The Square Well on the Web

Phasor Addition

http://www.jhu.edu/signals/phasorlecture2/indexphasorlect2.htm
http://www.jhu.edu/signals/phasorapplet2/phasorappletindex.htm
http://www.jhu.edu/signals/fourier2/index.html
http://www.jhu.edu/signals/listen-new/listen-newindex.htm
http://www.falstad.com/fourier/

The Square Well

http://www.falstad.com/qm1d
http://phet.colorado.edu/en/simulation/bound-states
http://webphysics.davidson.edu/faculty/dmb/singlesqwells/default.html

Bobby McFerrin

http://www.youtube.com/watch?v=ne6tB2KiZuk
http://www.youtube.com/watch?v=MVVUMNv1t9w
http://www.youtube.com/watch?v=d-diB65scQU
http://www.youtube.com/watch?v=mTB58ZmnudA
http://www.youtube.com/watch?v=GczSTQ2nv94
http://en.wikipedia.org/wiki/Pentatonic_scale

Time Independent Schrodinger Equation (TISE)

$$H|E_n >= E_n|E_n >$$

In position space

$$H_{op}\psi_n(x) = E_n\psi_n(x)$$

$$H_{op} = \frac{p_{op}^2}{2m} + V(x_{op})$$

$$p_{op} = -i\hbar\frac{d}{dx}$$

$$x_{op} = x$$

$$H_{op} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

For the square well

$$V(x) = 0$$

So TISE becomes this differential equation

$$H\psi_n = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) = E_n\psi_n(x)$$

Time Dependent Schrodinger Equation (TDSE)

$$H|\psi >= i\hbar \frac{d}{dt}|\psi >$$

Expand $|\psi >$ in the energy basis

$$|\psi(0) >= |\psi(0) >$$

$$|\psi(0) >= I_{op}\ |\psi(0) >$$

$$|\psi(0) >= \sum_{all\ n} |E_n >< E_n|\psi(0) >$$

$$|\psi(0) >= \sum_{all\ n} |E_n > a_n = \sum_{all\ n} a_n\ |E_n >$$

Write down $|\psi(t) >$ by inspection in energy basis

$$|\psi(t) >= \sum_{all\ n} a_n\ |E_n > exp(-iE_n t/\hbar)$$

$$\psi(x,t) = \sum_{all\ n} a_n\ \psi_n(x)\ exp(-iE_n t/\hbar)$$

This only works in the energy basis!!!

Chapter 5

Need a smoke. . .need a drink. . .no money. . .shirt reeks. . .shoes soaked. . .feet cold. . .two hours with this stupid shadow on my tail. . . Other than that, things are swell, just swell. Time to meet this clown. Yeah, the train station. . .past this marble corner. . .a moment. . .another moment. . . about right, turn. . . . The timing was perfect—face to face with the"shadowman." "Hey buddy, can I bum a smoke?" The shadow fumbled through his overcoat, then his jacket finally producing a pack of cigarettes. "Got a light?" He was quicker finding a lighter, but he was still so shaky that it took five tries to produce fire. Maybe send a signal to his boss. . .whoever that is. . . "Hey, buddy, let me tell you about Rutherford. They say he named the alpha particle. . ."

The Infinite Square Well

An atom in a molecule, an electron in an atom, and a nucleon in a nucleus are examples of particles confined to limited regions. Each demonstrates energy quantization while confined. Each limited region can be considered to be a "box" with "soft walls" formed by electrical or nuclear forces. The first step toward describing such realistic systems is to examine a one dimensional box with the simplest possible geometry and infinite or "hard walls". The potential energy function goes from zero in the region of confinement to infinity at each edge. This bit of unrealism makes the mathematics most tractable. The second step is to model "soft walls" by examining a one dimensional box where the potential energy function goes from zero in the region of confinement to a finite value at each edge. Both illustrate energy quantization. In fact, a particle subject to any type of confinement exhibits energy quantization.

Energy quantization is revealed in the form of allowed energy levels that are eigenenergies, or energy eigenvalues. These are the observable energies. Each eigenenergy has a corresponding eigenfunction, eigenstate, or eigenvector. A general wavefunction or state function may be an eigenfunction but will generally be a linear superposition of eigenfunctions.

As in the last two chapters, the postulates of quantum mechanics are not necessarily obvious in this development. The differential equation form of the time independent Schrodinger equation in position space dominates the discussion. Remember that it is simply a convenient form of the sixth postulate. Any eigenstate or any linear combination of eigenstates can comprise the state vector, as described by the first postulate. Measurements yield eigenvalues per the third postulate. We can attain probabilities for eigenstates or linear combinations of the eigenstates using the fourth postulate, and so on. The postulates are ever present.

As you work through this chapter, notice how the techniques of boundary value problems are used. Notice the mathematics used to attain eigenenergies and eigenfunctions. These things are useful and recurrent. Notice that position space is only one of many representations. Energy and momentum space representations are illustrative in this problem to further assimilate the idea that different representations may be more useful in other problems. Notice the impact of state vectors or wave functions that are linear combinations of eigenfunctions. Notice that results in two or three dimensions are generalizations of results in one dimension. The three dimensional problem may be pleasing because it is what we might first picture when we hear the phrase "particle in a box," which is the informal name of a square well.

---

1. Derive the eigenenergies of a particle in an infinite square well.

---

5. The Infinite Square Well

What we observe as material bodies and forces are nothing but shapes and variations in the structure of space. Particles are just *schaumkommen* (appearances). The world is given to me only once, not one existing and one perceived. Subject and object are only one. The barrier between them cannot be said to have broken down as a result of recent experience in the physical sciences, for this barrier does not exist.

- Erwin Schrodinger, on Quantum Theory

In science one tries to tell people, in such a way as to be understood by everyone, something that no one ever knew before. But in poetry, it's the exact opposite.

- P.A.M. Dirac

Particle in a Box

A model used to describe the behavior of particles of mass m, such as electrons in a metal, or plasma in a star, are constricted to a region. In this model, the energy eigenvalues of the bound particles are quantized.

For an infinite potential, or for a potential for which $V >> E$, the potential well will have **hard walls**, or two regions in which the wave function corresponding to quantized energy level within the well, will not be able to penetrate the classically forbidden region. For a finite potential, the potential well will have **soft walls**, or regions in which the quantized energy wave function is able to decay within the classically forbidden region.

Cosine and Sine Identities

- $\cos(a \pm b) = \cos a \cos b \mp \sin a \sin b$
- $\sin(a \pm b) = \cos a \sin b \pm \sin a \cos b$
- $\sin^2(a) = \frac{1}{2} - \frac{\cos 2a}{2}$
- $\cos^2(a) = \frac{1}{2} + \frac{\cos 2a}{2}$

LECTURE 9 7-14-08

THE WAVE FUNCTION AND ITS EQUATION

$\psi_n(x)$ no time

$\psi(x,t)$

SCHRODINGER EQUATION

$H\,\psi_n = E_n\,\psi_n$ TISE

$H\,\psi(x,t) = i\hbar \frac{d}{dt}\,\psi(x,t)$ TDSE

$\psi(x,t)$ is the probability amplitude to find the particle at x and t

$dP(x,t) = |\psi(x,t)|^2\,dx$

$= \psi^*(x,t)\,\psi(x,t)\,dx$

WAVE FCN

WAVE FCN SQUARED

$dP = |\psi|^2\,dx$ $\int dP = \int \psi^*(x)\,\psi(x)\,dx = 1$

$\psi(x,t)$ IS THE AMP EVERYWHERE IN SPACE

CONTAINS ALL THE INFORMATION ABOUT THE PARTICLE

CALCULATE $\psi(x,t)$ BY SOLVING THE SCHRODINGER EQN

IN THIS UNIT, STUDY SOLUTIONS TO TDSE AND TISE

SQUARE WELL

T and R

ATOMS

SCHRODINGER EQN

$$H \psi_n(x) = E_n \psi_n(x)$$

HAMILTONIAN

$$H = TE = KE + PE$$

$$H = \frac{p^2}{2m} + V(x) \qquad \text{CLASSICAL EQN}$$

TO CONVERT TO QM H

$$p = -i\hbar \frac{d}{dx}$$

$$x = x$$

$$H = \frac{p^2}{2m} + V(x) = \frac{p^2}{2m} + \frac{1}{2} K x^2$$

$$= \frac{\left(-i\hbar \frac{d}{dx}\right)\left(-i\hbar \frac{d}{dx}\right)}{2m} + \frac{1}{2} K (x^2)$$

$$= \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} K x^2$$

SHO

$$\left(\underbrace{\frac{-\hbar^2}{2m} \frac{d^2}{dx^2}}_{\text{OPERATOR}} + \frac{1}{2} K x^2 \right) \underbrace{\psi_n(x)}_{\text{EIGEN FCNS}} = \underbrace{E_n}_{\text{EIGENVALUES}} \psi_n(x)$$

LIKE LINEAR ALGEBRA

(MATRIX) (VECTOR) = (~~AN OTHER~~ DIFFERENT VECTOR)

(MATRIX) (EIGENVECTOR) = (NUMBER) (EIGEN VECTOR)

$$\begin{pmatrix} 3 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 5 \end{pmatrix} \underbrace{\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}}_{e\vec{v}} = \underbrace{3}_{ev} \underbrace{\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}}_{e\vec{v}}$$

$$\begin{pmatrix} 3 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 5 \end{pmatrix} \underbrace{\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}}_{e\vec{v}} = \underbrace{4}_{ev} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} 3 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 5 \end{pmatrix} \underbrace{\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}}_{e\vec{v}} = \underbrace{5}_{ev} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

3 x 3 MATRIX HAS 3 $e\vec{v}$'s

3 ev's

OBVIOUS WHEN MATRIX IS DIAGONAL

ALWAYS TRUE

HOW MANY ef's DOES $\frac{d^2}{dx^2}$ HAVE?

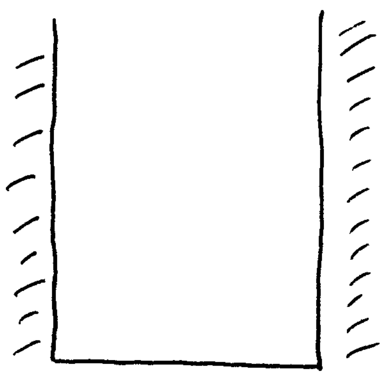
" " ev's " " " ?

WE NEED TO FIND ef's OF H

en's OF H

SQUARE WELL

aka, PARTICLE IN A BOX



INSIDE

$V(x) = 0$

AT BOUNDARY AND OUTSIDE $V(x) = \infty$

$\Rightarrow$ PARTICLE CANNOT GET OUTSIDE

even if only walls $= \infty$, particle cannot escape

TISE $\quad H\psi = E\psi$

$$\cancel{H\psi}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \cancel{V(x)}^{\,0}\right]\psi_n(x) = E_n\,\psi_n(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) = E_n\,\psi_n(x)$$

FIND THESE FCN S ef's

AND THESE NUMBERS en's

PUT $-\frac{\hbar^2}{2m}$ ON RHS

$$\frac{d^2}{dx^2}\psi_n(x) = -\frac{2mE_n}{\hbar^2}\psi_n(x)$$

$$= -c_n\psi_n(x)$$

WHAT FCNS HAVE SECOND DERIVATIVE = MINUS FCN ?

$$\frac{d^2}{dx^2}\sin(kx) = \frac{d}{dx}\left(\frac{d}{dx}\sin(kx)\right)$$

$$= \frac{d}{dx}\left(k\cos(kx)\right)$$

$$= -k^2\sin(kx)$$

$\sin(kx)$ is an ef WITH ev $= k^2$

$$\frac{d^2}{dx^2}\cos(kx) = \frac{d}{dx}\left(\frac{d}{dx}\cos(kx)\right)$$

$$= \frac{d}{dx}\left(-k\sin(kx)\right)$$

$$= \underbrace{-k^2}_{\text{ev}}\,\underbrace{\cos(kx)}_{\text{ef}}$$

$$\frac{d^2}{dx^2}\left(e^{ikx}\right) = \frac{d}{dx}\left(\cancel{e}\,\frac{d}{dx}\,e^{ikx}\right)$$

$$= \frac{d}{dx}\left(ik\,e^{ikx}\right)$$

$$= (ik)(ik)\,e^{ikx}$$

$$= -\underset{ev}{\underset{\uparrow}{k^2}}\;\underset{ef}{\underset{\nwarrow}{e^{ikx}}}$$

$$\frac{d^2}{dx^2}\left(e^{-ikx}\right) = \frac{d}{dx}\left(\frac{d}{dx}\,e^{-ikx}\right)$$

$$= \frac{d}{dx}\left(-ik\,e^{-ikx}\right)$$

$$= (-ik)(-ik)\,e^{-ikx}$$

$$= -\underset{ev}{\underset{\uparrow}{k^2}}\;\underset{ef}{\underset{\nwarrow}{e^{-ikx}}}$$

SINCE $\quad e^{i\theta} = \cos\theta + i\sin\theta$

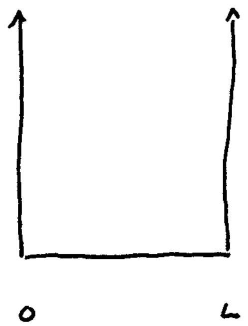
TWO SOLUTIONS: $\quad \cos(kx) \quad \sin(kx)$

$$e^{ikx} \qquad e^{-ikx}$$

NOW WE HAVE GENERAL SOLN

$$\psi(x) = A \sin(kx) + B \cos(kx) \qquad \text{inside the box}$$

APPLY BC's



$$\psi(0) = 0 \qquad A \sin(k \cdot 0) + B \cos(k \cdot 0) = 0$$

$$\Rightarrow B = 0$$

$$\psi(L) = 0 \qquad A \sin(kL) = 0$$

$$n(2\pi)$$

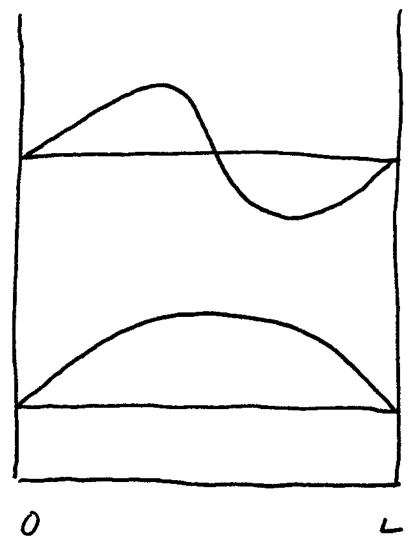
$$k = \frac{\pi}{L}$$

$$A \sin\left(n\left(\frac{\pi}{L}\right) L\right) = 0$$

SOLN'S INSIDE WELL

$$\psi_n(x) = A \sin(k_n x) \qquad \text{where } k_n = \left(\frac{\pi}{L}\right) n$$

DRAW SOLUTIONS $\psi_n(x)$

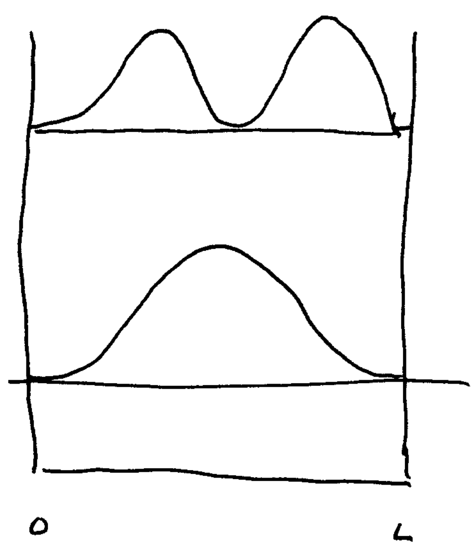


$n=2$ $\sin\left(\frac{2\pi x}{L}\right)$

$n=1$ $\sin\left(\frac{\pi x}{L}\right)$

ef's are called the stationary states

DRAW PROBABILITES



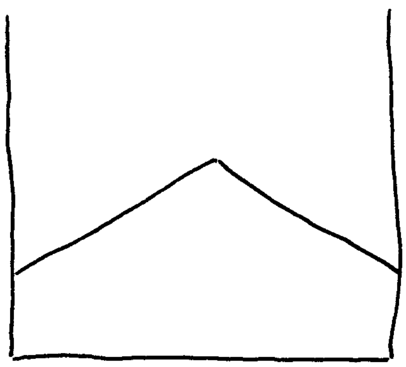
$n=2$ $\sin^2\left(\frac{2\pi x}{L}\right)$

$n=1$ $\sin^2\left(\frac{\pi x}{L}\right)$

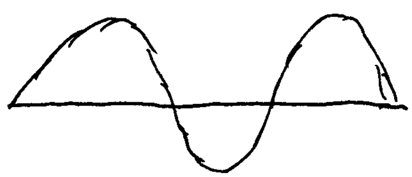
ANY ~~ø~~ WAVEFCN INSIDE WELL CAN BE EXPRESSED AS SUM OVER ef's

$$(\text{ANY WAVE FCN}) = \sum_{m=1}^{\infty} A_m \sin\left(\frac{m\pi x}{L}\right)$$

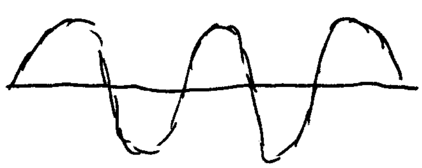
CALLED FOURIER SERIES EXPANSION



$m = 1$



$m = 3$



$m = 5$

ONLY ODD m's BECAUSE OF SYMMETRY

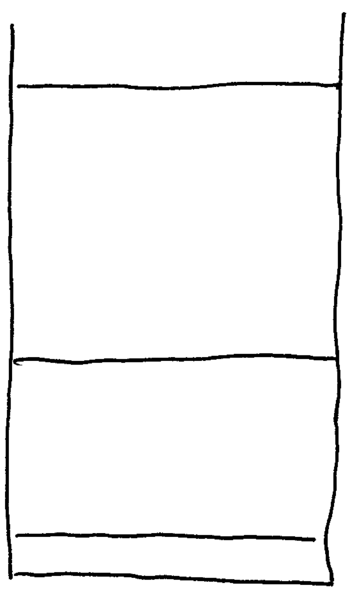
EIGENVALUES $\Rightarrow$ EIGEN ENERGIES

$$\frac{2m E_n}{\hbar^2} = k_n^2$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{p_n^2}{2m} \qquad p = \hbar k$$

$$k_n = \frac{n\pi}{L}$$

$$E_n = \left(\frac{\hbar^2 \pi^2}{2 m L}\right) n^2$$



$n = 3$ $\quad 9 E_1$

$n = 2$ $\quad 4 E_1$

$n = 1$ $\quad E_1$

n $\quad n^2 E_1$

LECTURE 10 7-16-08

LAST TIME

ENERGY EIGENSTATES $\psi_n(x)$
STATIONARY STATES
"STATES OF DEFINITE ENERGY" if you measure

TIME-INDEPENDENT SCHRODINGER EQUATION

TISE

$$H\,\psi_n(x) = E_n\,\psi_n(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) = E_n\,\psi_n(x)$$

GENERAL SOLUTIONS $\sin(kx)$ $\cos(kx)$ e^{ikx} e^{-ikx}

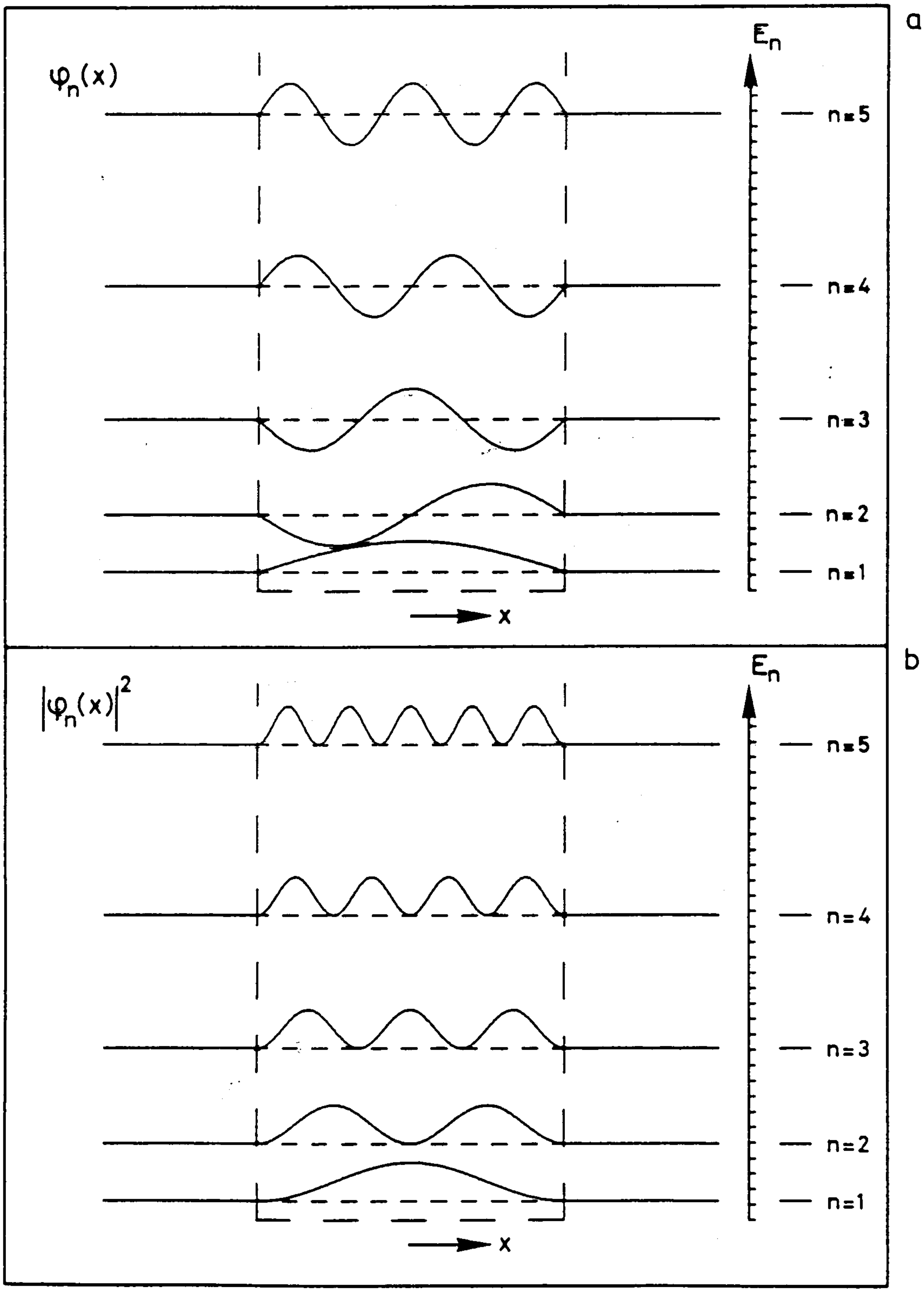
PARTICULAR SOLUTION

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right) = \sqrt{\frac{2}{L}}\sin(k_n x)$$

NORMALIZATION

$$k_n = \frac{n\pi}{L} \qquad E_n = \frac{p_n^2}{2m} = \frac{(\hbar k)^2}{2m} = \frac{\hbar^2}{2m}k_n^2$$

$$= \left(\frac{\pi^2\hbar^2}{2mL^2}\right)n^2 = (E_1)n^2$$



tes in an well. The ate ne). It vanishes / 2 and is ints cated as right side wn, and to rgies E_n of l states are tal lines. ated as left. They (a) the wave probability d states.

The energies of these bound states are

$$E_n = \frac{1}{2m}\left(\frac{\hbar n\pi}{d}\right)^2, \qquad n = 1, 2, 3, \ldots$$

as we easily verify by inserting φ_n into the time-independent Schrödinger equation,

$$\hbar^2 \quad d^2$$

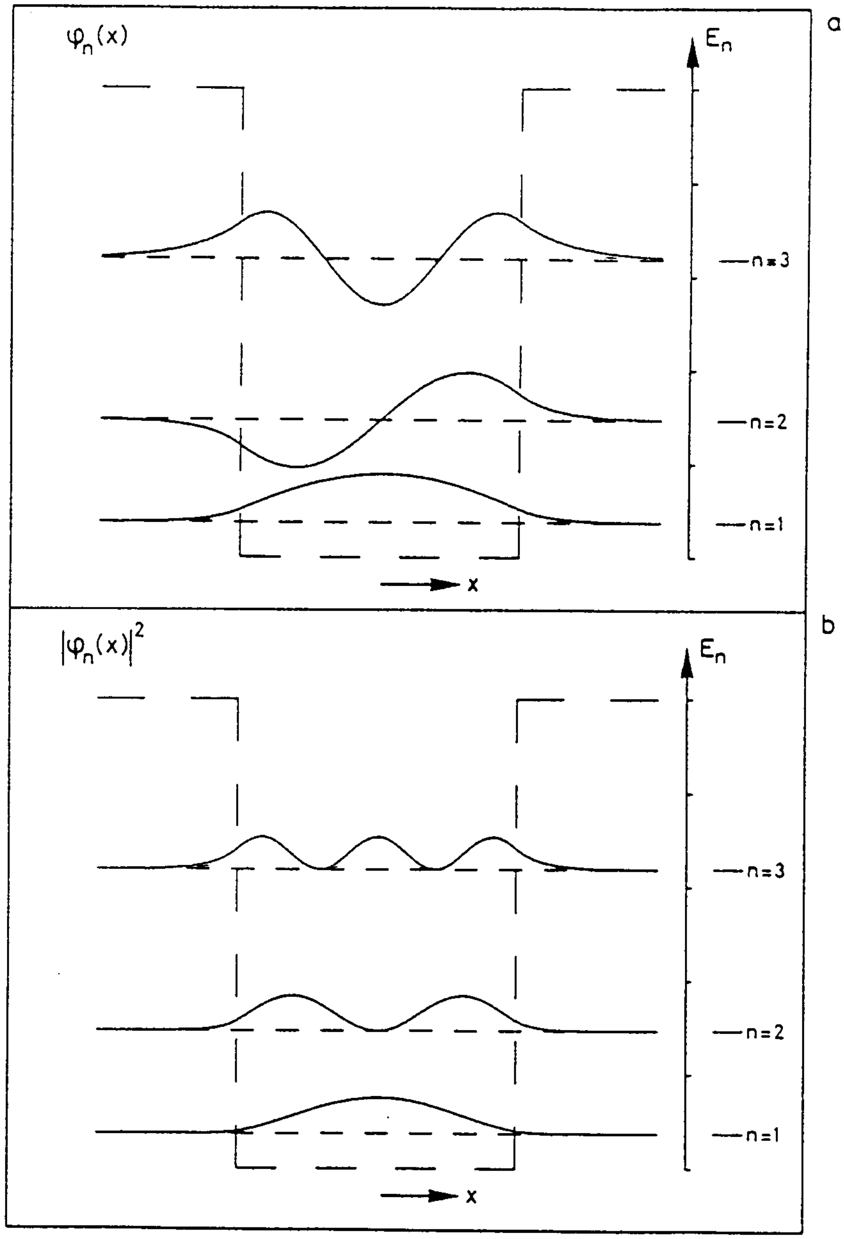


Figure 4.7 **(a) Wave functions and (b) probability densities of the bound states in a square-well potential. On the right side of the picture an energy scale is shown with marks for the bound-state energies ($n = 1, 2, 3$). The form of the potential $V(x)$ is indicated by the long-dash line, the energy E_n of the bound states by the horizontal short-dash lines. The horizontal dashed lines also serve as zero lines for the functions shown.**

Problems

4.1 Solve the stationary Schrödinger equation for energy E with a constant potential $V = V_0$.

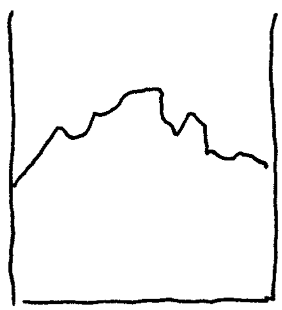
4.2 Discuss the behavior of the solutions for energies $E > V_0$, $E < V_0$. Which solutions correspond to the particular energy $E = V_0$? These three cases play a role in the

TODAY: TDSE

$$H\,\psi(x,t) = i\hbar \frac{d}{dt}\,\psi(x,t)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\,\psi(x,t) = i\hbar\frac{d}{dt}\,\psi(x,t)$$

LAST TIME: BUILD ANY WAVEFCN USING STATIONARY STATES



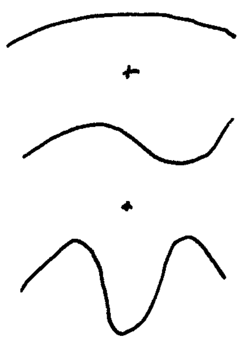
a_1 $\psi_1(x)$

+

a_2 $\psi_2(x)$

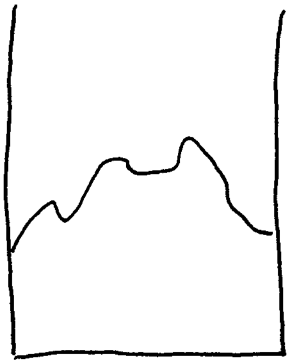
+

a_3 $\psi_3(x)$



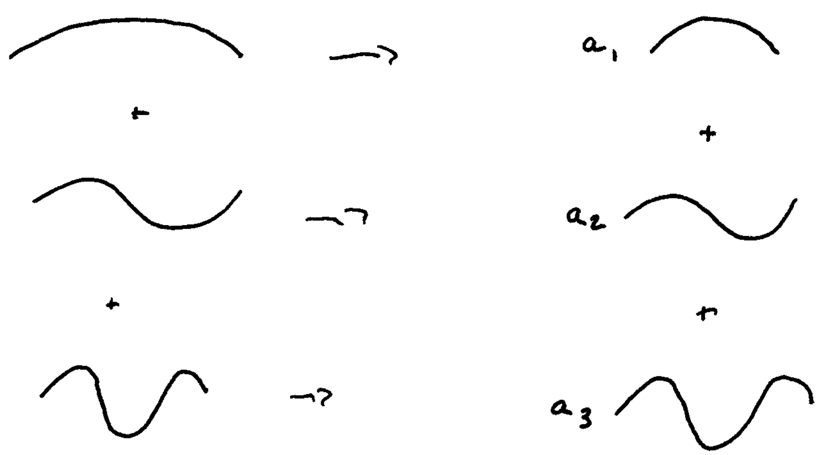
$\vdots$

$\Rightarrow$ ALL WE NEED IS THE TD OF ψ_n'S



AT $t=0$

TIME 0 | TIME t



$a_1 \rightarrow a_1 e^{-i\omega_1 t}$

$+$

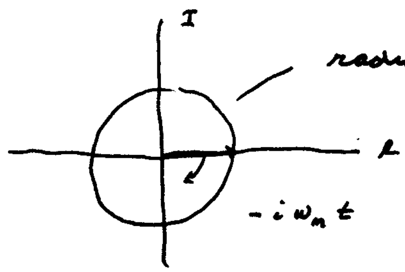
$a_2 \rightarrow a_2 e^{-i\omega_2 t}$

$+$

$a_3 \rightarrow a_3 e^{-i\omega_3 t}$

$+ \; \vdots$

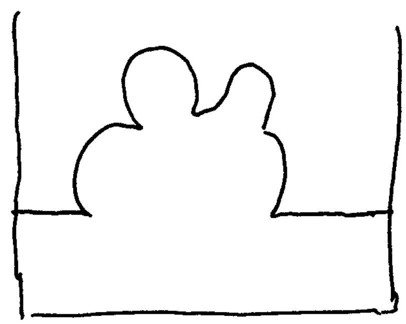
AT ANY X $\quad A_m e^{-i\omega_m t}$



radius circle $= A_m$

CAN EXPAND ANY FCN IN FOURIER SERIES

(inside well)



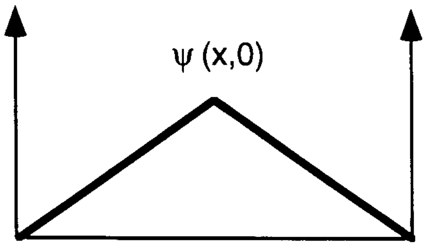
NO MICKEY MOUSE WAVE FCNS !

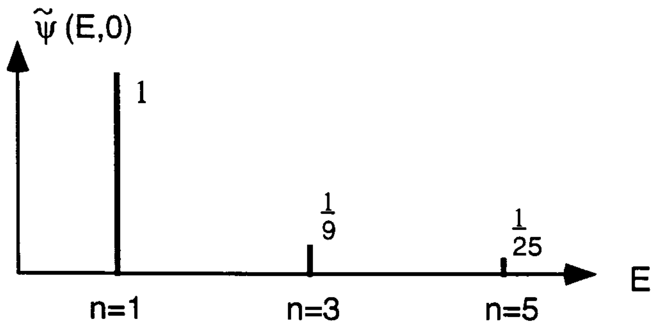
min curvature

momentum space

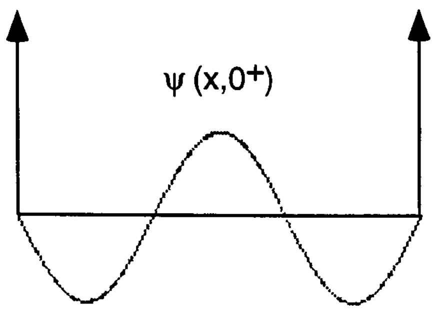
go to simulation

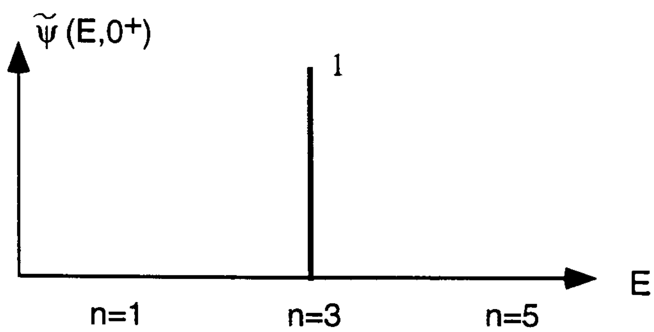
Immediately before the measurement, the two wavefunctions look like this





And immediately after the measurement, the two wavefunctions look like this





Remember, however that these two wavefunctions are just different representations of exactly the same state vectors—they are just $|\psi(0^-)>$ and $|\psi(0^+)>$ in two different bases!