } k\text{'s}} \quad (n = 1, 2, 3, \ldots)$$

$$\text{OR} \quad k_n = \frac{n\pi}{a}$$

labels allowed k

$$\boxed{\text{OR} \quad E_n = \frac{\hbar^2 k_n^2}{2m} = n^2 \frac{\pi^2 \hbar^2}{2ma^2} = n^2 \frac{h^2}{8ma^2} \quad (n = 1, 2, 3, \ldots)}$$

labels allowed energies

[Reiterate: It is ***physics*** (boundary conditions) that selects the allowed energies]

Back to (**):

$$\boxed{\psi(x) = A \sin k_n x = A \sin\left(\frac{n\pi x}{a}\right) \quad \text{for } 0 < x < a} \quad (\dagger)$$

$$\boxed{\text{We are done with solving TISE (or } \hat{H}\psi = E\psi \text{ eigenvalue problem)}}$$

How about the factor *A*?

- In QM, $\psi(x)$ in (†) works OK. It gives the relative probability of finding the particle via $|\psi(x)|^2$.

[Recall: This is how QM wavefunction different from classical waves]

- Usually, <u>normalizing</u> $\psi(x)$ is useful.
    - $\psi(x)$ goes to zero as $x \to \pm\infty$ (can be normalized)
    - $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$ normalization condition

$$\int_0^a |A|^2 \sin^2(k_n x)\, dx = 1 \overset{(Ex.)}{\Longrightarrow} A = \sqrt{\frac{2}{a}} \quad \text{(assuming real } A\text{)}$$

("A" happens not to depend on n for this problem)

All solutions to TISE (all eigenfunctions and eigenvalues of $\hat{H}$)

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) & \text{for } 0<x<a \\ 0 & \text{for}^{+}\ x \le 0 \text{ and } x \ge a \end{cases}$$

AND $E_n = \dfrac{n^2\pi^2\hbar^2}{2ma^2}$

$(n = 1, 2, 3, \ldots)$

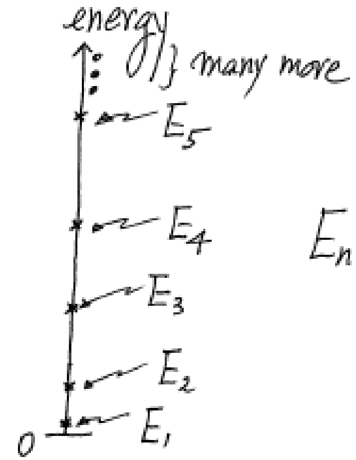
- Infinitely many $\psi_n(x)$ and E_n solved
- $\psi_1(x) \leftrightarrow E_1$, $\psi_2(x) \leftrightarrow E_2$, $\cdots$, $\psi_n(x) \leftrightarrow E_n$, $\cdots$ as stressed
- Each $\psi_n(x)$ is a state of definite energy (energy eigenfunction) with the energy E_n (energy eigenvalue)

These are exactly what we discussed under eigenvalue problems.

$^{+}$Note: Here I stress that $\psi(x)$ should be specified over all x, including outside the well/box.

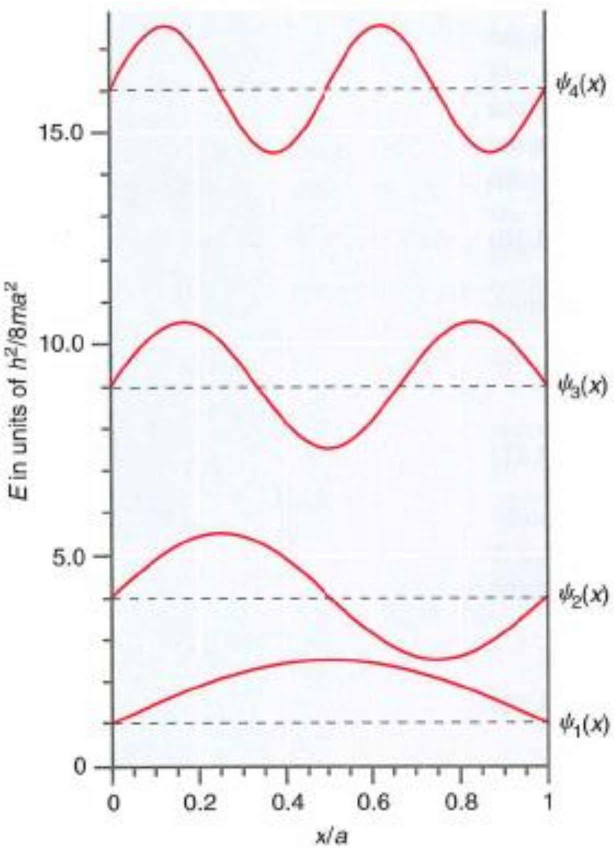
Displaying the TISE Solutions : Live with funny pictures

Stricty speaking: Allowed energies can be shown as dots (crosses) on an energy axis



$$E_n = n^2 \frac{\pi^2 \hbar^2}{2ma^2}$$

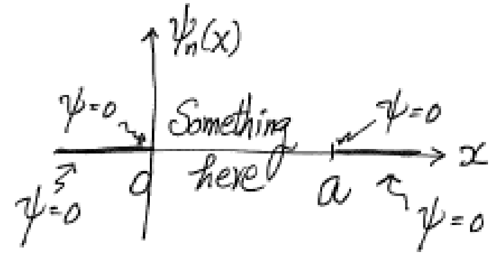
- Unfortunately, the energies are often displayed as horizontal lines together with the infinite well/box $U(x)$. Live with it!



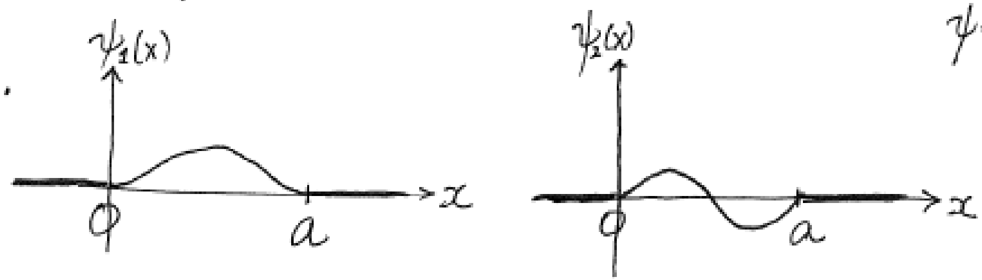
Energies are given in units of E_1

Allowed energies shown as dashed lines inside the well together with *U(x)*. But we need to be sure that the allowed energies (eigenvalues or eigenenergies) are energies. They do not depend on *x*. It is conventionally displayed like this. You must live with it on one hand and appreciate the information contained in the figure on the other.

Strictly speaking: Each $\psi_n(x)$ vs x plot is like



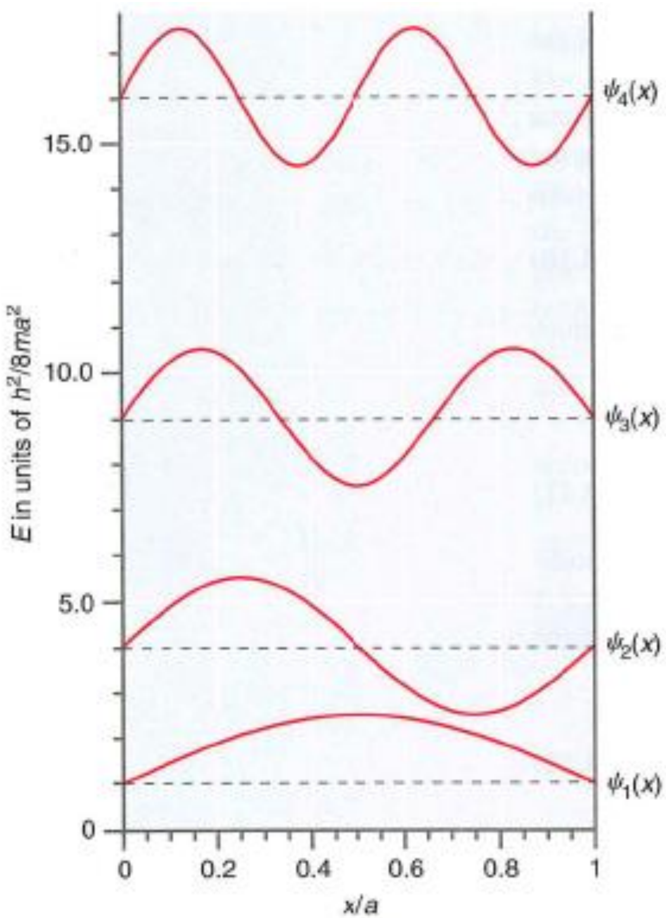
E.g.



etc.

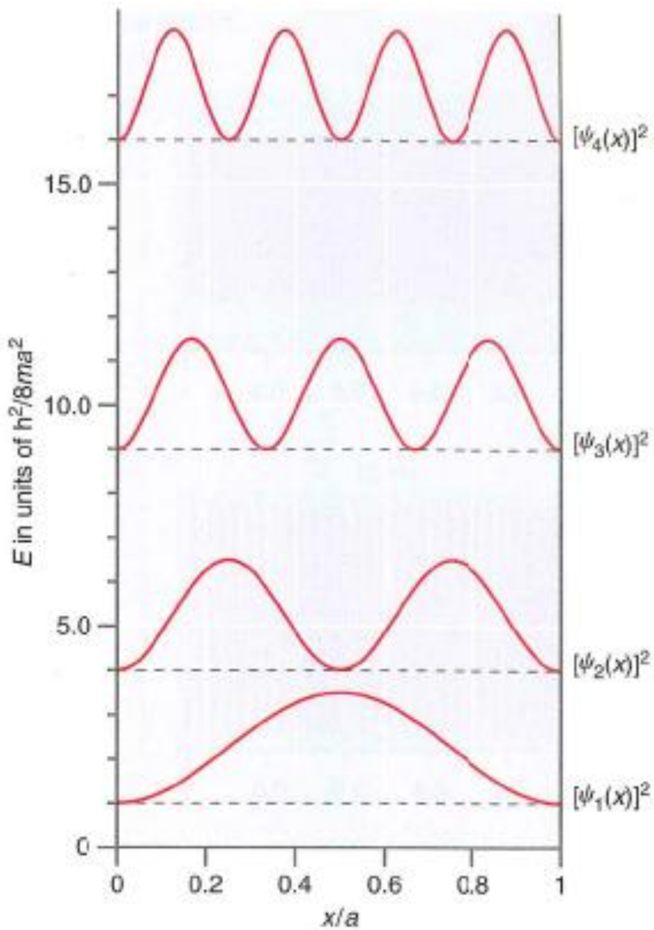
This is important because of the probability interpretation of wavefunction squared

- Unfortunately, $\psi_n(x)$ vs x are often drawn in funny way inside a picture of $U(x)$ and displaced by E_n. Live with it! But make sure you understand what the plots should look like formally.



Note that the wavefunctions are plotted in a funny way, with the x-axis (zero of the wavefunction) moved vertically up to where the allowed energy of the wavefunction locates! Live with it! But you need to be very sure where the zero of the wavefunctions really are! As the probability density is associated with the wavefunction squared, and thus where the zero is really matters!

Same "Live with it" comment on $|\psi_n(x)|^2$ vs x



Plot of probability densities for different energy eigenfunctions, but in a funny way as for the wavefunction. Live with it!
But make sure that you understand the meaning of the plots and how to make use of the information.

This ends the standard (baby level) treatment of the problem.

But there is much QM to learn from this simplest problem…

- How to “think like a physicist” in doing QM problems?
- Properties of energy eigenfunctions
- Using the set of energy eigenfunctions to answer initial value problems
- Is the set of “energy eigenfunctions” really special? Or the properties can be extended to other sets of eigenfunctions (of other QM operators)?
- How to calculate measureable quantities from wavefunctions?