9.1: Expectation Values of Hermetian Operators

$\hat{Q}$ is Hermetian if:

$$\int \Psi_1^* \hat{Q} \Psi_2 \, dx = \int (\hat{Q}\Psi_1)^* \Psi_2 \, dx$$

$$(\Psi_1, \Psi_2) \equiv \int \Psi_1^*(x) \Psi_2(x) \, dx$$

$$(a\Psi_1, \Psi_2) = a^*(\Psi_1, \Psi_2)$$

$$(\Psi_1, a\Psi_2) = a(\Psi_1, \Psi_2)$$

$\hat{Q}$ Hermitian

$$(\Psi_1, \hat{Q}\Psi_2) = (\hat{Q}\Psi_1, \Psi_2)$$

Expectation value $\hat{Q}$ in state $\Psi(x)$ <

$$\langle Q \rangle_\Psi = \int \Psi^* \hat{Q} \Psi \, dx = (\Psi, \hat{Q}\Psi)$$

$$\langle \hat{Q} \rangle_\Psi \in \mathbb{R}$$

$$(\langle \hat{Q} \rangle_\Psi)^* = \int (\Psi^* \hat{Q} \Psi)^* \, dx$$

$$= \int \Psi (Q\Psi)^* \, dx$$

$$= \int (\hat{Q}\Psi)^* \Psi \, dx$$

$$= \int \Psi^* Q \Psi = \langle \hat{Q} \rangle_\Psi$$

$$\Rightarrow \langle \hat{Q} \rangle \in \mathbb{R}$$

9.1: Expectation Values of Hermitian Operators (continued)

The eigenvalues of $\hat{Q}$ are Real

$$\hat{Q}\Psi_1 = q_1\Psi_1$$

q_1 is the eigenvalue
Ψ_1 is the eigenvector/eigenfunction

$$\langle\hat{Q}\rangle_{\Psi_1} = \int \Psi_1^* \hat{Q}\Psi_1 dx$$

$$= \int \Psi_1^* q_1 \Psi_1 dx = q_1 \int \Psi_1^* \Psi_1 \in \mathbb{R}$$

$$\rightarrow q_1 \in \mathbb{R}$$

for normalized Ψ_1
$\langle Q \rangle_{\Psi_1} = Q_1$

9.2: Eigenfunctions of a Hermitian Operator

The set of eigenfunctions for Hermitian Operators span the space of states

Consider the collection of eigenfunctions and eigenvalues of the Hermitian operator $\hat{Q}$

$$\hat{Q}\Psi_1 = q_1\Psi_1$$
$$\hat{Q}\Psi_2 = q_2\Psi_2$$
$$\vdots \qquad \vdots$$

The eigenfunctions can be organized to satisfy:

$$\int \Psi_i(x)\Psi_j(x)dx = \delta_{ij} = \text{Orthonormality}$$

9.2: Eigenfunctions of Hermitian Operators (continued)

If q_i is different from q_j

$$\int \Psi_i^* Q \Psi_j \, dx = \int \Psi_i^* q_j \Psi_j \, dx$$

$$= q_j \int \Psi_i^* \Psi_j \, dx$$

$$= \int (Q\Psi_i)^* \Psi_j \, dx$$

$$= \int (q_i \Psi_i)^* \Psi_j \, dx$$

$$= q_i \int \Psi_i^* \Psi_j \, dx$$

$$\rightarrow (q_i - q_j) \int \Psi_i^* \Psi_j = 0$$

since q_i is different from q_j:

$$\int \Psi_i^* \Psi_j \, dx = 0$$

Degeneracies must be acounted for!

9.3: Completeness of Eigenvectors

The eigenfunctions of $\hat{Q}$ form a set of basis functions. Any reasonable Ψ can be written as a superposition of $\hat{Q}$ eigenfunctions

$$\Psi(x) = \alpha_1 \Psi_1(x) + \alpha_2 \Psi_2(x) + \ldots = \sum_i \alpha_i \Psi_i(x)$$

$$(\Psi_i, \Psi) = \int \Psi_i^* \sum_j \alpha_j \Psi_j \, dx$$

$$= \sum_j \alpha_j \int \Psi_i^* \Psi_j \, dx$$

$$= \sum_j \alpha_j \delta_{ij} = \alpha_i$$

$$\alpha_i = (\Psi_i, \Psi)$$

$$\int |\Psi|^2 dx = 1$$

$$\int \left(\sum_i \alpha_i \Psi_i\right)^* \sum_j \alpha_j \Psi_j \, dx$$

$$= \sum_i \sum_j \alpha_i^* \alpha_j \underbrace{\int \Psi_i^* \Psi_j \, dx}_{\delta_{ij}}$$

$$= \sum_i \alpha_i^* \alpha_i = \sum_i |\alpha_i|^2$$

$$\sum_i |\alpha_i|^2 = 1$$

4.3: Completeness of Eigenvectors (continued)

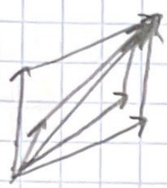
Measurement Postulate:

If we measure $\hat{Q}$ in the state Ψ, the possible values obtained are $q_1, q_2 \dots$

The probability p_i to measure q_i:

$$p_i = |\alpha_i|^2 = |(\Psi_i, \Psi)|^2$$

The outcome q_i the state of the system becomes $\Psi(x) = \Psi_i(x)$ which is the collapse of the wavefunction.



9.4: Consistency Condition

Suppose $\Psi = \sum \alpha_i \Psi_i$

Find $\langle \hat{Q} \rangle_\Psi$

$$\langle \hat{Q} \rangle = \int \Psi^* Q \Psi \, dx$$

$$= \int \left(\sum_i \alpha_i \Psi_i\right)^* Q \sum_j \alpha_j \Psi_j \, dx$$

$$= \sum_i \sum_j \alpha_i^* \alpha_j \underbrace{\int \Psi_i^* \underbrace{Q \Psi_j}_{q_j \Psi_j} \, dx}_{q_j \int \Psi_i^* \Psi_j \, dx = q_j \delta_{ij}}$$

$$= \sum_i \sum_j \alpha_i^* \alpha_j q_j \delta_{ij} = \sum_i |\alpha_i|^2 q_i$$

$$\langle \hat{Q} \rangle = \sum_i |\alpha_i|^2 q_i$$

Particle is on circle $x \in [0, L]$

$$\Psi = \sqrt{\frac{2}{L}} \left(\frac{1}{\sqrt{3}} \sin \frac{2\pi x}{L} + \sqrt{\frac{2}{3}} \cos \frac{6\pi x}{L} \right)$$

$\Psi(L) = \Psi(0)$

What are the possible values and their probabilities if momentum is measured?

$e^{\frac{2\pi i n x}{L}}$, $m \in \mathbb{Z}$ $(-\infty, \infty)$

$\Psi(x+L) = \Psi(x)$

9.4: Consistency Condition (continued)

$$\psi_m(x) \equiv \frac{1}{\sqrt{L}} e^{\frac{2\pi i m y}{L}}$$

$$\frac{\hbar}{i}\frac{\partial}{\partial x}\psi_m = \frac{\hbar 2\pi m}{L}\psi_m$$

$$P = \frac{\hbar 2\pi m}{L}$$

$$\sin x = \frac{e^{ix} - e^{-ix}}{2i}$$

$$\cos x = \frac{e^{ix} + e^{-ix}}{2i}$$

After:

$$\psi = \sqrt{\frac{2}{3}}\,\frac{1}{2i}\psi_1 - \sqrt{\frac{2}{3}}\,\frac{1}{2}\psi_{-1} + \frac{1}{\sqrt{3}}\psi_3 + \frac{1}{\sqrt{3}}\psi_{-3}$$

P values	Probabilities
$\frac{2\pi\hbar}{L}$	$\left\lvert\sqrt{\frac{2}{3}}\frac{1}{2i}\right\rvert^2 = \frac{2}{3}\frac{1}{4} = \frac{1}{6}$
$-\frac{2\pi\hbar}{L}$	$\frac{1}{6}$
$\frac{6\pi\hbar}{L}$	$\frac{1}{3}$
$-\frac{6\pi\hbar}{L}$	$\frac{1}{3}$

9.5: Defining Uncertainty

$Q_1 \dots Q_n$
$P_1 \dots P_n$

ΔQ = standard deviation

$$\bar{Q} = \sum_i P_i Q_i$$

$$(\Delta Q)^2 \equiv \sum_i P_i (Q_i - \bar{Q})^2 \geq 0$$

If $\Delta Q = 0$
$Q_i = \bar{Q} \Rightarrow$ not random anymore

$$(\Delta Q)^2 = \sum_i P_i Q_i^2 - 2\sum_i P_i Q_i \bar{Q} + \sum_i P_i \bar{Q}^2$$

$$= \overline{Q_i^2} - 2\bar{Q}\bar{Q} + (\bar{Q})^2$$

$$(\Delta Q)^2 = \overline{Q_i^2} - (\bar{Q})^2 \geq 0$$

Mean of square minus square of the mean

$$\overline{Q^2} \geq (\bar{Q})^2$$

Hermitian operator $\hat{Q}$

$$(\Delta \hat{Q})^2_\Psi = \langle \hat{Q}^2 \rangle_\Psi - \langle Q \rangle^2_\Psi$$

$$(\Delta Q)^2_\Psi = \langle (\hat{Q} - \langle Q \rangle)^2 \rangle$$

$$(\Delta Q)^2_\Psi = \int_{-\infty}^{\infty} |(Q - \langle Q \rangle)\Psi|^2 dx$$

10.1: Uncertainty and Eigenstates

$(\Delta\hat{Q})^2_\Psi = \langle\hat{Q}^2\rangle_\Psi - \langle\hat{Q}\rangle^2_\Psi$

1) $(\Delta\hat{Q})^2 = \langle(\hat{Q}-\langle Q\rangle)^2\rangle$ •

2) $(\Delta\hat{Q})^2 = \int |(\hat{Q}-\langle Q\rangle)\Psi(x,t)|^2 dx$ ••

• $(\Delta\hat{Q})^2 \overset{\text{pf}}{=} \langle\hat{Q}^2 - 2\hat{Q}\langle\hat{Q}\rangle + \langle\hat{Q}\rangle^2\rangle$

$= \langle\hat{Q}^2\rangle - 2\langle\hat{Q}\rangle\langle\hat{Q}\rangle + \langle\hat{Q}\rangle^2$

$= \langle Q^2\rangle - \langle Q\rangle^2$

•• Start with $\langle(\hat{Q}-\langle Q\rangle)^2\rangle = \int \Psi^*(x,t)(\hat{Q}-\langle\hat{Q}\rangle)(\hat{Q}-\langle\hat{Q}\rangle)\Psi(x,t)dx$

$= \int ((\hat{Q}-\langle\hat{Q}\rangle)\Psi(x,t))^*((\hat{Q}-\langle\hat{Q}\rangle)\Psi(x,t))dx$

$= \int |(\hat{Q}-\langle\hat{Q}\rangle)\Psi(x,t)|^2 dx$

If Ψ is an eigenstate of $\hat{Q}$:

$\hat{Q}\Psi = \lambda\Psi$

$\int \Psi^* Q \Psi dx = \lambda \int \Psi^*\Psi dx = \lambda \equiv \langle\hat{Q}\rangle$

$\hat{Q}\Psi = \langle\hat{Q}\rangle_\Psi \Psi$

$(\hat{Q}-\langle Q\rangle)\Psi = 0$

$\Delta Q = 0$

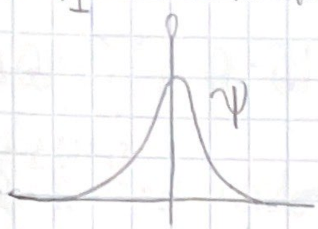
10.1: Uncertainty and Eigenstates (Continued)

If $\Delta Q = 0$

$\hookrightarrow \int |(\hat{Q} - \langle \hat{Q} \rangle)\Psi(x,t)|^2 dx = 0$

$(\hat{Q} - \langle \hat{Q} \rangle)\Psi = 0$

$(\Delta Q)_{\Psi} = 0 \iff \Psi$ is an eigenstate of $\hat{Q}$



$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$

Gaussian surface

$\downarrow$

Gaussian Integral

$\Delta x \Delta p \geq \frac{\hbar}{2}$

10.2: Stationary States

Simple and useful of the Schrödinger Equation

A stationary state has a factorized space and time dependency

$\Psi(x,t) = g(t)\psi(x)$

Time independent observables have no time dependencies

$\frac{d}{dt}\langle x\rangle = \frac{\langle p\rangle}{m}$

$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\Psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\Psi(x,t)$

$i\hbar\psi(x)\frac{d}{dt}g(t) = g(t)\underbrace{\hat{H}\psi(x)}_{f(x)}$

Divide by Ψ

$i\hbar\frac{1}{g}\frac{dg}{dt} = \frac{1}{\psi(x)}\hat{H}\psi(x)$

$= \text{constant} = E$ [energy]

$i\hbar\frac{dg}{dt} = Eg$

$g(t) = Ce^{-i\frac{Et}{\hbar}}$

10.2: Stationary States (continued)

$g(t) = Ce^{-\frac{iEt}{\hbar}}$

$\hat{H}\psi(x) = E\psi(x)$

$$\underbrace{\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi(x)}_{\text{Time Independent Schrodinger Equation}}$$

$\Psi(x,t) = c\psi(x)e^{-\frac{iEt}{\hbar}}$

$\int \Psi^*(x,t)\Psi(x,t)\,dx = 1$

$\int \psi^*(x)e^{\frac{iEt}{\hbar}}\psi(x)e^{-\frac{iEt}{\hbar}}\,dx = 1$

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

10.3: Expectation Values on Stationary States

$$\langle \hat{H} \rangle_{\Psi(x,t)} = \int \Psi^*(x,t)\, \hat{H}\, \Psi(x,t)\, dx$$

$$= \int \psi^*(x) e^{\frac{iEt}{\hbar}} \hat{H} e^{-\frac{iEt}{\hbar}} \psi(x)\, dx$$

$$= \int \psi^*(x)\, \hat{H}\, \psi(x)\, dx$$

$$= \langle \hat{H} \rangle_{\psi(x)}$$

$$= E \int \psi^* \psi\, dx = E$$

Expected value of any time independent operator $\hat{Q}$ in a stationary state is time independent.

$$\langle \hat{Q} \rangle_{\Psi(x,t)} = \int \Psi^*(x,t)\, \hat{Q}\, \Psi(x,t)$$

$$= \int \psi^*(x) e^{\frac{iEt}{\hbar}} \hat{Q} \left(\psi(x) e^{-\frac{iEt}{\hbar}} \right) dx$$

$$= \int \psi^* \hat{Q} \psi\, dx = \langle \hat{Q} \rangle_{\psi(x)}$$

The superposition of two stationary states of different energy is not stationary.

10.4: Comments on Spectrum and Continuity Conditions

$\hat{H}\Psi(x) = E\Psi(x)$

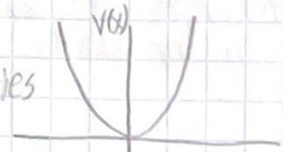
$\hat{H}$ is hermitian

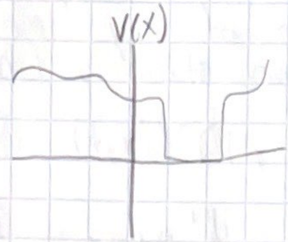
$\hat{H}$: the eigenfunctions form an orthonormal set that spans!

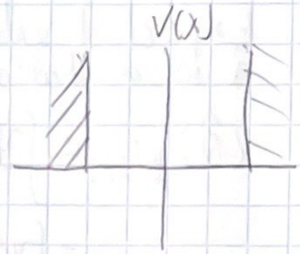
$$\left.\begin{matrix} \Psi_1(x) & E_1 \\ \Psi_2(x) & E_2 \\ \vdots & \vdots \end{matrix}\right\} \text{spectrum of the theorem}$$

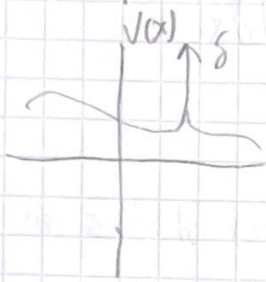
$$\frac{d^2\Psi}{dx^2} = \frac{2m}{\hbar^2}\left(V(x) - E\right)\Psi(x)$$

V(x) have many properties

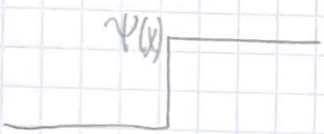








$\Psi(x)$ has to be continuous



$\Psi'(x) \sim \delta(x) \quad \Psi''(x) \sim \delta'(x)$

10.4: Comments on Spectrum and Continuity Conditions (continued)

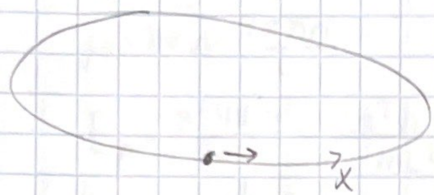
$\Psi'(x)$ is continuous unless $V(x)$ has a δ function

If Ψ' is discontinuous,

then $\Psi''(x) \sim \delta$ function

$\hookrightarrow V$ will have a δ function

10.5: Particle on a Circle



$x \sim x + L$

$\Psi(x+L) = \Psi(x)$

$V(x) \equiv 0 \Rightarrow \hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$

$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = E\Psi$

10.5: Particle on a Circle (continued)

$$\int_0^L \psi^* \, dx = -\frac{\hbar^2}{2m}\int \psi^*(x)\frac{d}{dx}\frac{d}{dx}\psi(x)$$

$$= E\underbrace{\int \psi^*\psi(x)\,dx}_{1}$$

$$= E$$

$$-\frac{\hbar^2}{2m}\int \frac{d}{dx}\left(\psi^*\frac{d\psi}{dx}\right) - \frac{d\psi^*}{dx}\frac{d\psi}{dx}\,dx = E$$

$$-\frac{\hbar}{2m}\psi^*\frac{d\psi}{dx}\Big|_0^L + \frac{\hbar^2}{2m}\int_0^L \left|\frac{d\psi}{dx}\right|^2 dx = E > 0$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi, \; k \in \mathbb{R}$$

$$E = \frac{\hbar^2 k^2}{2m} \quad p = \hbar k$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi \qquad \begin{cases} \sin(kx) \\ \cos(kx) \\ e^{ikx} \end{cases}$$

$$\psi = e^{ikx}$$

11.1: Energy Eigenstates For Particle on a Circle

$\psi(x+L)=\psi(x)$

$\psi''(x)=-\frac{2mE}{\hbar^2}=-k^2\psi$, proved $E>0$

$\psi(x)\sim e^{ikx}$

$e^{ik(x+L)}=e^{ikx}$

$e^{ikL}=1$

$kL=2\pi n,\ n\in\mathbb{Z}$

$k_n=\frac{2\pi n}{L}$

$p_n=\hbar k_n=\frac{2\pi\hbar n}{L}$

$E_n=\frac{\hbar^2 4\pi^2 n^2}{2mL^2}=\frac{2\pi^2\hbar^2 n^2}{mL^2}$

$\psi_n(x)\sim e^{ik_nx}$

$\int_0^L|\psi_n|^2dx=1$

$\int_0^L N^2dx=1\rightarrow LN^2=1$

$\rightarrow N=\frac{1}{\sqrt{L}}$

$\psi_n(x)=\frac{1}{\sqrt{L}}e^{ik_nx}$

$=\frac{1}{\sqrt{L}}e^{\frac{2\pi inx}{L}}$

$\Psi_n(x,t)=\psi_n(x)e^{\frac{-iE_nt}{\hbar}}$

11.1: Energy Eigenstates for Particle on a Circle (continued)

$\psi_n(x,t)$, $n \in (-\infty, \infty)$

$\psi_0(x) = \frac{1}{\sqrt{L}}$

ψ_{-1}, ψ_1 are degenerate states with energy $E_1 = E_{-1}$

ψ_2, ψ_{-2} are degeneracies as well

$\left.\psi_k, \psi_{-k}\right\}$ Degeneracies

$\hat{p}\psi_n(x) = p_n \psi_n$

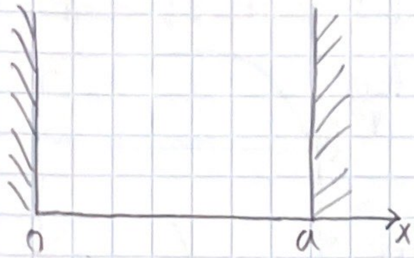
Any $\psi(x)$ periodic can be written:

$$\psi(x) = \sum_{n \in \mathbb{Z}} a_n \psi_n(x)$$

$$\left.\begin{array}{l} \psi_k + \psi_{-k} \sim \cos kx \\ \psi_k - \psi_{-k} \sim \sin kx \end{array}\right\} \text{energy eigenstates}$$

Not $\hat{p}$ eigenstates anymore

11.2: Infinite Square Well Energy Eigenstates



$$V(x) = \begin{cases} 0, & 0 < x < a \\ \infty, & x \leq 0,\ x \geq a \end{cases}$$

$\psi(x) = 0,\ x < 0,\ x > a \longrightarrow \left.\begin{array}{l} \psi(0) = 0 \\ \psi(a) = 0 \end{array}\right\}$ by continuity

$$\psi'' = -\frac{2mE}{\hbar^2}\psi(x)$$

$$= -k^2\psi(x)$$

$$\psi(x) = C_1 \cos kx + C_2 \sin kx$$

$$\psi(x=0) = 0 = C_1$$

$$\psi(x) = C_2 \sin kx$$

$$\psi(x=a) = 0 = C_2$$

$$ka = n\pi$$

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

11.2: Infinite Square Well Energy Eigenstates (continued)

$n \neq 0$

$n=-2,\ n=2$

$\sin(-kx) = -\sin kx$

$n = 1, 2, 3, \ldots \Rightarrow k_n = \frac{\pi n}{a}$

$\psi_n(x) \sim \sin\left(\frac{n\pi x}{a}\right)$

$$\int_0^a |\psi_n|^2 dx = N^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx$$

$$= N^2 \cdot \frac{1}{2} a = 1$$

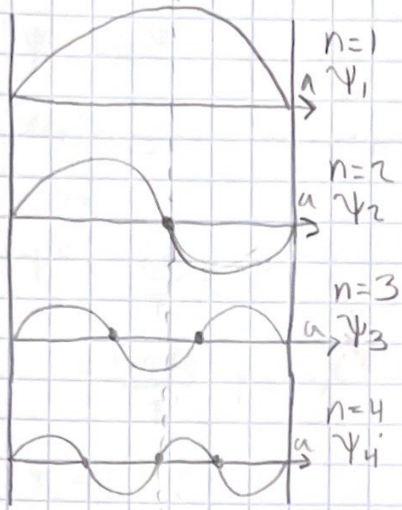
$$\Rightarrow N = \sqrt{\frac{2}{a}}$$

$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right),\ n = 1, 2, \ldots \infty$

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

11.3: Nodes and Symmetries of the Infinite Square Well

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



ground state

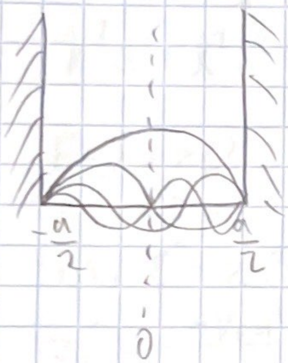
1 node

2 nodes

3 nodes

The ground state has no nodes

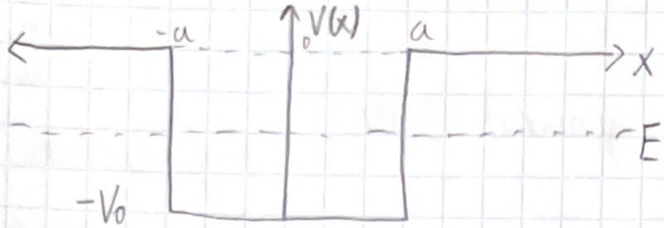
node is a zero of the wave function not at the end of the domain



Bound states of a symmetric potential are either odd or even

$V(-x) = V(x)$

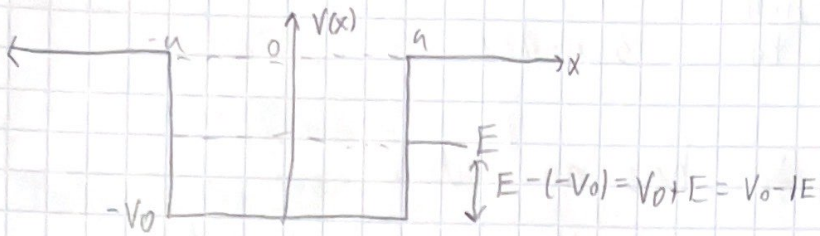
11.4: Setting Up Finite Square Well



$V_0 > 0$

Look for bound states with $E<0$

$$\psi'' = -\frac{2m}{\hbar}(E - V(x))\psi$$



$$\psi'' = \underbrace{-\frac{2m}{\hbar}(E - V(x))}_{\alpha}\psi$$

$\alpha < 0$, $|x| < \alpha$ trigonometric

$\alpha > 0$, $|x| > \alpha$ exponential

Even solutions:

$\psi(-x) = \psi(x)$

$-a < x < a$

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E - (-V_0))\psi$$

$$= -\frac{2m}{\hbar^2}(V_0 - |E|)\psi$$

11.4: Setting Up Finite Square Well (continued)

$$k^2 \equiv \frac{2m}{\hbar^2}(V_0 - |E|) > 0 \quad (1)$$

$$\psi'' = -k^2\psi$$

$$\psi(x) = \cos kx, \quad -a < x < a \quad (2)$$

$x > a$

$$\psi'' = -\frac{2m}{\hbar^2}E\psi$$

$$= \frac{2m|E|}{\hbar^2}\psi, \quad \kappa^2 = \frac{2m|E|}{\hbar^2} \quad (3)$$

$$\psi'' = \kappa^2\psi$$

- solutions: $\psi \sim e^{\pm\kappa x}$

$$\psi(x) = Ae^{-\kappa x}, \quad x > a \quad (4)$$

$$\kappa^2 + k^2 = \frac{2mV_0}{\hbar^2}$$

$$k^2a^2 + \kappa^2a^2 = \frac{2mV_0a^2}{\hbar^2}$$

$$\left.\begin{aligned} &\xi = \kappa a > 0 \\ &\eta = ka > 0 \\ &\eta^2 + \xi^2 = z_0^2 \\ &z_0^2 = \frac{2mV_0a^2}{\hbar^2} \end{aligned}\right\} \text{new definitions}$$

11.5: Finite Square Well Energy Eigenstates

ψ is continuous at $x=a$

$\cos ka = A e^{-\kappa a}$

ψ' must be continuous at $x=a$

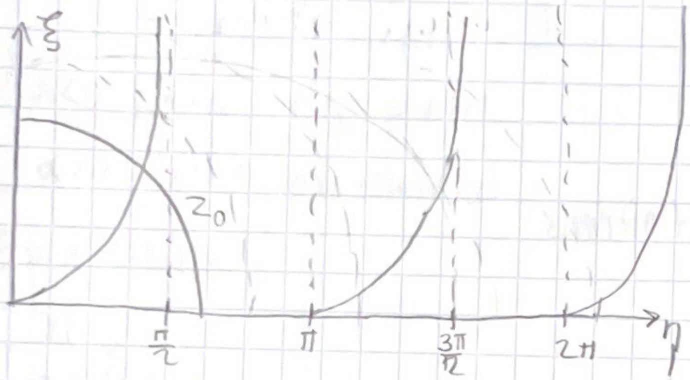
$-k\sin ka = -\kappa A e^{-\kappa a}$

$k \tan ka = \kappa$

$\xi = \eta \tan \eta$

$$\xi = \kappa^2 a^2 = \frac{2m|E|a^2}{\hbar^2}$$
$$= \frac{2mV_0 a^2}{\hbar^2}\left(\frac{|E|}{V_0}\right)$$

$$\frac{|E|}{V_0} = \left(\frac{\xi}{z_0}\right)^2$$



$\xi = -\eta \cot \eta$