Modern Physics

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Lesson X
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Born's rule

- Probability amplitude ψ ☞ complex function used to describe behaviour of systems
- Probability density (probability per unit length in one dimension)

$$P(x)\,dx = |\psi(x)|^2 dx \tag{1}$$

- Probability to find particle between two points x_1 and x_2

$$P(x_1 < x < x_2) = \int_{x_1}^{x_2} |\psi(x)|^2\,dx \tag{2}$$

- Normalization ☞ probability to find particle between $(-\infty, +\infty)$

$$\int_{-\infty}^{+\infty} |\psi(x)|^2\,dx = 1 \tag{3}$$

Expectation value

- We can no longer speak with certainty about particle position
- We can no longer guarantee outcome of single measurement (of any physical quantity that depends on position)
- Expectation value ☞ most probable outcome for single measurement which is equivalent to average outcome for many measurements
- E.g. ☞ determine expected location of particle
  Performing a large number of measurements we calculate average position

$$\langle x \rangle = \frac{n_1 x_1 + n_2 x_2 + \cdots}{n_1 + n_2 + \cdots} = \frac{\sum_i n_i x_i}{\sum_i n_i} \tag{4}$$

Expectation value (cont'd)

- Number of times n_i that we measure each position x_i
  is proportional to probability $P(x_i)\,dx$
  to find particle in interval dx at x_i

- Making substitution and changing sums to integrals

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} P(x)\, x\, dx}{\int_{-\infty}^{+\infty} P(x)\, dx} \Rightarrow \langle x \rangle = \int_{-\infty}^{+\infty} x |\psi(x)|^2\, dx \qquad (5)$$

- Expectation value of any function $f(x)$

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} f(x) |\psi(x)|^2\, dx \qquad (6)$$

Dirac notation

- State vector or wave-function ψ ☞ represented as "ket" $|\psi\rangle$
- We express any n-dimensional vector in terms of basis vectors
- We expand any wave function in terms of basis state vectors

$$|\psi\rangle = \lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle + \cdots \tag{7}$$

- Alongside the ket ☞ we define "bra" $\langle\psi|$
- Together ☞ bra and ket define *scalar product*

$$\langle\phi|\psi\rangle \equiv \int_{-\infty}^{+\infty} dx\; \phi^*(x)\; \psi(x) \Rightarrow \langle\phi|\psi\rangle^* = \langle\psi|\phi\rangle \tag{8}$$

- As for n-dimensional vector ☞ Schwartz inequality holds

$$\langle\psi|\phi\rangle \leq \sqrt{\langle\psi|\psi\rangle\langle\phi|\phi\rangle} \tag{9}$$

Operators and Observables

- Operator $\hat{A}$ ☞ maps state vector into another $\hat{A}|\psi\rangle = |\phi\rangle$
- Eigenstate (or eigenfunction) of $\hat{A}$ with eigenvalue a

$$\hat{A}|\psi\rangle = a|\psi\rangle$$

- Observable ☞ any particle property that can be measured
- For any observable A ☞ there is an operator $\hat{A}$

$$\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle = \int_{-\infty}^{+\infty} dx\, \psi^*(x)\, \hat{A}\psi(x) \tag{10}$$

- $A^\dagger$ is called hermitian conjugate of $\hat{A}$ if

$$\int_{-\infty}^{+\infty} (\hat{A}^\dagger\phi)^*\, \psi\, dx = \int_{-\infty}^{+\infty} \phi^*\, \hat{A}\psi\, dx \Rightarrow \langle A^\dagger\phi|\psi\rangle = \langle\phi|A\psi\rangle \tag{11}$$

- $\hat{A}$ is called hermitian if $\hat{A}^\dagger = \hat{A}$ ☞ $\langle A\phi|\psi\rangle = \langle\phi|A\psi\rangle$

Commutator

- Operators are associative but not (in general) commutative

$$\hat{A}\hat{B}|\psi\rangle = \hat{A}(\hat{B}\psi\rangle) = (\hat{A}\hat{B})|\psi\rangle \neq \hat{B}\hat{A}|\psi\rangle \quad (12)$$

- Example ☞ $(\hat{x}\hat{p} - \hat{p}\hat{x})\psi(x) = -i\hbar \left\{ x\frac{\partial \psi}{\partial x} - \frac{\partial}{\partial x}[x\psi(x)] \right\}$ (13)

  by product rule of differentiation

$$(\hat{x}\hat{p} - \hat{p}\hat{x})\psi(x) = i\hbar\psi(x) \quad (14)$$

- Since this must hold for any function $\psi(x)$

$$\hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar \quad (15)$$

- Short-hand notation:

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$$

- A "free" particle ☞ no external forces acting upon it $\Rightarrow V(x) = V_0$
- State represented by its wave function ☞ $\psi(x) = Ae^{ikx}$
- Schrödinger equation has 4 possible solutions

$$\frac{2m}{\hbar^2}(E - V_0)\psi(x) = -\frac{\partial^2}{\partial x^2}\psi(x) = k^2\psi(x) \qquad \pm k \in \Re \text{ or } \Im \tag{16}$$

  - 2 travelling waves solutions

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad k = \pm\frac{1}{\hbar}\sqrt{2m(E - V_0)} \quad (E > V_0) \tag{17}$$

  - 2 exponentially decaying solutions

$$\psi(x) = Ae^{\kappa x} + Be^{-\kappa x} \qquad i\kappa = \pm i\frac{1}{\hbar}\sqrt{2m(V_0 - E)} \qquad (E < V_0) \tag{18}$$

- Allowed energies are

$$E = \frac{\hbar^2 k^2}{2m} + V_0 \tag{19}$$

- $E > V_0$ ☞ classically allowed
- $E < V_0$ ☞ classically forbidden
- Traveling wave solutions ☞ time evolution of probability density

$$P(x,t) = \psi^*(x,t)\psi(x,t) = \psi^*(x)e^{i\omega t}\psi(x)e^{-i\omega t} = \psi^*(x)\psi(x) \quad (20)$$

independent of time!

- Particle traveling in only one (say $+x$) direction

$$P(x,t) = \psi^*(x)\psi(x) = A^*e^{-ikx}Ae^{ikx} = A^*A \quad (21)$$

independent of position ☞ particle completely delocalized!

- Superposition of both positive and negative going waves

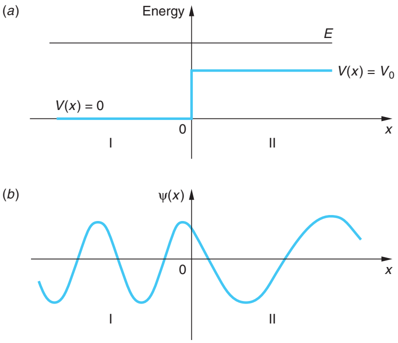
$$\begin{aligned} P(x,t) &= \left(Ae^{ikx} + B^{-ikx}\right)^* (Ae^{ikx} + Be^{-ikx}) \\ &= A^*A + B^*B + 2\Re\{A^*Be^{-2ikx} + B^*Ae^{2ikx}\} \end{aligned}$$

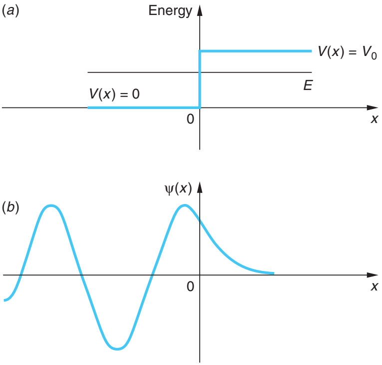
- For real-valued coefficients A and B

$$P(x,t) = A^2 + B^2 + 2ABcos(2kx) \quad (22)$$

which is equation for standing wave

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x \geq 0 \end{cases} \quad (23)$$





Case1: $E > V_0$

- $x < 0$ ☞
$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad k_1 = \sqrt{2mE}/\hbar \tag{24}$$
- $x > 0$ ☞
$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} \qquad k_2 = \sqrt{2m(E - V_0)}/\hbar \tag{25}$$
- Assume particle initially comes from $-x$ direction ☞ $D = 0$
- Continuity constraints @ $x = 0$

$$\psi_1(0) = \psi_2(0) \Rightarrow A + B = C \tag{26}$$

$$\psi'(0) = \psi_2'(0) \Rightarrow ik_1(A - B) = ik_2C \tag{27}$$

- Combining these and eliminating C

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2} = \frac{1 - k_2/k_1}{1 + k_2/k_1} \tag{28}$$

Case1: $E > V_0$ (cont'd)

- Reflection coefficient of barrier ☞ reflectivity

$$R = \left|\frac{B}{A}\right|^2 = \left|\frac{1 - k_2/k_1}{1 + k_2/k_1}\right|^2 \quad (29)$$

- Due to conservation of particle number
(or probability depending on how you think about wave function)
transmissivity is simply given by

$$T = 1 - R = 1 - \left|\frac{1 - k_2/k_1}{1 + k_2/k_1}\right|^2 \quad (30)$$

- In going from region I to region II
de Broglie wavelength becomes longer for increased potential step

Case2: $E < V_0$

- $x < 0$ ☞
$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad k_1 = \sqrt{2mE}/\hbar \tag{31}$$
- $x > 0$ ☞
$$\psi_2(x) = Ce^{\kappa_2 x} + De^{-\kappa_2 x} \qquad \kappa_2 = \sqrt{2m(V_0 - E)}/\hbar \tag{32}$$
- $C = 0$ since ψ cannot grow infinitely large as $x \to \infty$
- Continuity constraints @ $x = 0$

$$\psi_1(0) = \psi_2(0) \Rightarrow A + B = D \tag{33}$$

$$\psi_1'(0) = \psi_2'(0) \Rightarrow ik_1(A - B) = \kappa_2 D \tag{34}$$

Combining these and eliminating D

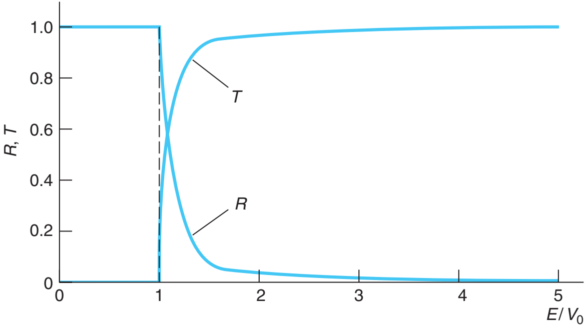
$$\frac{B}{A} = \frac{k_1 - i\kappa_2}{k_1 + i\kappa_2} \tag{35}$$

Case2: $E < V_0$ (cont'd)

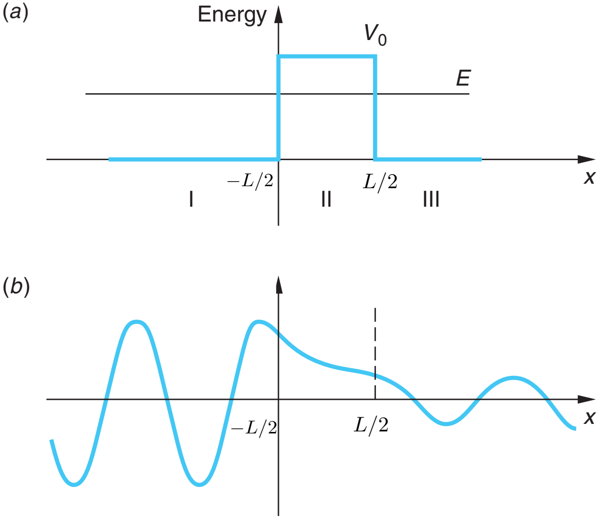
- Reflectivity of barrier

$$R = \left|\frac{B}{A}\right|^2 = \left(\frac{k_1 - i\kappa_2}{k_1 + i\kappa_2}\right)\left(\frac{k_1 + i\kappa_2}{k_1 - i\kappa_2}\right) = 1 \quad (36)$$

- Although $P \neq 0$ to penetrate into classically forbidden region particle will always be reflected (eventually)



$$V(x) = \begin{cases} V_0 & \text{for } -L/2 < x < L/2 \\ 0 & \text{otherwise} \end{cases} \quad (37)$$



wave function

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx} \quad \psi_2(x) = Ce^{\kappa x} + De^{-\kappa x} \quad \psi_3(x) = Fe^{ikx} + Ge^{ikx}$$

wave vector

$$k = \sqrt{2mE}/\hbar \qquad \kappa = \sqrt{2m(V_0 - E)}/\hbar$$

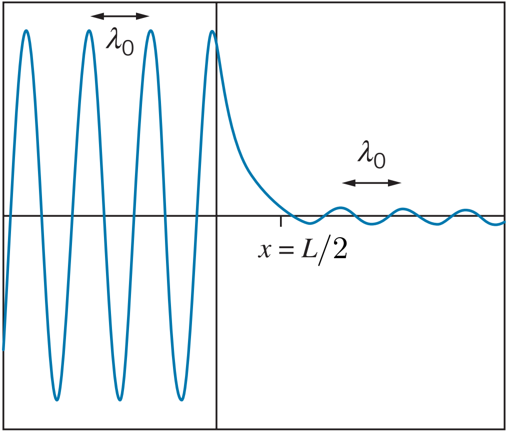
- Assuming particle initially starts on left of barrier ☞ $G = 0$

boundary conditions

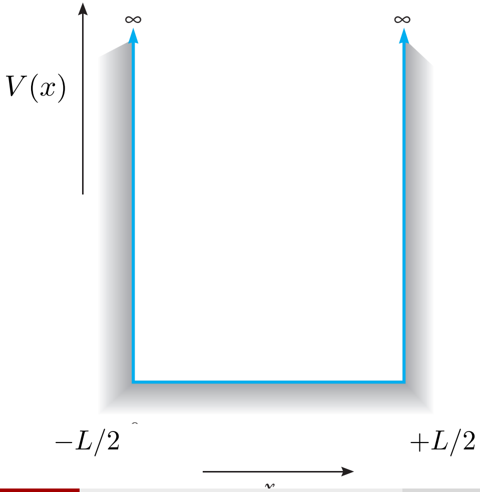
$$\begin{aligned}
e^{-ikL/2} + \frac{B}{A} e^{ikL/2} &= \frac{C}{A} e^{-\kappa L/2} + \frac{D}{A} e^{\kappa L/2} \\
ik\left(e^{-ikL/2} - \frac{B}{A} e^{ikL/2}\right) &= \kappa \left(\frac{C}{A} e^{-\kappa L/2} - \frac{D}{A} e^{\kappa L/2}\right) \\
ik\left(\frac{F}{A} e^{ikL/2}\right) &= \kappa \left(\frac{C}{A} e^{\kappa L/2} - \frac{D}{A} e^{-\kappa L/2}\right) \\
\frac{F}{A} e^{ikL/2} &= \frac{C}{A} e^{\kappa L/2} + \frac{D}{A} e^{-\kappa L/2}
\end{aligned}$$

Solving for transmission coefficient

$$T = \left| \frac{F}{A} \right|^2 = \frac{4k^2\kappa^2}{(k^2+\kappa^2)^2 \cosh(2\kappa L) - (k^4+\kappa^4+6k^2\kappa^2)} \tag{38}$$



$$V(x) = \begin{cases} \infty & \text{for } x < L/2 \\ V_0 & \text{for } -L/2 \leq x \leq L/2 \\ \infty & \text{for } x > L/2 \end{cases} \quad (39)$$



- wave function outside box

$$\psi(x) = 0 \qquad x < -L/2 \wedge x > L/2 \tag{40}$$

- wave function inside box

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad -L/2 \leq x \leq L/2 \tag{41}$$

- energy and wave vector

$$E = \frac{\hbar^2 k^2}{2m} + V_0 \Rightarrow k^2 = \frac{2m(E - V_0)}{\hbar^2} \tag{42}$$

- boundary conditions for wave function

$$\psi(-L/2) = Ae^{-ikL/2} + Be^{ikL/2} = 0 \tag{43}$$

$$\psi(+L/2) = Ae^{ikL/2} + Be^{-ikL/2} = 0 \tag{44}$$

- adding (43) to (44) gives

$$2(A+B)\cos(kL/2) = 0 \tag{45}$$

- while subtracting (43) from (44) gives

$$2i(A-B)\sin(kL/2) = 0 \tag{46}$$

- both conditions in (45) and (46) must be met
  - when $A = B$ (46) is met and to satisfy (45)

$$k = \frac{2\pi n_1}{L} + \frac{\pi}{L} \qquad n_1 = 0, 1, 2, 3, \cdots \tag{47}$$

  - when $A = -B$ in which (45) is met and to satisfy (46)

$$k = \frac{2\pi n_2}{L} \qquad n_2 = 1, 2, 3, \cdots \tag{48}$$

• Consolidate quantization conditions rewriting

$$k = \frac{\pi n}{L} \qquad n = 1, 2, 3 \cdots \tag{49}$$

and solution to time-independent Schrödinger equation

$$\psi_n(x) = A \begin{cases} \cos(n\pi x/L) & \text{for } n \text{ odd} \\ \sin(n\pi x/L) & \text{for } n \text{ even} \end{cases} = A \sin\left[\frac{n\pi}{L}\left(x + \frac{L}{2}\right)\right] \tag{50}$$

• Not only is the wave vector quantized ☞ but also

$$p = \hbar k = \hbar \pi n/L \tag{51}$$

and

$$E = V_0 + \frac{\hbar^2 k^2}{2m} = V_0 + \frac{\hbar^2 \pi^2 n^2}{2mL^2} \tag{52}$$

- Amplitude can be found by considering normalization condition

$$\int_{-\infty}^{+\infty} |\psi_n(x)|^2 dx = \int_{-L/2}^{+L/2} \left| A \sin\left[\frac{n\pi}{L}\left(x + \frac{L}{2}\right)\right]\right|^2 dx = |A|^2 \frac{L}{2}, \quad (53)$$

recall ☞

$$\int_{-L/2}^{+L/2} \left| \sin\left[\frac{n\pi}{L}\left(x + \frac{L}{2}\right)\right]\right|^2 dx = \frac{L}{2}. \quad (54)$$

- Since we require ☞ $|A|^2 L/2 = 1$

$$A = \sqrt{\frac{2}{L}} \Rightarrow \psi_n(x) = \sqrt{\frac{2}{L}} \sin\left[\frac{n\pi}{L}\left(x + \frac{L}{2}\right)\right] \quad (55)$$

- Normalization can be met for a range of complex amplitudes

$$A = e^{i\phi}\sqrt{\frac{2}{L}} \quad (56)$$

in which phase ϕ is arbitrary

- This implies outcome of measurement about particle position (which is proportional to $|\psi(x)|^2$) is invariant under *global* phase factor

Hamiltonian operator

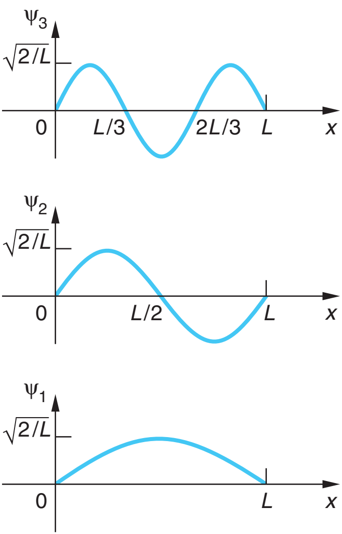
- Each solution $\psi_n(x)$ ☞ satisfies the eigenvalue problem

$$\hat{H}\psi_n(x) = E_n\psi_n(x) \qquad \hat{H} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right] \tag{57}$$

- Solutions are orthogonal to one another

$$\int_{-L/2}^{+L/2} \psi_m^*(x)\,\psi_n(x)\,dx = \delta_{mn} \tag{58}$$

$$\delta_{mn} \begin{cases} 1 & m = n \\ 0 & m \neq n \end{cases} \tag{59}$$



ψ3
√2/L
0
L/3
2L/3
L
x
ψ3²
2/L
0
L/3
2L/3
L
x
ψ2
√2/L
0
L/2
L
x
ψ2²
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2/L
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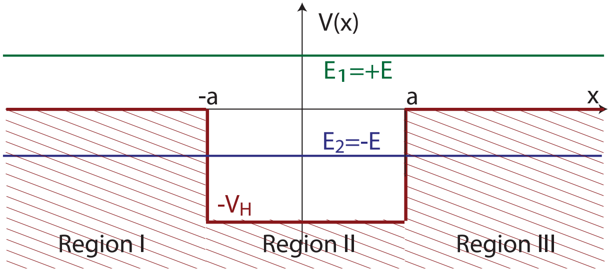
x



$$E_1 = +E \Rightarrow \begin{cases} -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx} = E\psi(x) & \text{in region I} \\ -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx} = (E+V_H)\psi(x) & \text{in region II} \\ -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx} = E\psi(x) & \text{in region III} \end{cases}$$

$$E_2 = -E \Rightarrow \begin{cases} -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx} = -E\psi(x) & \text{in region I} \\ -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx} = (V_H-E)\psi(x) & \text{in region II} \\ -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx} = -E\psi(x) & \text{in region III} \end{cases}$$

- E_1 ☛ Expect to find solution in terms of travelling waves
  Not so interesting ☞ describes case of unbound particle
- E_2 ☛ Expect waves inside the well and imaginary momentum
  (yielding exponentially decaying probability of finding particle)
  in outside regions
- More precisely
  - Region I: $k' = i\kappa \Rightarrow \kappa = \sqrt{\frac{-2mE_2}{\hbar^2}} = \sqrt{\frac{-2mE}{\hbar^2}}$
  - Region II: $k = \sqrt{\frac{2m(V_H+E_2)}{\hbar^2}} = \sqrt{\frac{2m(V_H+E)}{\hbar^2}}$
  - Region III: $k' = i\kappa \Rightarrow \kappa = \sqrt{\frac{-2mE_2}{\hbar^2}} = \sqrt{\frac{-2mE}{\hbar^2}}$
- And wave function is
  - Region I: $C'e^{-\kappa|x|}$
  - Region II: $A'e^{ikx} + B'e^{-ikx}$
  - Region III: $D'e^{-\kappa x}$

  In first region can write either $C'e^{-\kappa|x|}$ or $C'e^{\kappa x}$
  First notation makes it clear we have exponential decay

- Potential even function of x
- Differential operator also even function of x
- Solution has to be odd or even for equation to hold
- A and B must be chosen such that

$$\psi(x) = A' e^{ikx} + B' e^{-ikx}$$

is either even or odd

- Even solution ☛ $\psi(x) = A\cos(kx)$
- Odd solution ☛ $\psi(x) = A\sin(kx)$

Odd solution

- $\psi(-x) = -\psi(x)$ setting $C' = -D'$ ☛ rewrite $-C' = D' = C$
  - Region I $\psi(x) = -Ce^{\kappa x}$ and $\psi'(x) = -\kappa Ce^{\kappa x}$
  - Region II $\psi(x) = A\sin(kx)$ and $\psi'(x) = kA\cos(kx)$
  - Region III $\psi(x) = Ce^{-\kappa x}$ and $\psi'(x) = -\kappa Ce^{-\kappa x}$

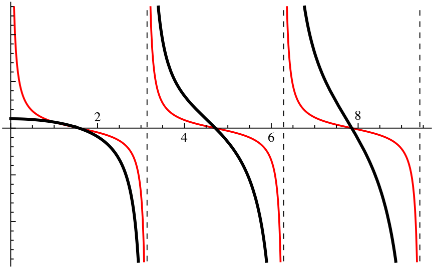
- Since $\psi(-x) = -\psi(x)$ ☞ consider boundary condition @ $x = a$
- Two equations are

$$\begin{cases} A\sin(ka) = Ce^{-\kappa a} \\ Ak\cos(ka) = -\kappa Ce^{-\kappa a} \end{cases}$$

- Substituting first equation into second

$$Ak\cos(ka) = -\kappa A\sin(ka)$$

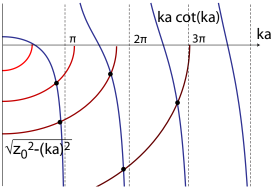
- Constraint on eigenvalues k and κ ☞ $\kappa = -k\cot(ka)$
- $\cot z$ (red) and $z\cot z$ (black)

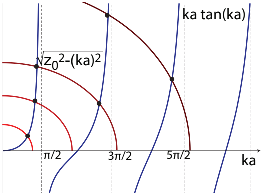


- Change of variable
  - multiply both sides by a
  - setting $ka = z$ and $\kappa a = z_1$ ☞ $z_1^2 = \frac{2mE}{\hbar^2} a^2$ and $z^2 = \frac{2m(V_H - E)}{\hbar^2} a^2$
  - setting $z_0^2 = \frac{2mV_H}{\hbar^2} a^2$ ☞ $z_1^2 = z_0^2 - z^2$ or $\kappa a = \sqrt{z_0^2 - z^2}$
- Transcendental equation for z (and hence E) as function of z_0

$$\kappa a = -ka \cot(ka) \Rightarrow z_1 = -z \cot(z) \Rightarrow \sqrt{z_0 - z^2} = -z \cot(z)$$

- To find solutions ☞ plot both sides and look for crossings
  - $y_1(z) = -\sqrt{z_0^2 - z^2}$ ☞ quarter circle of radius $z_0 = \sqrt{2mV_H a^2/\hbar^2}$
  - $y_2(z) = z \cot(z)$

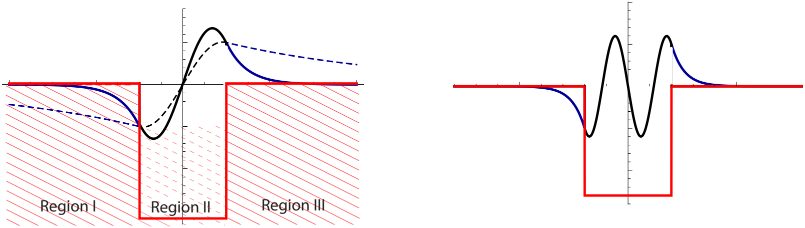




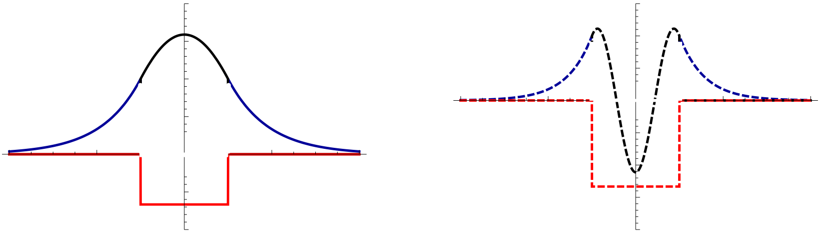
- Coefficient A (and hence C and D) can be found (once eigenfunctions have been found)
  by imposing eigenfunction is normalized
- If $z_0 < \pi/2 \Rightarrow$ no solutions ☞ $1^{\rm st}$ curve never crosses curves well is too shallow $\Rightarrow$ no bound solutions ☞ particle can escape
- Only if $V_H > \frac{\hbar}{ma^2}\frac{\pi^2}{8}$ there's bound solution
- For $z_0 > \pi/2$ ☞ infinite number of solutions
- e.g.
  - for $\pi/2 \leq z_0 \leq 3\pi/2$ ☛ only one solution
  - for $3\pi/2 \leq z_0 \leq 5\pi/2$ ☛ two solutions
  - etc.
- Bound state is always possible if we consider even solution
- Equation to be solved for even solution is

$$\kappa a = ka \tan(ka)$$

- Odd solutions



- Even solutions



Expansion in orthogonal eigenfunctions

- Time dependence of quantum states

$$\psi_n(x,t) = \psi_n e^{-iE_n t/\hbar} \tag{60}$$

- Solution for "particle in a box"
  can be expressed as a sum of different solutions

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x,t) \tag{61}$$

c_n must obey normalization condition ☞ $\sum_{n=1}^{\infty} |c_n|^2 = 1$

- Modulus squared of each coefficient
  gives probability to find particle in that state

$$P_n = |c_n|^2 \tag{62}$$

Example

- Particle initially prepared
  in symmetric superposition of ground and first excited states

$$\Psi^{(+)}(x,t=0)=\frac{1}{\sqrt{2}}\left[\psi_1(x)+\psi_2(x)\right] \tag{63}$$

- Probability to find particle in state 1 or 2 is 1/2
- State will then evolve in time according to

$$\begin{aligned}\Psi^{(+)}(x,t) &= \frac{1}{\sqrt{2}}\left[\psi_1(x)e^{-i\omega_1 t}+\psi_2(x)e^{-i\omega_2 t}\right] \\ &= e^{-i\omega_1 t}\frac{1}{\sqrt{2}}\left[\psi_1(x)+\psi_2(x)e^{-i\Delta\omega t}\right]\end{aligned} \tag{64}$$

- Probability to find particle in initial superposition state
  is not time independent