Chapter 2

Time-independent Schroedinger Equation

To solving TDSE, first solve TISE

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial^2 x} + V\Psi$$

- Assume $V=V(x)$ only so that we can use separation of variables method

Separation of variables

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial^2 x} + V\Psi$$

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

Φ, *φ* are pronounced as /ˈfaɪ/

$$\frac{\partial\Psi}{\partial t} = \psi\frac{d\varphi}{dt}, \frac{\partial^2\Psi}{\partial^2 x} = \frac{d^2\psi}{dx^2}\varphi$$

$$i\hbar\psi\frac{\partial\varphi}{\partial t} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\varphi + V\varphi\psi$$

$$i\hbar\frac{1}{\varphi}\frac{d\varphi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V(x)$$

Separation of variables

$$i\hbar\frac{1}{\varphi}\frac{d\varphi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V(x) = E$$

LHS is a function of t alone while the RHS is a function of x alone. Equation 2.4 is true only if both sides equal to a *constant*. We will call this constant E

$$\frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi \qquad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

The solution to the time-dependent part

$$\varphi(t) = e^{-iEt/\hbar}$$

Exercise: Show this.

TISE

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

The main tasks in ZCT 205 is to learn how to solve this equation for different types of $V(x)$.

Stationary states

Solutions to the TDSE in the form of

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

are said to be “stationary states”.

$$|\Psi(x,t)|^2 = \Psi^*\Psi = \psi^* e^{+iEt/\hbar}\psi e^{-iEt/\hbar} = |\psi(x)|^2$$

$$\langle Q(x,p)\rangle = \int \Psi^* Q\left(x, -i\hbar\frac{d}{dx}\right)\Psi dx = \int \psi^* Q\left(x, -i\hbar\frac{d}{dx}\right)\psi dx$$

For a particle in a stationary state, every expectation value is constant in time. So is its probability density function $|\Psi(x,t)|^2$

Why is *t* drops out in stationary states?

t drops out from $|\Psi(x,t)|^2$ and $\langle Q(x,p)\rangle$ for stationary states because these states take on the particular separable form

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

Stationary state is a solution to TDSE, but the inverse is not necessarily so

Note: It is possible for the solutions to TDSE to take a form other than $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$

For example, $\Psi(x,t) = c_1\psi_1(x)e^{-iE_1t/\hbar} + c_2\psi_2(x)e^{-iE_2t/\hbar}$
is also a solution. But this solution is not a stationary state.

A stationary state is a solution to TDSE; but a solution to TDSE is not necessarily a stationary state.

Hamiltonian

- The operator for total energy (an observable) is Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

- The expectation value for total energy

$$\langle H \rangle = \int \psi^* (\hat{H}\psi) dx$$

Time independent SE in terms of Hamiltonian

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

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

$$\hat{H}\psi = E\psi$$

Note: *E* is the separable constant introduced during the separation of variables procedure

Expectation value of *H*

By definition, the expectation value of *H* is the expected total energy

$$\langle H \rangle = \int \psi^* (\hat{H}\psi) dx = E \int |\psi|^2 dx = E.$$

The separable constant *E* actually is the expected total energy.

Variance of *H*

$$\sigma_H^2 = \langle H^2 \rangle - \langle H \rangle^2 = E^2 - E^2 = 0$$

No 'spread' in the measured value of total energy for a particle in stationary state.

Measurements of the total energy is certain to return the same value *E*.

- So, we say,

Stationary states are states of definite total energy.

Contrast this to other observables, such as *p*, *x*, where the variances in general are non-zero.

In the case of e.g., *p*, stationary states are not states of definite momentum.

TISE has infinite many separable solutions, each with a different constant, E_i

$$\Psi_1(x,t) = \psi_1(x)e^{-iE_1t/\hbar}, \Psi_2(x,t) = \psi_2(x)e^{-iE_2t/\hbar}, \cdots$$

$\{E_1,\ E_2, \cdots\}$ are known as "the allowed energies" (separable constants)

The solutions in the form

$$\psi_n(x)\,e^{-\frac{iE_n t}{\hbar}}$$

are sometimes referred to as the "eigenstates" or eigensolutions, and E_n "eigenenergies"

Linear combination of the separable solutions (eigensolutions) is also a solution

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-itE_n/\hbar}$$

This is known as “the total solution”, the most general form of solution to the TISE.

Show that the total solution is a solution to the TDSE

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-itE_n/\hbar}$$

A solution to

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial^2 x} + V\Psi$$

To completely solve the TISE

- Amounts to finding the coefficients c_n in that match the initial condition, usually in the form of an initial spatial profile of the wave function,
- $$\Psi(x, t=0) = f(x)$$

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-itE_n/\hbar}$$

Procedures

- 1. Solve the TISE for the complete set of stationary states
- $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

$$\{E_1, E_2, \cdots\}$$

$$\{\psi_1(x), \psi_2(x), \cdots\}$$

Procedures

- 2. Find the general solution at $t = 0$, i.e.,

$$\Psi(x,0) = \sum_{n=0}^{\infty} c_n \psi_n(x)$$

- by finding the coefficients c_n that fit the initial and boundary conditions.

- $f(x)$ "initial profile"

Procedures

3. Once all the c_n are found, the general time-dependent solution is obtained as

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-itE_n/\hbar} = \sum_{n=0}^{\infty} c_n \Psi_n(x,t) \qquad (2.7)$$

Example:
Non-stationary states

Example 2.1 Suppose a particle starts out in a linear combination of just *two* stationary states:

$$\Psi(x, 0) = c_1\psi_1(x) + c_2\psi_2(x).$$

(To keep things simple I'll assume that the constants c_n and the states $\psi_n(x)$ are *real*.) What is the wave function $\Psi(x, t)$ at subsequent times? Find the probability density, and describe its motion.

Solution

the wave function $\Psi(x,t)$ at subsequent times

$$\Psi(x,t) = c_1\psi_1(x)e^{-iE_1t/\hbar} + c_2\psi_2(x)e^{-iE_2t/\hbar}$$

where E_1 and E_2 are the energies associated with ψ_1 and ψ_2

the probability density is time-dependent

$$|\Psi(x,t)|^2 = (c_1\psi_1 e^{iE_1t/\hbar} + c_2\psi_2 e^{iE_2/\hbar})(c_1\psi_1 e^{-iE_1t/\hbar} + c_2\psi_2 e^{-iE_2/\hbar})$$

$$= c_1^2\psi_1^2 + c_2^2\psi_2^2 + 2c_1c_2\psi_1\psi_2\cos[(E_2 - E_1)t/\hbar].$$

Comment 1

- The state

$$\Psi(x,t) = c_1\psi_1(x)e^{-iE_1t/\hbar} + c_2\psi_2(x)e^{-iE_2t/\hbar}$$

- is not a stationary state (why is this so?)

The state $\Psi(x, t)$, also a solution to the TDSE, is formed by a linear combination of two TISE solutions ψ_1 , ψ_2 with weights c_1 and c_2.

Although ψ_1 and ψ_2 are stationary states by themselves, the linear combination of them is not.

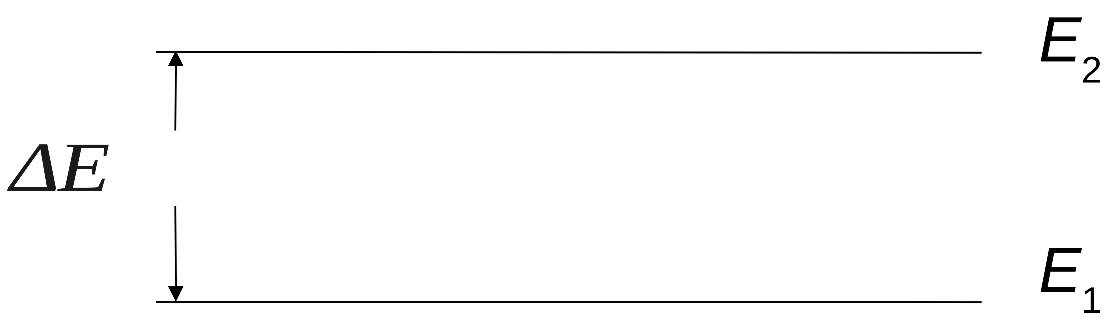
Comment 2

$$\Psi(x,t) = c_1\psi_1(x)e^{-iE_1t/\hbar} + c_2\psi_2(x)e^{-iE_2t/\hbar}$$

- The state is a “mixed” state.
- It oscillates between the two states

  $\psi_1(x)e^{-iE_1t/\hbar}$ and $\psi_2(x)e^{-iE_2t/\hbar}$

- at an angular frequency $\omega = \dfrac{\Delta E}{\hbar} = \dfrac{|E_2 - E_1|}{\hbar}$



Another mathematical property of TISE

∗**Problem 2.2** Show that E must exceed the minimum value of $V(x)$, for every normalizable solution to the time-independent Schrödinger equation. What is the classical analog to this statement? *Hint:* Rewrite Equation 2.5 in the form

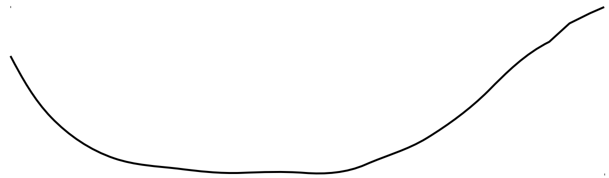
$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}[V(x) - E]\psi;$$

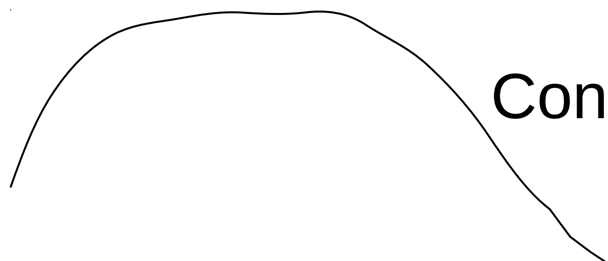
if $E < V_{\min}$, then ψ and its second derivative always have the *same sign*—argue that such a function cannot be normalized.

Proof

Concave upwards

$$\frac{d^2\Psi}{dx^2} > 0 \; \forall \; x,$$





$$\frac{d^2\Psi}{dx^2} > 0 \; \forall \; x,$$

Concave downwards

Proof

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

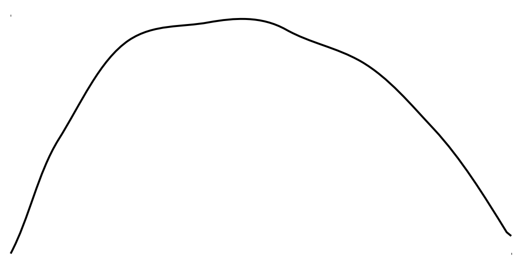
- If $E < V_{min}$,

$$\frac{d^2\psi(x)}{dx^2} = +k^2\psi(x), where k^2 some positive real value$$

Case I: $\psi(x) > 0$

Concave upwards

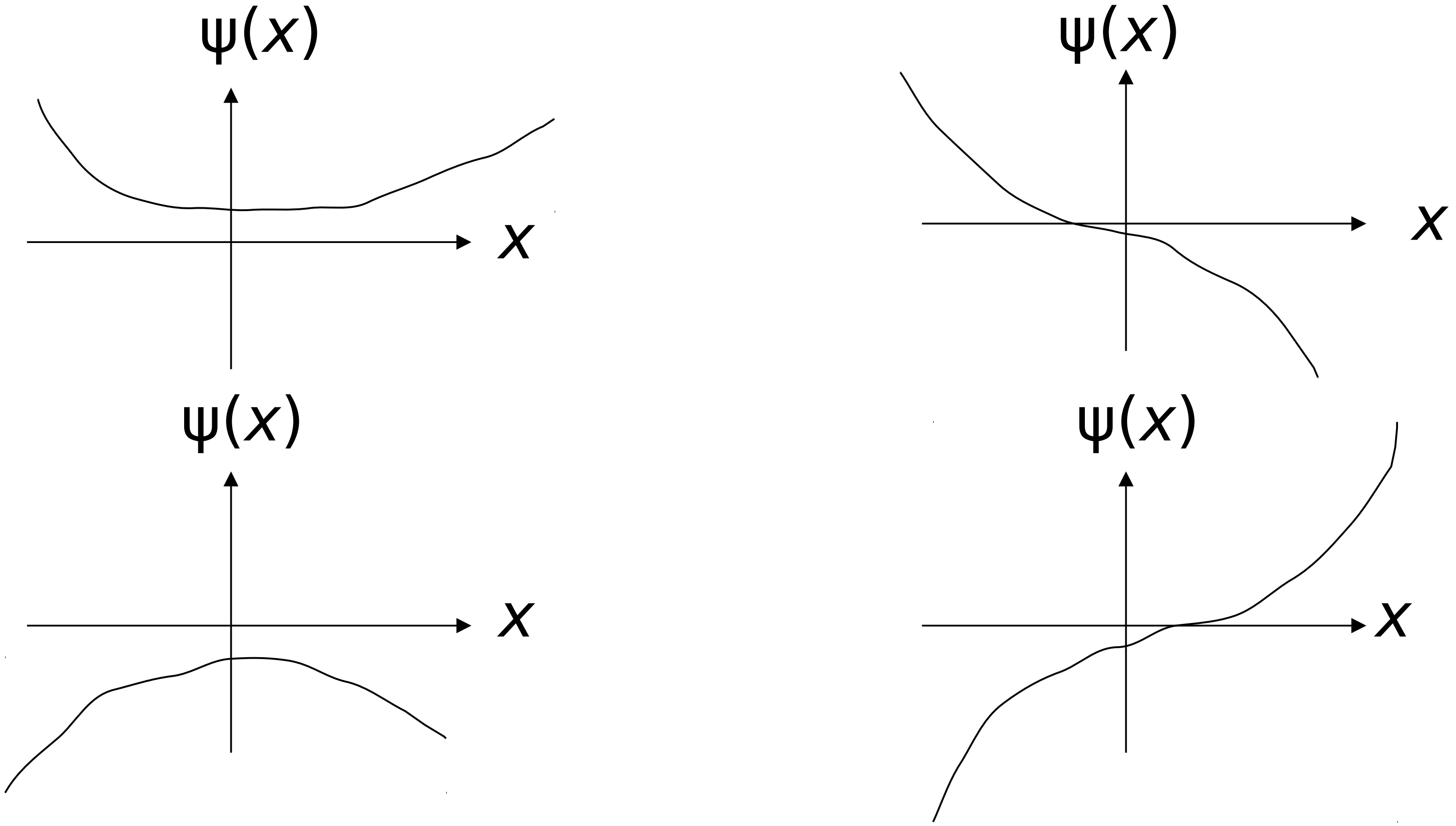
Case II: $\psi(x) < 0$



Concave downwards

Proof

$$\frac{d^2\psi(x)}{dx^2} = +k^2\psi(x), where k^2 some positive real value$$



In all possible cases, ψ(*x*) will shoot to positive or negative infinity as *x* increase ⇒ ψ(*x*) would not be normalised

Infinite square well

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

$$V(x) = \begin{cases} 0, & \text{if } 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases}$$

Figure 2.2: The infinite square well potent

Solution

$\psi(x)$ outside the infinite well is zero.

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

$$\Big\downarrow \; 0 \le x \le a, V$$

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

$$V(x) = \begin{cases} 0, & \text{if } 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases}$$

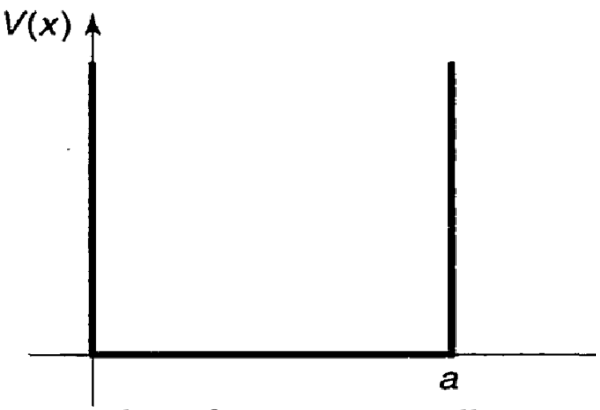


Figure 2.2: The infinite square well potent

or

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \text{ where } k \equiv \frac{\sqrt{2mE}}{\hbar}; k^2 \ge 0$$

The general solution

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \text{ where } k \equiv \frac{\sqrt{2mE}}{\hbar}; k^2 \geq 0$$

E, must be positive

WHY ?

k is real and positive

$$\psi(x) = C_1 e^{ikx} + C_2 e^{-ikx}$$

↓ Do you know how to show this?

$$= A \sin kx + B \cos kx$$

Use Euler relation

The general solution

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \text{ where } k \equiv \frac{\sqrt{2mE}}{\hbar}; k^2 \geq 0$$

E, must be positive

WHY ?

k is real and positive

$$\psi(x) = C_1 e^{ikx} + C_2 e^{-ikx}$$

Do you know how to show this?

$$= A \sin kx + B \cos kx$$

Use Euler relation

The general solution

$$\psi(x) = A \sin kx + B \cos kx$$

$$\psi(x) = 0 \text{ for } x \leq 0, x \geq a$$

The arbitrary constants *A*, *B* are fixed by the boundary conditions of the problem.

$$V(x) = \begin{cases} 0, & \text{if } 0 \leq x \leq a \\ \infty, & \text{otherwise} \end{cases}$$

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

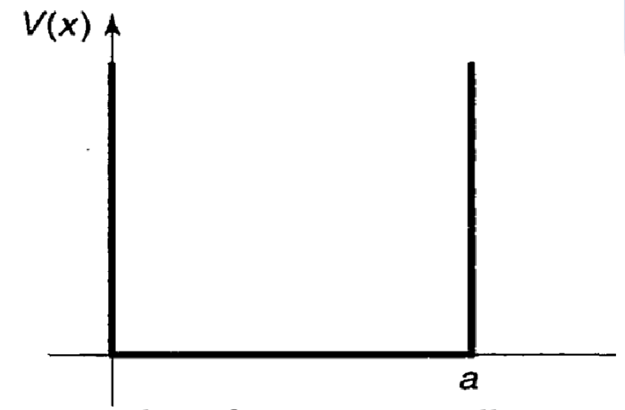


Figure 2.2: The infinite square well potent

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

$$B = 0$$

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

The constant *k* is quantised due to the boundary condition

$$\psi(x) = 0 \text{ for } x \leq 0, x \geq a$$

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

$$\psi(a) = A \sin ka = 0$$

$$\text{Since } A \neq 0$$

$$ka = 0, \pm\pi, \pm 2\pi, \pm 3\pi, \cdots$$

$$k \neq 0$$

$$k_n = \frac{n\pi}{a}, \text{ with } n = 1, 2, 3, \cdots$$

$$V(x) = \begin{cases} 0, & \text{if } 0 \leq x \leq a \\ \infty, & \text{otherwise} \end{cases}$$

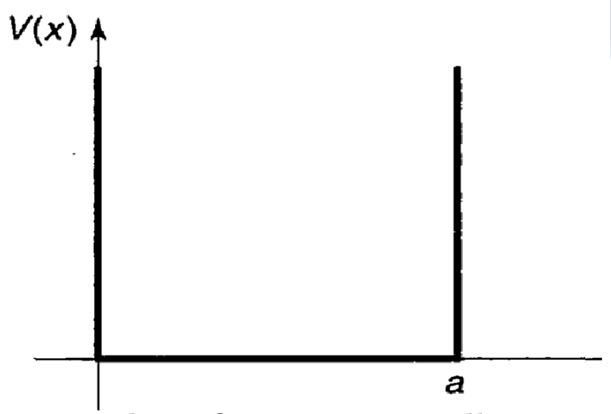


Figure 2.2: The infinite square well potent

The allowed energies

$$k_n = \frac{n\pi}{a}, \text{ with } n = 1, 2, 3, \cdots$$

the possible values of E are

$$E_n = p_n^2/2m = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

$$V(x) = \begin{cases} 0, & \text{if } 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases}$$

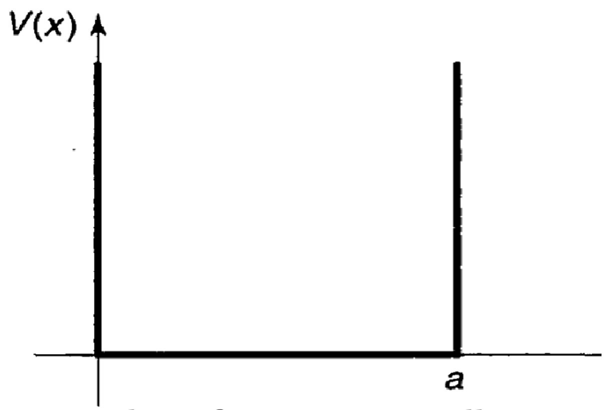


Figure 2.2: The infinite square well potent

Normalisation

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

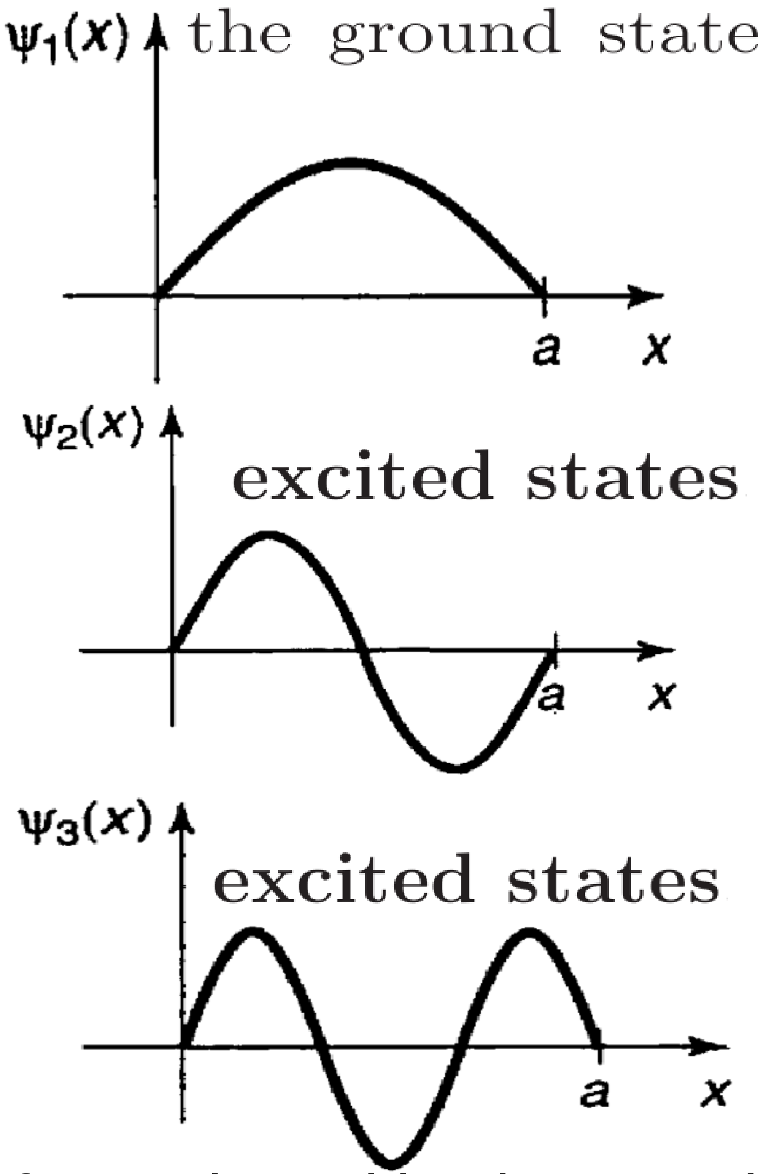
$$\int_0^a |\psi|^2 dx = 1$$

$$A = \sqrt{2/a}$$

$$Exercise:\ Show\ this.$$

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

$$\psi(x) = 0 \text{ for } x \leq 0, x \geq a$$

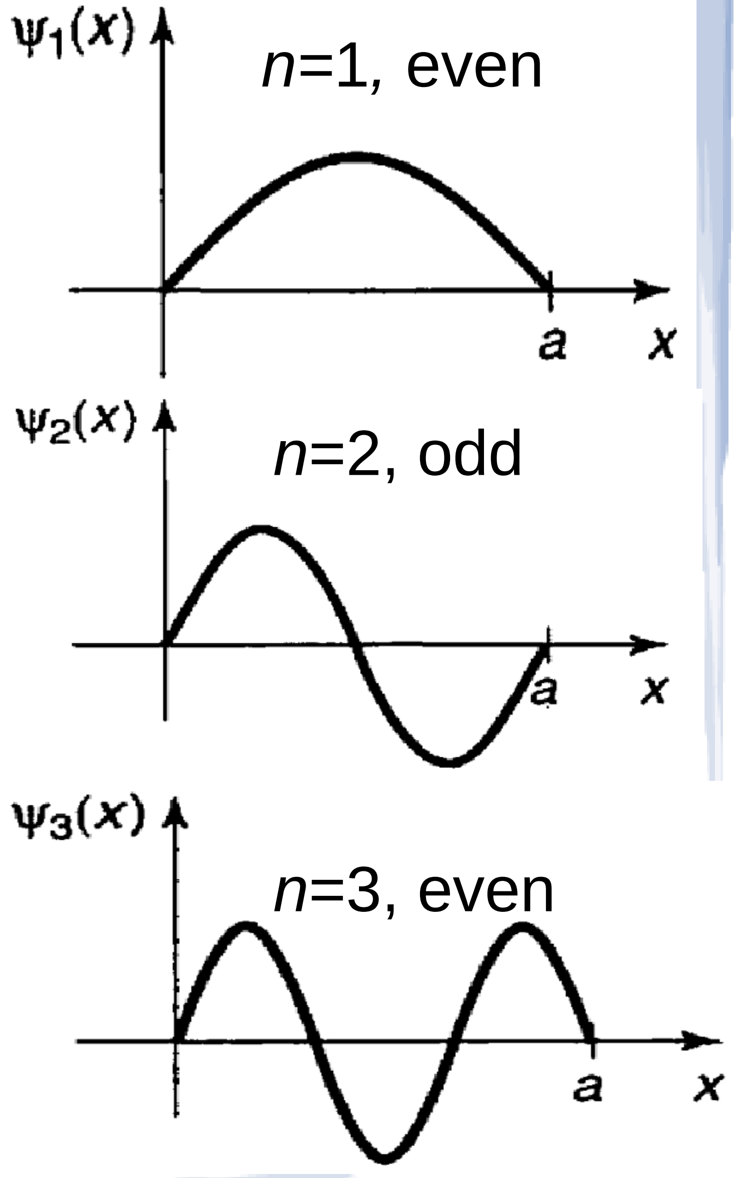


The TISE has an infinite set of solutions (one for each positive integer *n*).

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

1. ψ_n are alternately even and odd, with respect to the center of the well (i.e., $x = a/2$).

2. As n increases, each successive states has one more node.



The TISE solutions are mutually orthogonal

$$\int \psi_m(x)^* \psi_n(x) dx = \delta_{mn}$$

Exercise: Proof this

This is a very important properties used repeatedly in many subsequent calculations

Kronecker delta function

$$\delta_{mn} = \begin{cases} 0, & \text{if } m \neq n \\ 1, & \text{if } m = n \end{cases}$$

The TISE solutions are complete

Any other function $f(x)$ can be expressed as linear combination of $\{\psi_n(x)\}$:

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a} x\right)$$

This is analogous to the three Cartesian unit vectors $\{\hat{x}, \hat{y}, \hat{z}\}$

for which any vector can be expressed as linear combination of them

$$\vec{r} = x\hat{x} + y\hat{y} + z\hat{z}$$

Fourier's trick

Given any function $f(x)$ expressed in the form of the linear combination

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

The coefficients c_n can be projected out via

$$c_n = \int \psi_n(x)^* f(x) dx$$

Proof

$$c_n = \int \psi_n(x)^* f(x) dx$$

This can be simply proven by making use of the orthogonality of the TISE solutions

$$\int \psi_m(x)^* \psi_n(x) dx = \delta_{mn}$$

The stationary states of the particle in the infinite quantum well

- The stationary states associated with the TISE solution are

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-itE_n/\hbar}$$

With eigenenergies

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

The most general solution

- The most general solution to the TDSE is a linear combination of stationary states:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)$$
$$= \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-itE_n/\hbar}$$

Check that indeed $\Psi(x, t)$ is a solution to the TDSE.

The coefficients c_n

c_n in $\Psi(x, t)$ can be obtained if the initial condition ("initial profile") is given (in the form of a specific form $\Psi(x, t=0) = f(x)$)

$$c_n = \int \psi_n(x)^* f(x) dx = \int_{-\infty}^{\infty} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) f(x) dx$$

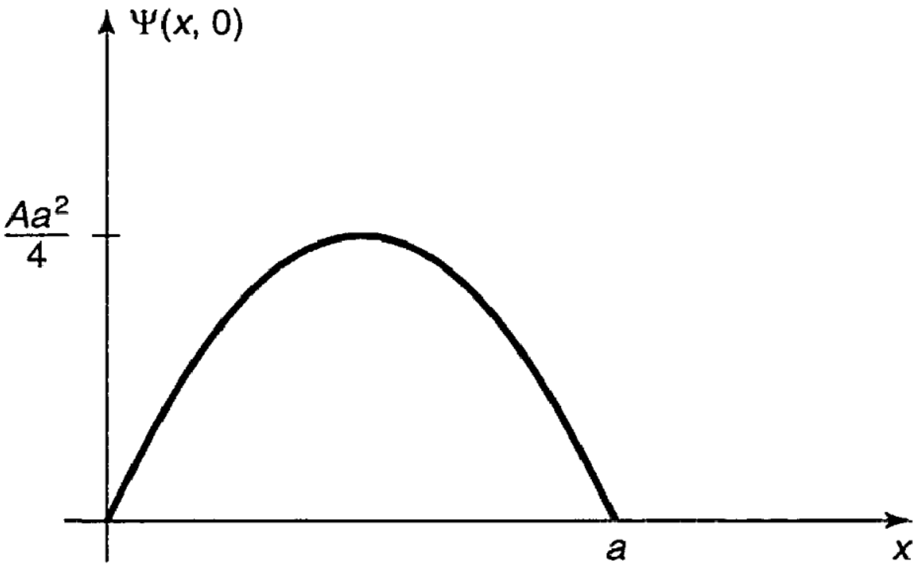
$$= \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a} x\right) f(x) dx$$

Example

A particle in the infinite square well has the initial wave function

$$\Psi(x,0) = Ax(a-x), \quad (0 \le x \le a).$$

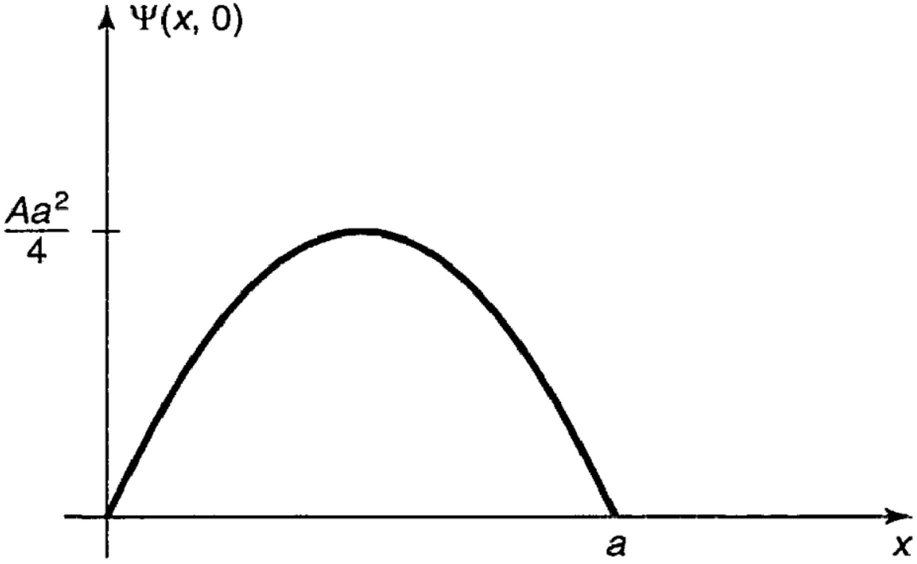
Find $\Psi\left(x,t\right)$



Normalisation

$$1 = \int_0^a |\Psi(x,0)|^2\,dx = |A|^2 \int_0^a x^2(a-x)^2\,dx = |A|^2 \frac{a^5}{30}$$

$$A = \sqrt{\frac{30}{a^5}}$$



The coefficients c_n

$$c_n = \int \psi_n(x)^* f(x) dx = \int_{-\infty}^{\infty} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) f(x) dx$$

f(*x*) here plays the role of the initial profile

$$f(x) \equiv \Psi(x, 0) = Aa(a - x)$$

Coefficient c_n

$$c_n = \int \psi_n(x)^* f(x) dx = \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a} x\right) f(x) dx$$

$$c_n = \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a} x\right) \sqrt{\frac{30}{a^5}}\, x(a-x)\, dx$$

$$= \frac{2\sqrt{15}}{a^3}\left[a \int_0^a x \sin\left(\frac{n\pi}{a}x\right) dx - \int_0^a x^2 \sin\left(\frac{n\pi}{a}x\right) dx\right]$$

$$= \frac{2\sqrt{15}}{a^3}\left\{a\left[\left(\frac{a}{n\pi}\right)^2 \sin\left(\frac{n\pi}{a}x\right) - \frac{ax}{n\pi}\cos\left(\frac{n\pi}{a}x\right)\right]\Bigg|_0^a\right.$$

$$\left. - \left[2\left(\frac{a}{n\pi}\right)^2 x \sin\left(\frac{n\pi}{a}x\right) - \frac{(n\pi x/a)^2 - 2}{(n\pi/a)^3}\cos\left(\frac{n\pi}{a}x\right)\right]\Bigg|_0^a\right\}$$

$$= \frac{2\sqrt{15}}{a^3}\left[-\frac{a^3}{n\pi}\cos(n\pi) + a^3\frac{(n\pi)^2 - 2}{(n\pi)^3}\cos(n\pi) + a^3\frac{2}{(n\pi)^3}\cos(0)\right]$$

$$= \frac{4\sqrt{15}}{(n\pi)^3}\left[\cos(0) - \cos(n\pi)\right]$$

$$= \begin{cases} 0, & \text{if } n \text{ is even.} \\ 8\sqrt{15}/(n\pi)^3, & \text{if } n \text{ is odd.} \end{cases}$$

Final answer

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-itE_n/\hbar}$$

$$c_n = \begin{cases} 0, & \text{if } n \text{ is even.} \\ 8\sqrt{15}/(n\pi)^3, & \text{if } n \text{ is odd.} \end{cases}$$

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

$$\Psi(x,t) = \sqrt{\frac{30}{a}} \left(\frac{2}{\pi}\right)^3 \sum_{n=1,3,5\ldots} \frac{1}{n^3} \sin\left(\frac{n\pi}{a}x\right) e^{-in^2\pi^2\hbar t/2ma^2}$$

Interpretation of c_n

- Every time you measure the observable energy of a quantum particle in state Ψ, you will obtain a discrete number E_n. $|c_n|^2$ is the probability of getting the particular value E_n when you make a measurement.

Normalisation of c_n

- The probability when summed over all allowed states *n* must be normalised:

$$\sum_{n=1}^{\infty} |c_n|^2 = 1$$

Exercise: Proof this relation for any arbitrary t-dependent state $\Psi(x,t)$

Proof of normalisation of c_n

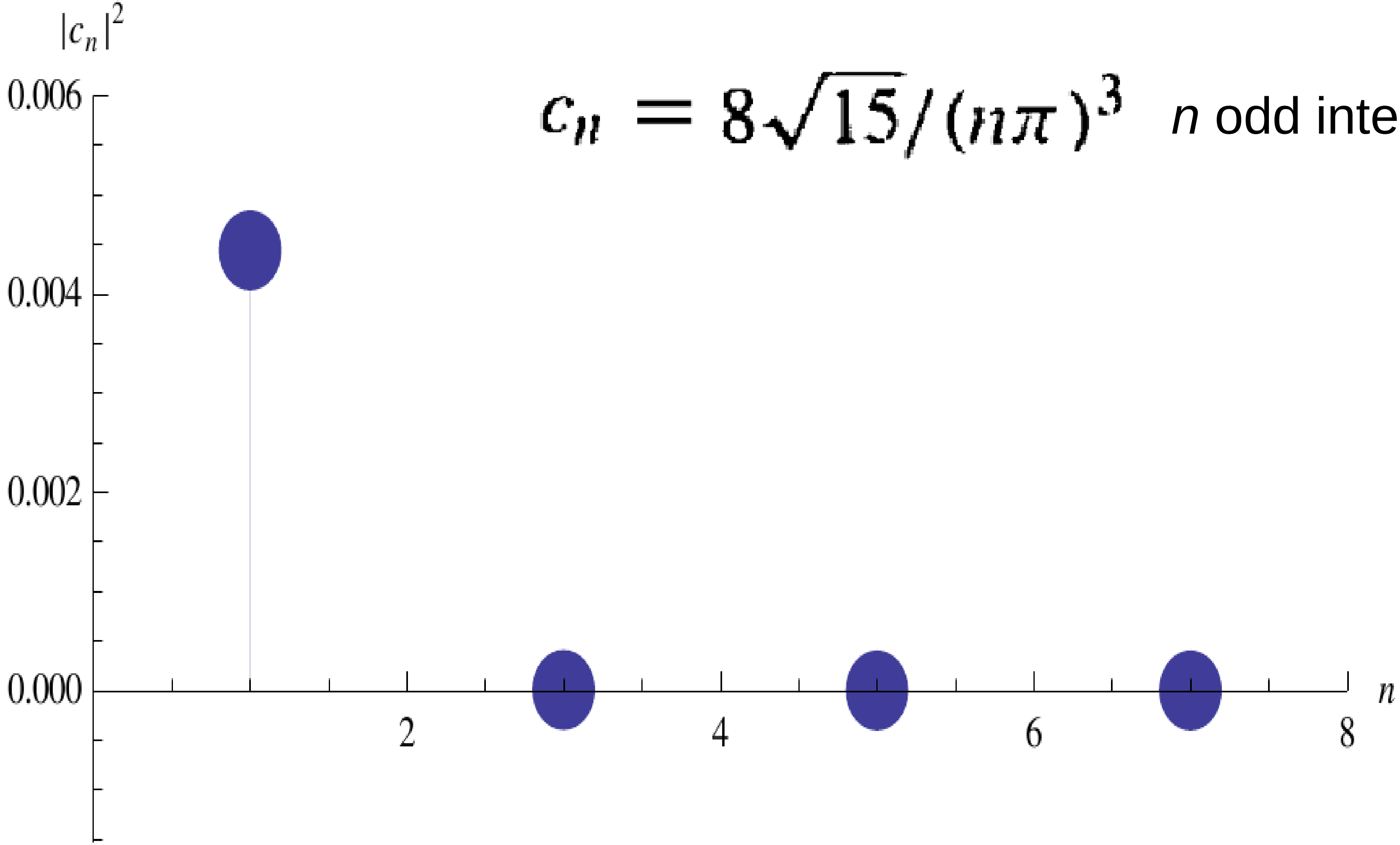
- Use $\int |\Psi(x,t)|^2 = 1$

and $\int \psi_n^*(x)\psi_m(x)dx = \delta_{mn}$

to prove

$$\sum_{n=1}^{\infty} |c_n|^2 = 1$$

$|c_n|^2$ vs. n



$$c_n = 8\sqrt{15}/(n\pi)^3$$ *n* odd integer

Comment: only the first c_n (n=1) contribute significantly; the other n's (n=3,5,7,...) contribution is almost negligible.

Expectation value of the energy

$$\langle H \rangle = \sum_{n=0}^{\infty} |c_n|^2 E_n$$

This can be proven via

$$(1)\ \textit{the definition}\ \langle H \rangle = \int \Psi^* H \Psi$$

$$(2)\ \textit{the TISE in terms of Hamiltonian},$$

$$H\Psi_n = E_n \Psi_n$$

$$(3)\ \Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-itE_n/\hbar}$$

Note that the expectation value of energy is a constant. This is a manifestation of conservation of energy in QM.

Expectation value of the energy

$$\langle H \rangle = \sum_{n=0}^{\infty} |c_n|^2 E_n$$

$$c_n = \begin{cases} 0, & \text{if } n \text{ is even,} \\ 8\sqrt{15}/(n\pi)^3, & \text{if } n \text{ is odd.} \end{cases}$$

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

$$\langle H \rangle = \sum_{n=1,3,5,\ldots}^{\infty} \left(\frac{8\sqrt{15}}{n^3 \pi^3} \right)^2 \frac{n^2 \pi^2 \hbar^2}{2ma^2} = \frac{480\hbar^2}{\pi^4 ma^2} \sum_{n=1,3,5,\ldots}^{\infty} \frac{1}{n^4} = \frac{5\hbar^2}{ma^2}$$

Use Murray Spiegel or revisit your ZCA 110 for the series sum

$$\sum_{n=1,3,5,\cdots} \frac{1}{n^4}$$

Online resource

- Murray Spiegel, Mathematical Handbook of Formulas and Tables (Schaum's outline series)
- https://archive.org/details/MathematicalHandbook

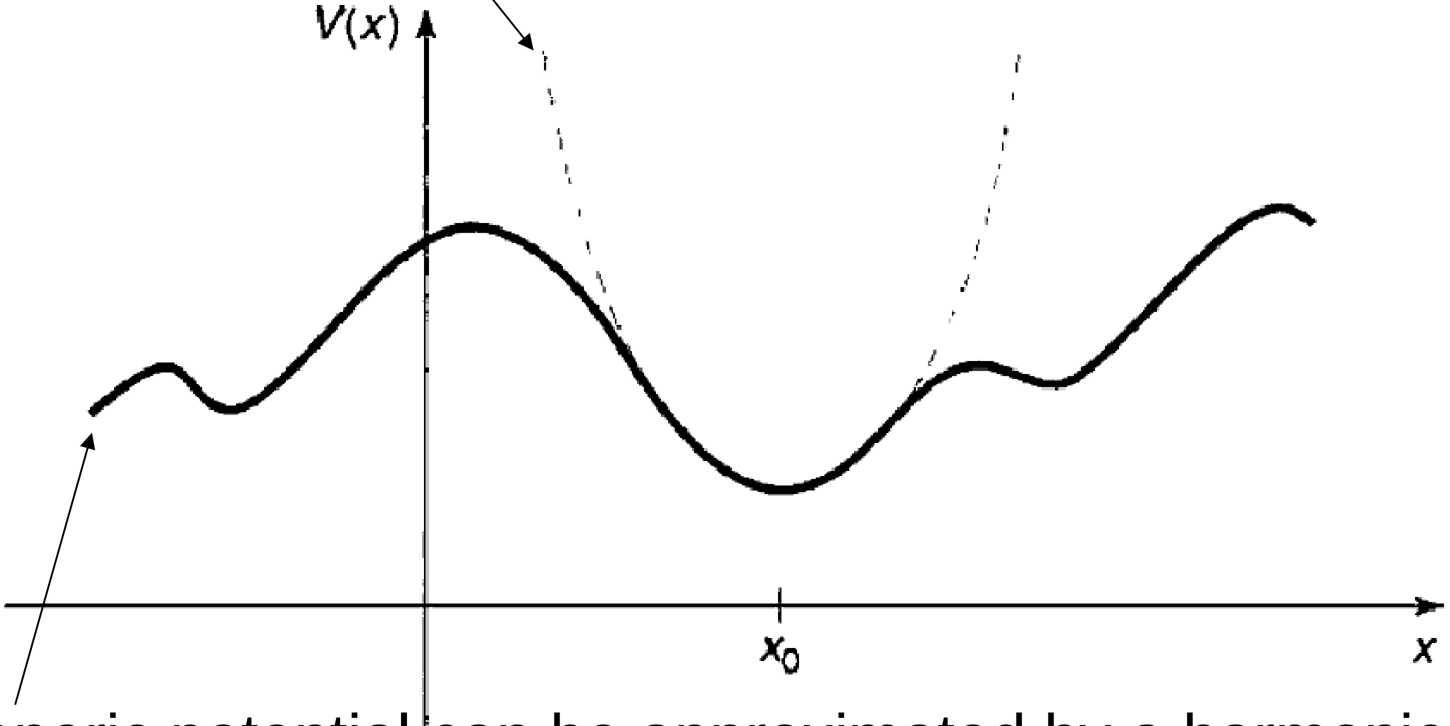
Check your common sense

Is $\langle H \rangle$ larger, equal or smaller than the ground state energy $E_1 = \frac{\pi^2 \hbar^2}{2ma^2}$?

Explain why.

The harmonic oscillator

$$V(x) = \frac{1}{2}m\omega^2 x^2$$



A generic potential can be approximated by a harmonic potential in the neighborhood of a local minimum ($x = x_0$)

TISE for a 1D harmonic oscillator

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{2x^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi$$

Change variable from *x* to ξ (ξ is pronounced as "/ˈzaɪ/, /ˈksaɪ/". I prefer to pronounce it "cacing")

$$\xi=x\sqrt{\frac{m\omega}{\hbar}}$$

$$\frac{d^2\psi}{d\xi^2}=(\xi^2-K)\psi \qquad K\equiv\frac{2E}{\hbar\omega}$$

Solving $\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi$

- Strategy:
- First solve it in the $\xi \rightarrow \infty$ limit.
- Then use the info of the solution in this limit to solve the more general case of intermediate ξ .

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi$$

$$\big\downarrow \ \xi \rightarrow \infty$$

$$\frac{d^2\psi}{d\xi^2} = \xi^2\psi$$

Dropping the *B* coefficient

$$\frac{d^2\psi}{d\xi^2} = \xi^2\psi$$

$$\psi(\xi) = Ae^{-\xi^2/2} + Be^{+\xi^2/2}$$

Prove this

What is *B*?

The *B* term blows up as $|\xi| \to \infty$, hence has to be dropped in order to preserve normalisability.

As such, $\psi(\xi) \sim e^{-\xi^2/2} \text{ at large } \xi$

In the intermediate range of ξ

$$\psi(\xi) = h(\xi)e^{-\xi^2/2}$$

where the (yet unknown) functions $h(\xi)$ behave in such a way that

$$\psi(\xi) \sim e^{-\xi^2/2} \text{ at large } \xi$$

Recast the TISE

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi$$

$$\psi(\xi) = h(\xi)e^{-\xi^2/2}$$

Show this

$$\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K-1)h = 0.$$

Solving $\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K-1)h = 0.$

- Power series method

$$h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j$$

What we really want are the values of the coefficients a_j for all j.

Solving $\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K-1)h = 0$

Differentiating $h(\xi)$ with respect to ξ once and twice, then substitute the results back into $\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K-1)h = 0$

$$\sum_{j=0}^{\infty}\left[(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j\right]\xi^j = 0$$

Show this

The coefficients to ξ_j must be zero for every j

ξ^j

Non-zero, because the are the solution (wave function) we are after

Recursion formula

Setting

$$[(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j] = 0$$

↓

$$a_{j+2} = \frac{2j+1-K}{(j+1)(j+2)}a_j$$

The recursion formula allows us to obtain all a_j based on two "seed" coefficients (unknown at this stage), a_0 and a_1.

a_0 generate all even coefficients $a_j, j = 2, 4, 6, \cdots$

a_1 generate all odd coefficients $a_j, j = 3, 5, 7, \cdots$

Recursion formula

$$a_{j+2} = \frac{2j+1-K}{(j+1)(j+2)} a_j$$

Example:

$$j=0: a_2 = \frac{(2\cdot 0+1-K)}{(0+1)(0+2)} a_0 = \frac{(1-K)}{2} a_0$$

$$j=1: a_3 = \frac{(2\cdot 1+1-K)}{(1+1)(1+2)} a_1 = \frac{(3-K)}{6} a_1$$

$$j=2: a_4 = \frac{(2\cdot 4+1-K)}{(2+1)(2+2)} a_2 = \frac{(5-K)}{12} a_2 = \frac{(5-K)}{12} \frac{(1-K)}{2} a_0$$

$$j=3: a_5 = \frac{(2\cdot 5+1-K)}{(3+1)(3+2)} a_2 = \frac{(11-K)}{20} a_3 = \frac{(11-K)}{20} \frac{(3-K)}{6} a_1$$

a_{even} is in terms of a_0

a_{odd} is in terms of a_1

The solution $h(\xi)$ as sum of two parts with definite parity

$$h(\xi) = h_{even}(\xi) + h_{odd}(\xi),$$

$$h_{even}(\xi) \equiv a_0 + a_2\xi^2 + a_4\xi^4 + \cdots ,$$

$$h_{odd}(\xi) \equiv a_1 + a_3\xi^3 + a_5\xi^5 + \cdots .$$

a_0, a_1 are to be fixed by normalisation

Odd and even solutions.
Looks familiar?

Explicitly

$$h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j$$

$$= \left(a_0 \xi^0 + a_2 \xi^2 + a_4 \xi^4 + \ldots \right) + \left(a_1 \xi^1 + a_3 \xi^3 + a_5 \xi^5 + \ldots \right)$$

Constraint

Constraint has to be imposed on

$$a_{j+2} = \frac{2j+1-K}{(j+1)(j+2)} a_j$$

so that $\psi(\xi) = h(\xi) e^{-\xi^2/2}$ does not blow up in the $\xi \to \infty$ limit

How to design such a constraint?

Introducing the non-negative integer n

$$a_{j+2} = \frac{2j+1-K}{(j+1)(j+2)}a_j$$

Introduce a non-negative integer *n* to truncate the series

$$h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j$$

beyond the *n*-term.

If there exist a non-negative integer *n* such that

$$K = 2n + 1$$

then, for any $j \geq n$

$$a_{2+n} = \frac{(2n+1)-K}{(n+1)(n+2)} a_n = 0$$

Note: a_{2+n}=0 but not a_n

In other words, if $K = 2n + 1$, then ...

- For any given odd n,
- $a_m = 0$ for all odd m, m > n
- Example: If n=3, $\underbrace{a_1, a_3}_{0}; \underbrace{a_5, a_7, a_9, \ldots}_{=0}$
- a_n even terms are not affected by $K = 2n + 1$ if n is odd.

In other words, if $K = 2n + 1$, then ...

- For a given even n,
- $a_k = 0$ for all even k, k > n
- Example: If n = 4, $\underbrace{a_0, a_2, a_4}_{0}; \underbrace{a_6, a_8, a_{10}, \ldots}_{=0}$
- a_n odd terms are not affected by $K = 2n + 1$ if n is even.

Further condition to be imposed "by hand"

- As an independent consideration, we have to impose another condition by hand on a_j to make $\psi(\xi)$ well behaved in the limit $\xi \to \infty$:

$a_0 = 0$ if n is odd (hence, all even $a_j = 0$)

$a_1 = 0$ if n is even (hence, all odd $a_j = 0$)

Numerical illustration

$$a_{j+2} = \frac{2j + 1 - K}{(j+1)(j+2)} a_j$$

$K = 2n + 1$

$a_0 = 0$ if n is odd (hence, all even $a_j = 0$)

$a_1 = 0$ if n is even (hence, all odd $a_j = 0$)

n	$K = 2n+1$	Odd a_j	Even a_j	$h_n(\xi)$ a_0
0	1	0	$a_0 \neq 0$; $a_2 = a_4 = a_6 = \ldots = 0$	$a_1 \xi$
1	3	$a_1 \neq 0$; $a_3 = a_5 = a_7 = \ldots = 0$	0	$a_0 + a_2 \xi^2$ $a_1 \xi + a_3 \xi^3$
2	5	0	$a_0 \neq 0$; $a_2 = 2a_0$ $a_4 = a_6 = \ldots = 0$	$a_0 + a_2 \xi^2 + a_4 \xi^4$
3	7	$a_1 \neq 0$; $a_3 = a_1/3$; $a_5 = a_7 = \ldots = 0$	0	$a_1 \xi + a_3 \xi^3 + a_5 \xi^5$

The values of a_0 or a_1 are not important; only the relatives values of a_j are

- The absolute values of a_0 or a_1 are not important.
- Only the relative values of a_j with respect to a_0 or a_1 are.

Normalisation

$$\psi_n(\xi) = e^{-\xi^2/2} h_n(\xi)$$

We can normalise the solution $\psi_n(\xi)$ for a particular *n* via

$$\int |\psi_n(\xi)|^2 dx = 1$$

This in turn will fix the value of a_0 (in the case n is even) or a_1 (in the case n is odd) for that particular n value.

Some examples of the solutions ψ_n

- ψ_n for the first few odd and even integers are shown in the next two slides.

$$\psi_n(\xi) = e^{-\xi^2/2} h_n(\xi)$$

Even n

$$\psi_n(\xi) = e^{-\xi^2/2} h_n(\xi)$$

$n = 0$

$A_n = 0.751126$

$h_n(\xi) = 1$

$\psi_n(\xi) = 0.751126\, e^{-0.5\,\xi^2}$

$n = 2$

$A_n = 0.531126$

$h_n(\xi) = 1 - 2\xi^2$

$\psi_n(\xi) = 0.531126\, e^{-0.5\,\xi^2}\left(1 - 2\xi^2\right)$

$n = 4$

$A_n = 0.459969$

$$h_n(\xi) = 1 - 4\xi^2 + \frac{4\xi^4}{3}$$

$$\psi_n(\xi) = 0.459969\, e^{-0.5\,\xi^2}\left(1 - 4\xi^2 + \frac{4\xi^4}{3}\right)$$

Odd n $\psi_n(\xi) = e^{-\xi^2/2} h_n(\xi)$

$n = 1$

$A_n = 1.06225$

$h_n(\xi) = \xi$

$\psi_n(\xi) = 1.06225\, e^{-0.5\,\xi^2}\, \xi$

$n = 3$

$A_n = 1.30099$

$$h_n(\xi) = \xi - \frac{2\,\xi^3}{3}$$

$$\psi_n(\xi) = 1.30099\, e^{-0.5\,\xi^2} \left(\xi - \frac{2\,\xi^3}{3}\right)$$

$n = 5$

$A_n = 1.45455$

$$h_n(\xi) = \xi - \frac{4\,\xi^3}{3} + \frac{4\,\xi^5}{15}$$

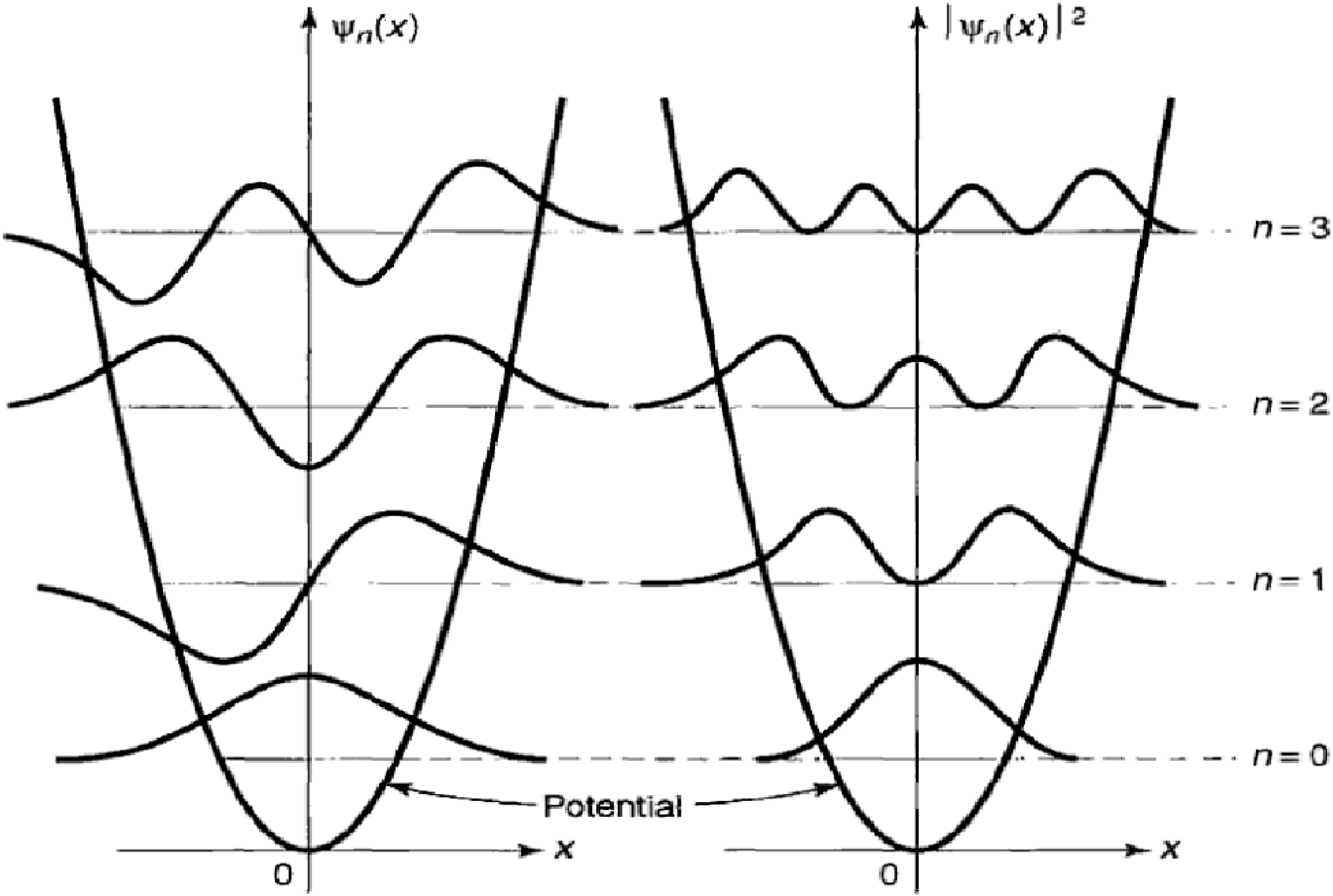
$$\psi_n(\xi) = 1.45455\, e^{-0.5\,\xi^2} \left(\xi - \frac{4\,\xi^3}{3} + \frac{4\,\xi^5}{15}\right)$$

Checking whether ψ is well behaved in the limit $\xi \to \infty$

Using Mathematica code, we verify that,

$$\psi_n(\xi) = e^{-\xi^2/2} h_n(\xi)$$

indeed converges to zero at the limit $|\xi| \to \infty$



$\psi_n(x)$
$|\psi_n(x)|^2$
$n = 3$
$n = 2$
$n = 1$
$n = 0$
Potential
x
0
x
0

Quantisation of energy

- $K = 2n + 1$;
- $K = 2E/(\hbar\omega)$
- $E = (n + 1/2)\hbar\omega$

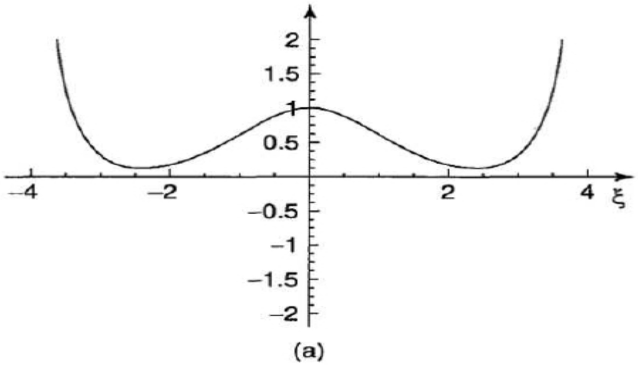
Mathematica code for QHO

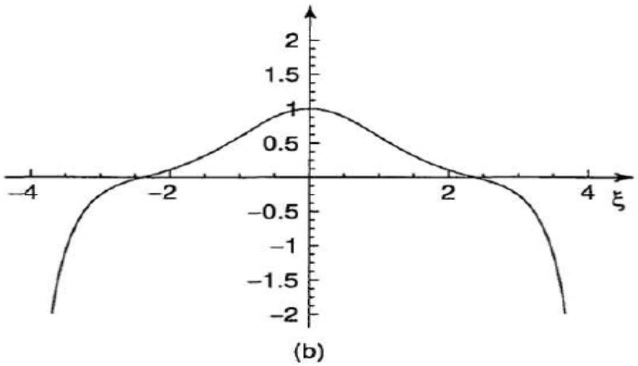
The code, download-able from

www2.fizizk.usm.my/tlyoon/teaching/ZCT205_1314/QHO.nb

shows you how to generate the QHO solution using Mathematica

- Numerically, if *E* assume a value other that allowed, (say $E = 0.49\ \hbar\omega$ or $0.51\ \hbar\omega$), the solution $\psi(\xi)$ will blow beyond the the furthest nodes.
- See also QHO.nb





Exercise

- Assume *n* is 1, write down $h(\xi)$, hence the stationary wave function, $\psi_1(x)$.
- Assume *n* is 2, write down $h(\xi)$, hence the stationary wave function, $\psi_2(x)$.

Hermite polynomial, $H_n(\xi)$

$$\psi_n(x) = h_n(\xi)e^{-\xi^2/2} = \frac{1}{\sqrt{2^n n!}} H_n(\xi)e^{-\xi^2/2}$$

TABLE 2.1: The first few Hermite polynomials, $H_n(\xi)$.

$$H_0 = 1,$$
$$H_1 = 2\xi,$$
$$H_2 = 4\xi^2 - 2,$$
$$H_3 = 8\xi^3 - 12\xi,$$
$$H_4 = 16\xi^4 - 48\xi^2 + 12,$$
$$H_5 = 32\xi^5 - 160\xi^3 + 120\xi.$$

Rodrigues formula

$$H_n(\xi) = (-1)^n e^{\xi^2} \left(\frac{d}{d\xi}\right)^n e^{-\xi^2}$$

Recursion relation

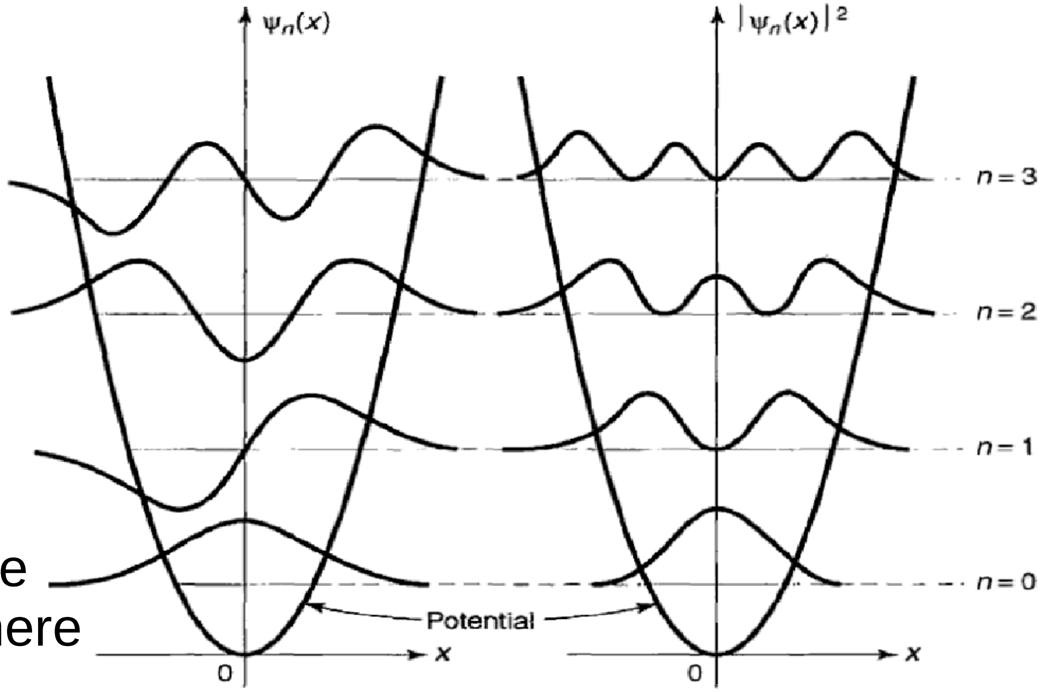
$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2nH_{n-1}(\xi)$$

Exercise

- Derive H_1, H_2, H_3 from the Rodrigues formula.
- Derive H_3, H_4 from H_1, H_2 using the recursion relation.
- As a check, the function H_3 derived using both methods must agree.

Features of the QM solutions for the harmonic oscillator I

$$1.\ |\psi_n|^2 \neq 0 \text{ outside the harmonic well}$$

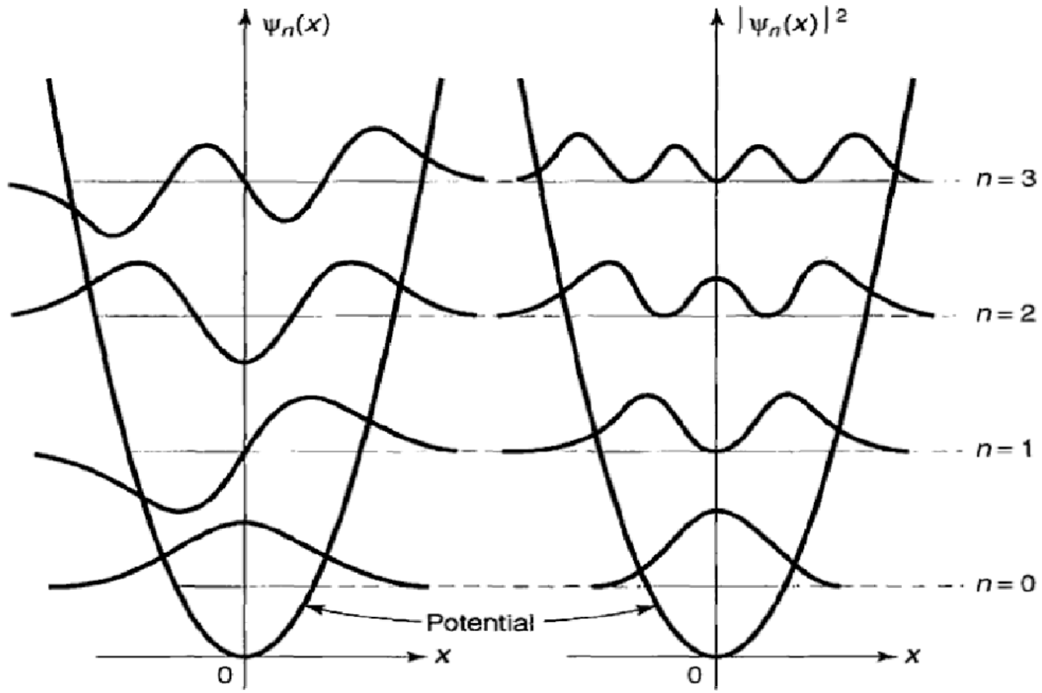


The particle has non zero probability to be found in classically forbidden regions, where $E < V$

Quantum Tunelling effect

Features of the QM solutions for the harmonic oscillator II

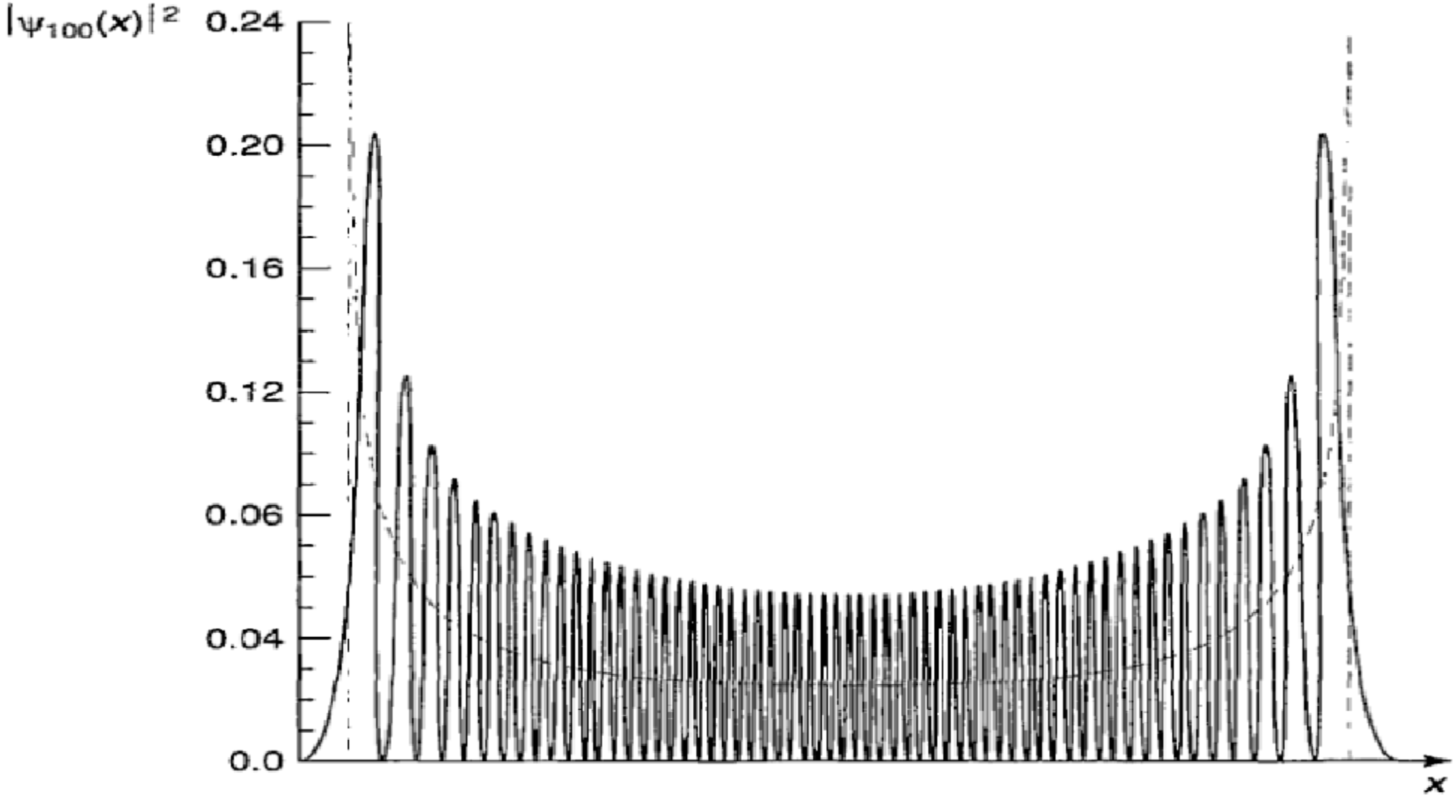
2. In the odd states, probability to find the oscillator is always zero at the center ($x = 0$) of the potential.



Features of the QM solutions for the harmonic oscillator III: Correspondence principle

3. As $n \to \infty$, $|\psi_n(x)|^2$ behaves much like what is expected of a classical harmonic oscillator.

The correspondence principle: in the $n \to \infty$ limit, results of a quantum calculation must reduce to that of classical calculation.



Free particle

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

↓

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \text{ where } k \equiv \frac{\sqrt{2mE}}{\hbar}$$

Equivalent to setting $a \to \infty$ in infinite quantum well

The time-independent solution

$$\psi_k(x) = Ae^{ikx} + Be^{-ikx}$$

But no boundary condition (as in the case of infinite quantum well).

Hence, *E* is not quantised (so is *k*).

This is an essential difference between a 'confined' system and a free particle.

The time-dependent "stationary" solution is a traveling plane wave

$$\Psi_k(x,t) = \psi_k(x)e^{-itE/\hbar} = \psi_k(x)e^{-\frac{it\hbar k^2}{2m}}$$

$$= Ae^{ik(x-\frac{\hbar k}{2m}t)} + Be^{-ik(x+\frac{\hbar k}{2m}t)}$$

Compactly,

$$\Psi_k(x,t) = Ae^{ik(x-\frac{\hbar k}{2m}t)};$$

$$k \equiv \pm\frac{\sqrt{2mE}}{\hbar}, \text{ with}$$

$$\begin{cases} k > 0 \Rightarrow \text{traveling to the positive direction} \\ k < 0 \Rightarrow \text{traveling to the negative direction} \end{cases}$$

Normalisation of the traveling wave "stationary" solution

$$\int_{-\infty}^{\infty} \Psi_k^* \Psi_k dx \to \infty$$

SHOW THIS! IT"S EASY

Disturbing !!!
A stationary state is one which has a definite energy.
But since the state Ψ_k can't be normalised, there is nothing such as a free particle with a definite energy.

Total solution to the TDSE

- To properly interpret

$$\Psi_k(x,t) \quad = \quad Ae^{ik(x-\frac{\hbar k}{2m}t)}$$

- we must look at the total solution instead of just the individual stationary solution per se.

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)\psi_k(x,t)e^{-itE/\hbar}dk$$

Compare this with as in the case of quantised E_n (confined system)

$$\Psi(x,t) = \sum_{\text{all } n} c_n\psi_n(x)e^{-itE_n/\hbar}$$

Comparison

Quantised system	Free particle
$\Psi(x,t) = \sum_{\text{all } n} c_n \psi_n(x) e^{-itE_n/\hbar}$	$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) \psi_k(x,t) e^{-itE/\hbar} dk$
E_n, k_n (discrete)	E, k (continuous)
c_n	$\frac{1}{\sqrt{2\pi}} \phi(k) dk$
$\sum_n c_n (\cdots)$	$\int_{-\infty}^{\infty} (\cdots) \phi(k) dk$
1	$\frac{1}{\sqrt{2\pi}}$ A new factor introduced introduced for the sake of later convenience (so that it is consistent with the definition of Fourier transformation)
Normalisable	Normalisable

A free particle must be represented as a wave packet (so that it remains normalisable)

- A free particle cannot be in a "stationary state" $\Psi_k(x,t) = \psi_k(x)e^{-itE/\hbar}$ as it is not normalisable.
- But

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \phi(k)\psi_k(x,t)e^{-itE/\hbar}dk$$

is normalisable.

- Hence, a free particle must be represented as a wave packet in the form of $\Psi(x,t)$
- Note that $\Psi(x,t)$ has a large spread of wave number *k* (hence a large spread in energy *E*).

Plancherel's theorem

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ikx} dk \Leftrightarrow F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx.$$

$F(k)$ is the Fourier transform of $f(x)$

$f(x)$ inverse Fourier transform of $F(k)$

Finding $\phi(k)$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m}t)} dk.$$

$\downarrow$ $t = 0$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}}\int \phi(k) e^{ikx} dk$$

given $f(x) \equiv \Psi(x,0)$ we want to know what $\phi(k)$ is.

A classic Fourier transformation problem

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx$$

Example

$$\Psi(x,0) = \begin{cases} A, & \text{if} -a < x < a, \\ 0, & \text{otherwise}, \end{cases}$$

$$\text{Find } \Psi(x,t).$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)} dk.$$

This amounts to finding $\phi(k)$

Normalisation

$$\int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = 1 \Rightarrow A = \frac{1}{\sqrt{2a}}.$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \int_{-a}^{a} e^{-ikx} dx$$

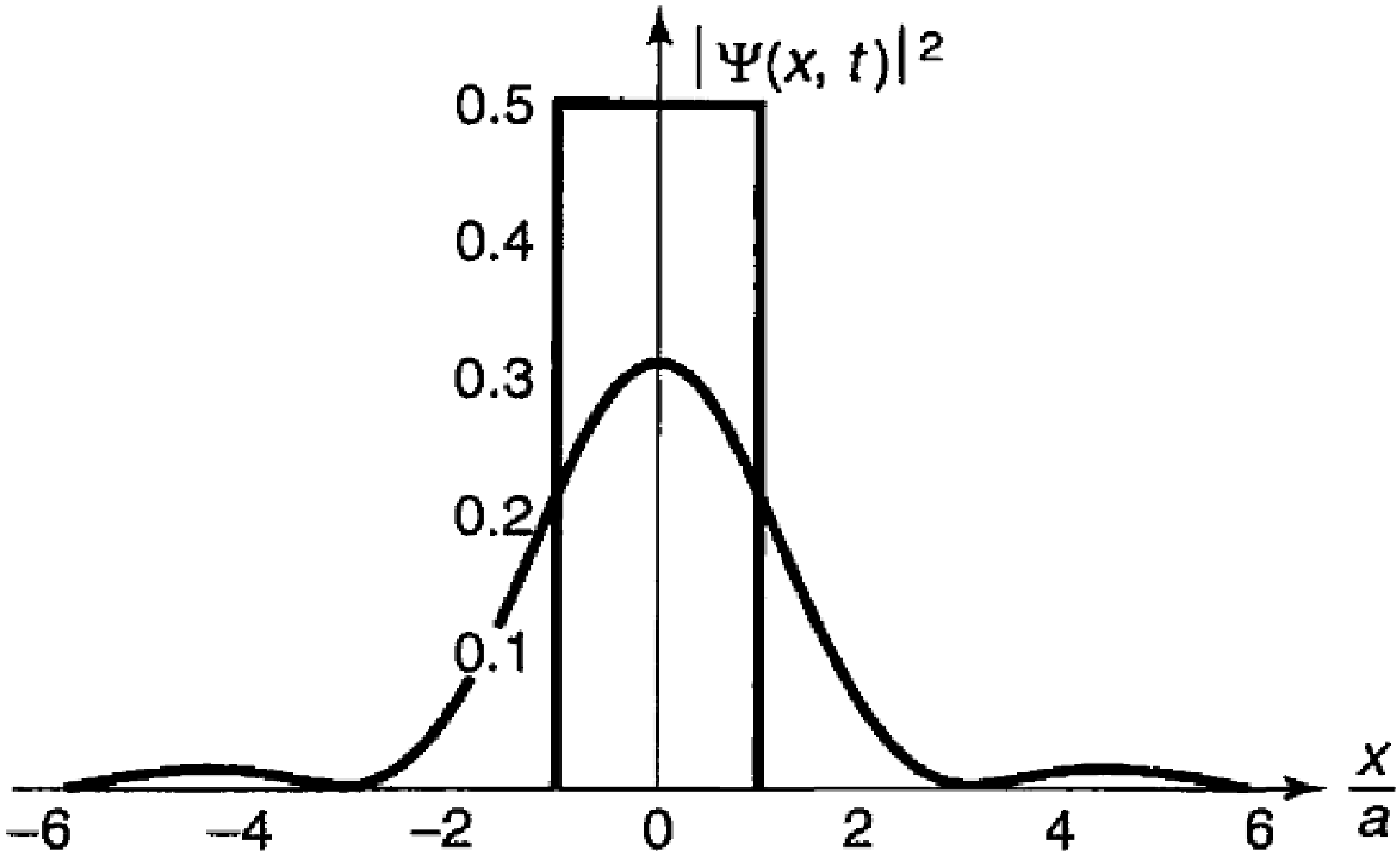
$$= \cdots = \frac{1}{\sqrt{a\pi}} \frac{\sin(ka)}{k} \quad \text{(show this)}$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)} dk.$$

$$\phi(k) = \frac{1}{\sqrt{a\pi}} \frac{\sin(ka)}{k}$$

$$= \frac{1}{\pi\sqrt{2a}} \int_{-\infty}^{\infty} \frac{\sin(ka)}{k} e^{i(kx - \frac{\hbar k^2}{2m} t)} dk$$

$\Psi(x,t)$ begins to spread in width as $t > 0$



$$\Psi(x,t) = \frac{1}{\pi\sqrt{2a}} \int_{-\infty}^{\infty} \frac{\sin(ka)}{k} e^{i(kx - \frac{\hbar k^2}{2m}t)} dk$$

at $t = 0$

Description in *x*-space vs. Description in *k*-space

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{i(kx-\frac{\hbar k^2}{2m}t)}dk.$$

vs

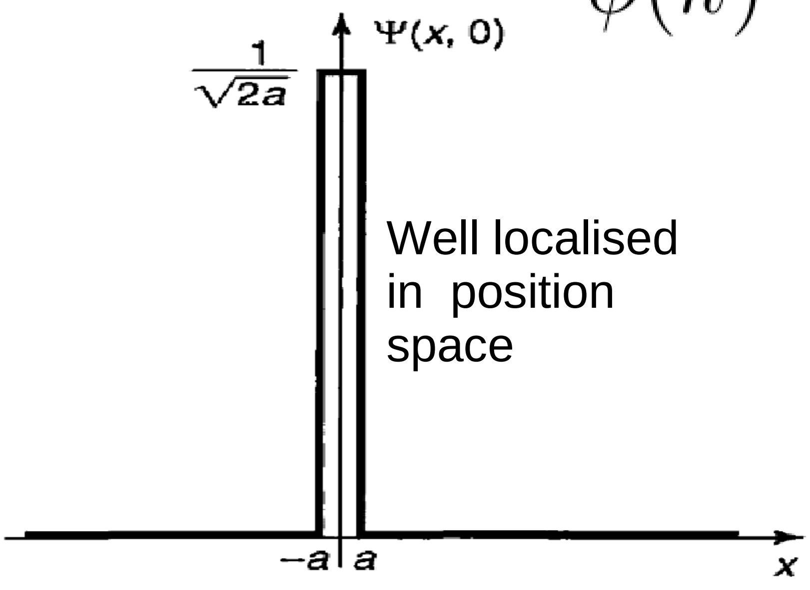
$$\phi(k) = \frac{1}{\sqrt{a\pi}}\frac{\sin(ka)}{k}$$

$\phi(k)$ describes the free particle (at $t = 0$) in terms of $k = p/\hbar$

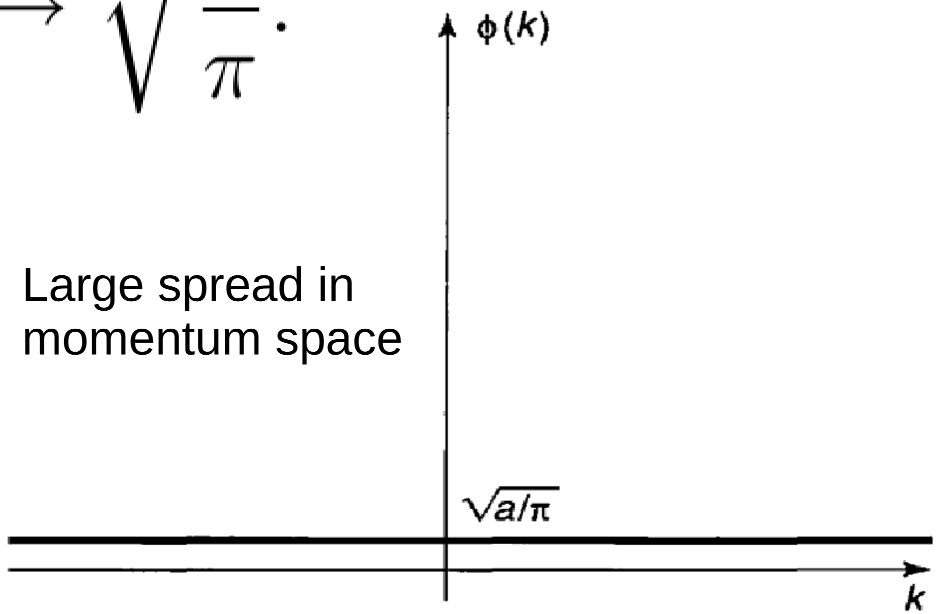
$\Psi(x,0)$ describes the free particle (at $t = 0$) in terms of position, x.

In the *a* << 1 limit at *t* = 0

$$\phi(k) \xrightarrow{a\ll 1} \sqrt{\frac{a}{\pi}}.$$



(a)

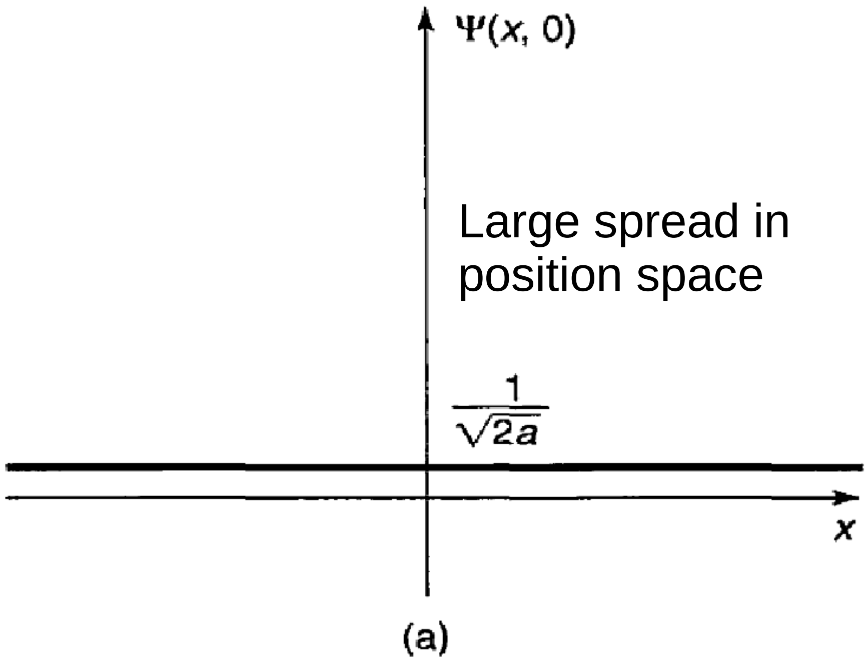


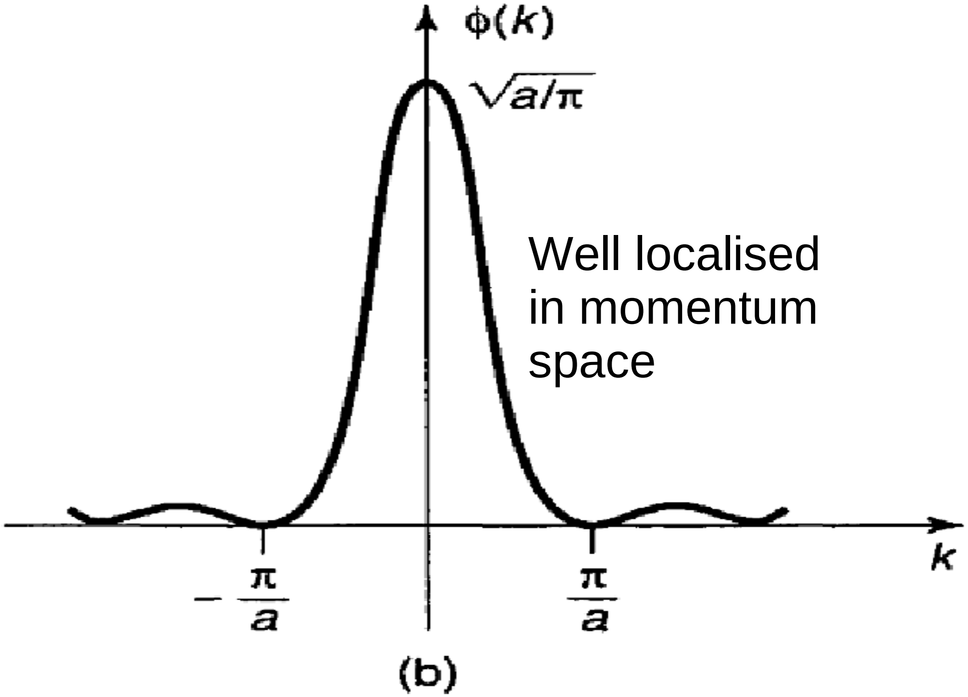
(b)

A small spread in position space, $\sigma_x \simeq a$ (where $a \ll 1$) is associated with a large spread in momentum space, i.e., $\sigma_k \rightarrow \infty$.

In the a >> 1 limit at t = 0

$$\phi(k) = \sqrt{\frac{a}{\pi}} \frac{\sin(ka)}{ka}$$





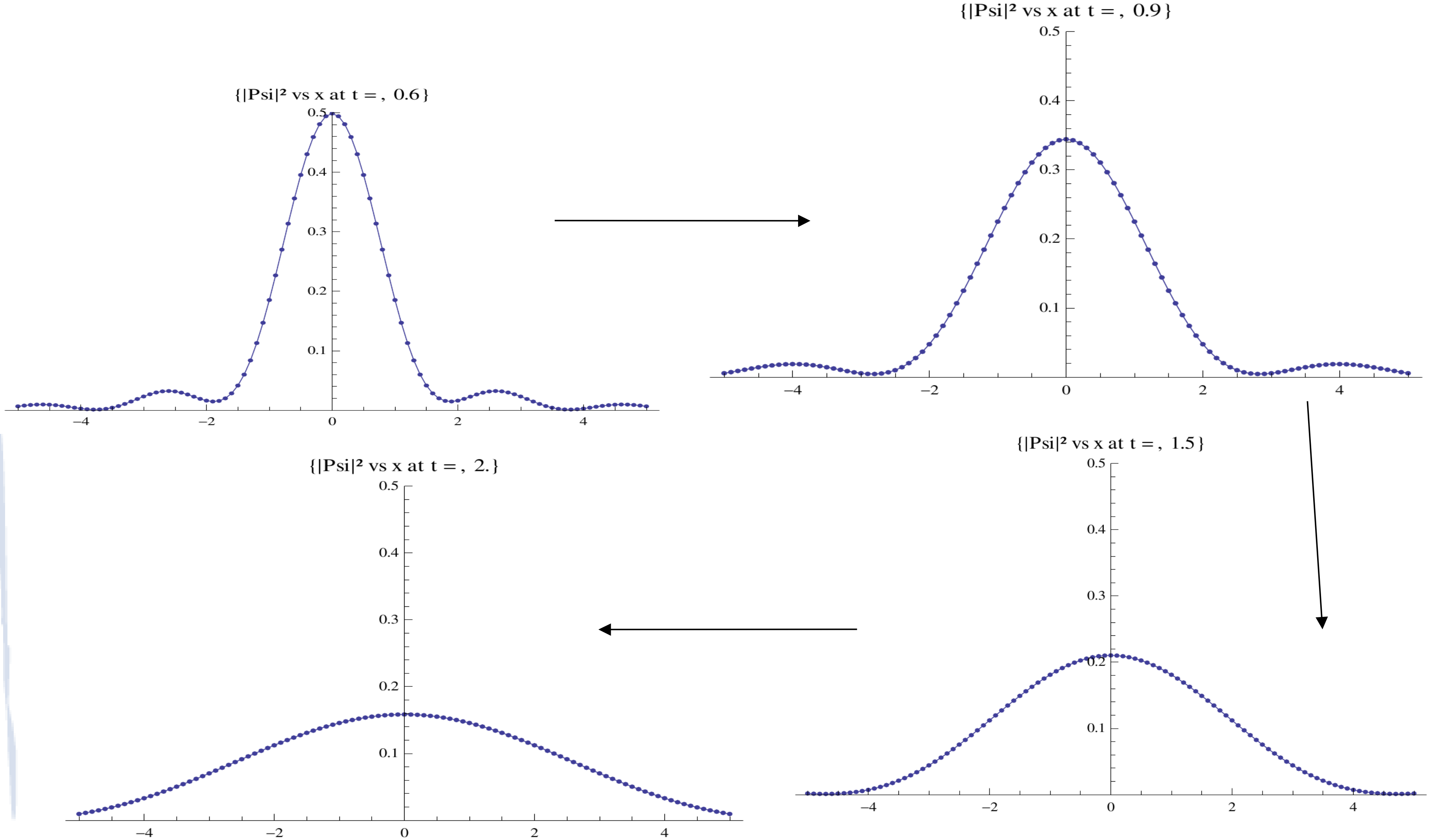
A small spread in momentum space, $\sigma_k \approx \frac{2\pi}{a}$

is associated with a large spread in position space,

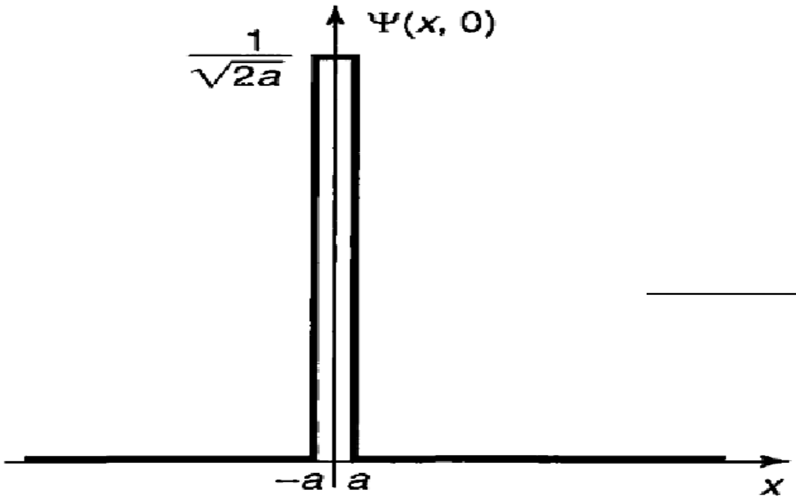
i.e., $\sigma_x \to \infty$.

When time evolution is switched on

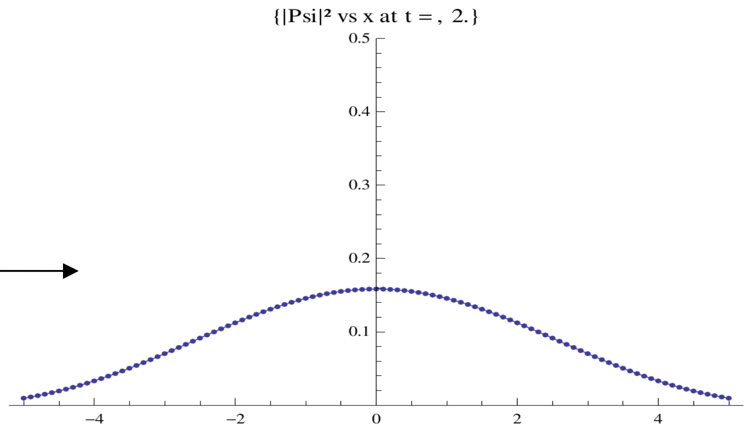
www2.fizik.usm.my/tlyoon/teaching/ZCT205_1314/freeparticle.nb



In position space



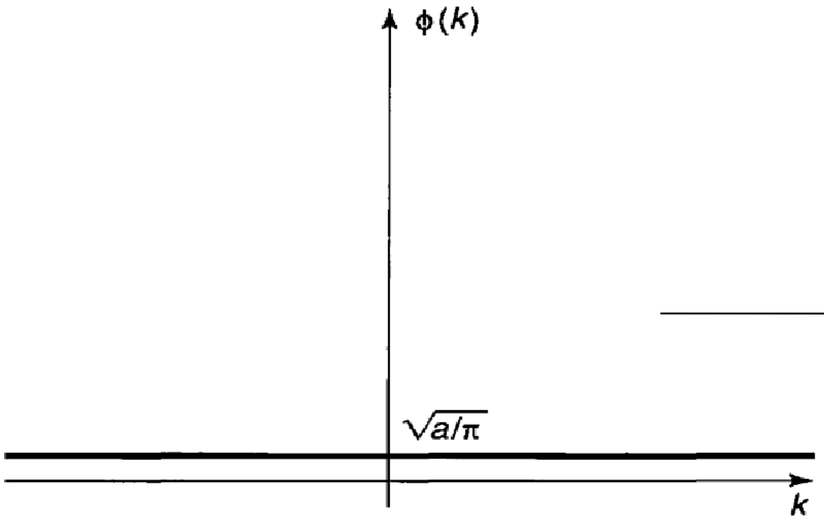
Position well defined

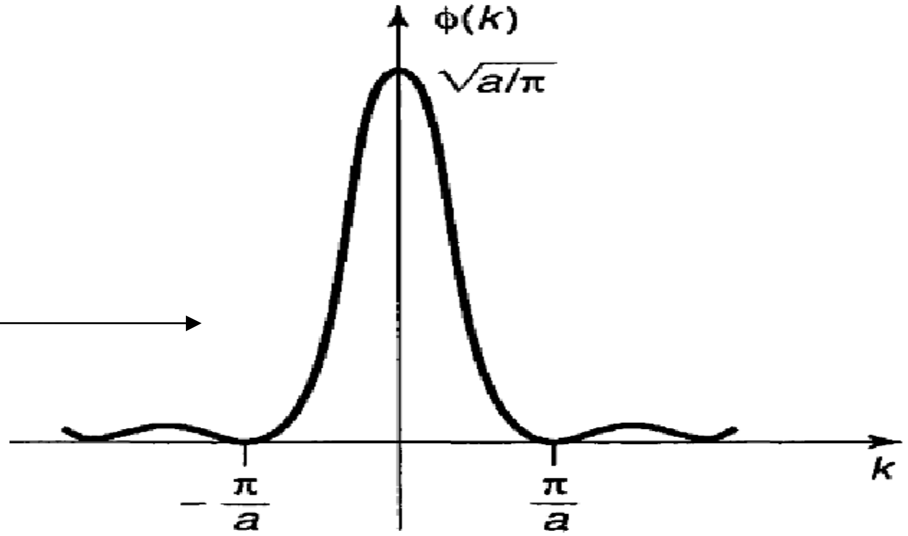


Position not well defined, large spread in *x*

$$\sigma_x(t=0) = 2a \longrightarrow \sigma_x(t \to \infty) \to \infty$$

In momentum space





Wavelength not well defined (large spread in *k*)

Wavelength better defined

$$\sigma_k(t=0) \rightarrow \infty \longrightarrow \sigma_k(t \rightarrow \infty) \rightarrow 2\pi/a$$

the HUP is in action

$$\sigma_x \sigma_k \geq \hbar/2\pi$$

Continuous vs. discrete energy solutions

Two different kind of TISE solutions $\psi(x)$ (stationary states):

1. $\psi_n(x)$, renormalisable, labeled by a discrete index n (QHO, infinite well.)

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-itE_n/\hbar}$$

2. $\psi_k(x)$, non-renormalisable, labeled by continuous variable k, as in the free particle.

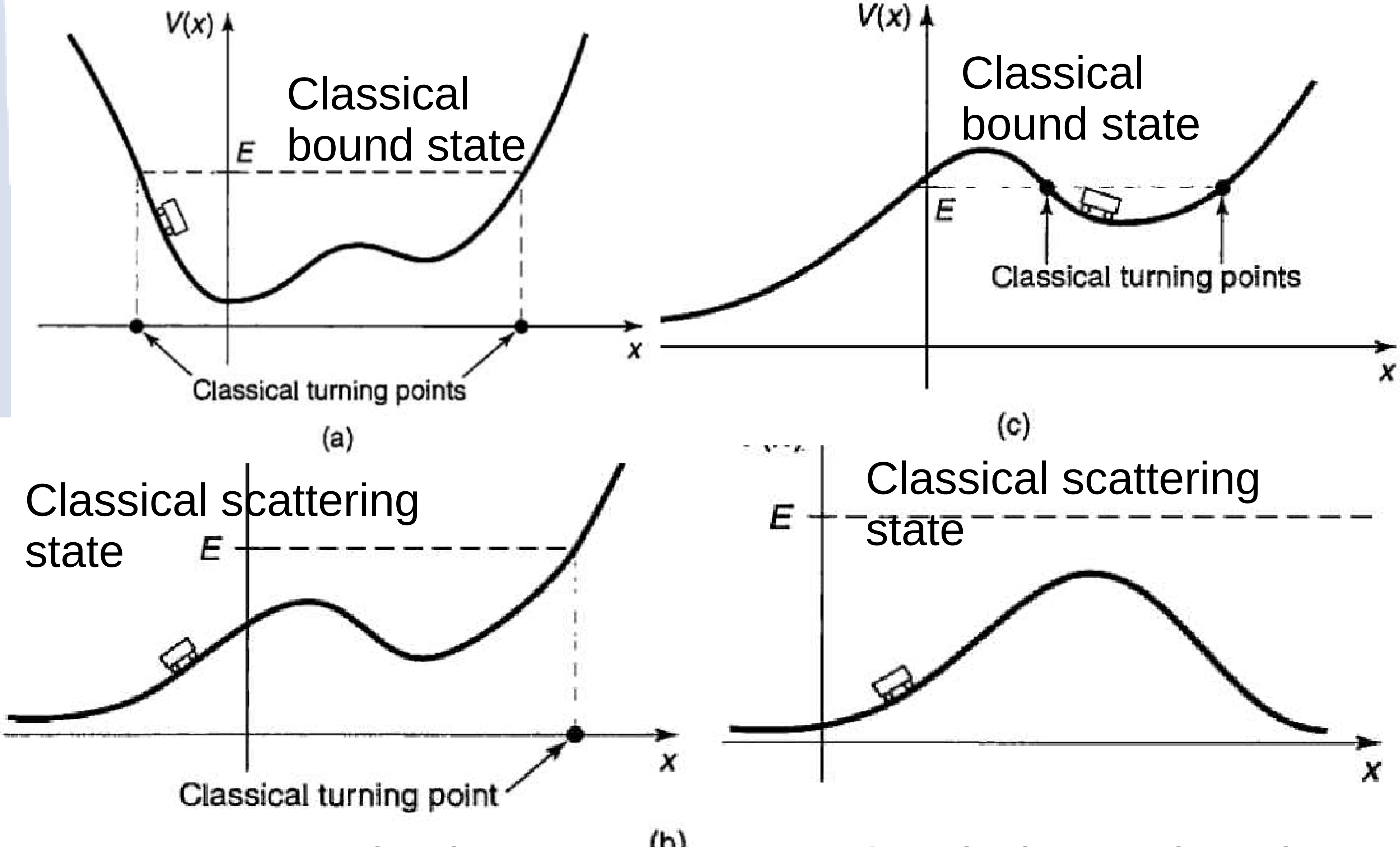
$$\Psi(x,t) = \int_{k=-\infty}^{k=\infty} \phi(k) \psi_k(x) e^{-i\frac{\hbar k^2}{2m}t} dk$$

What's the difference?

- What is the difference between a discretely indexed $\psi_n(x)$ and a continuously indexed $\psi_k(x)$?

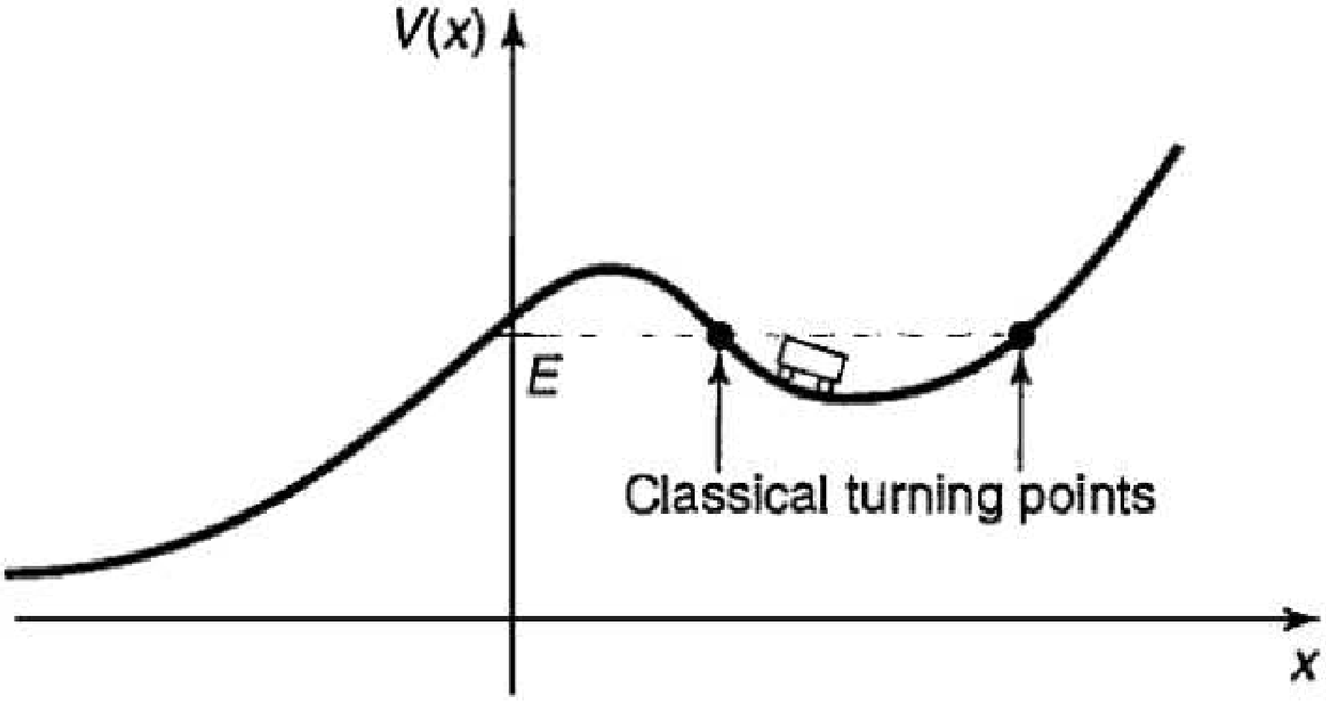
- $\psi_n(x)$: bound states
- $\psi_k(x)$: scattering states

In classical mechanics



In CLASSICAL mechanics, a particle can only exist in a region where *E* > *V*

In quantum mechanics



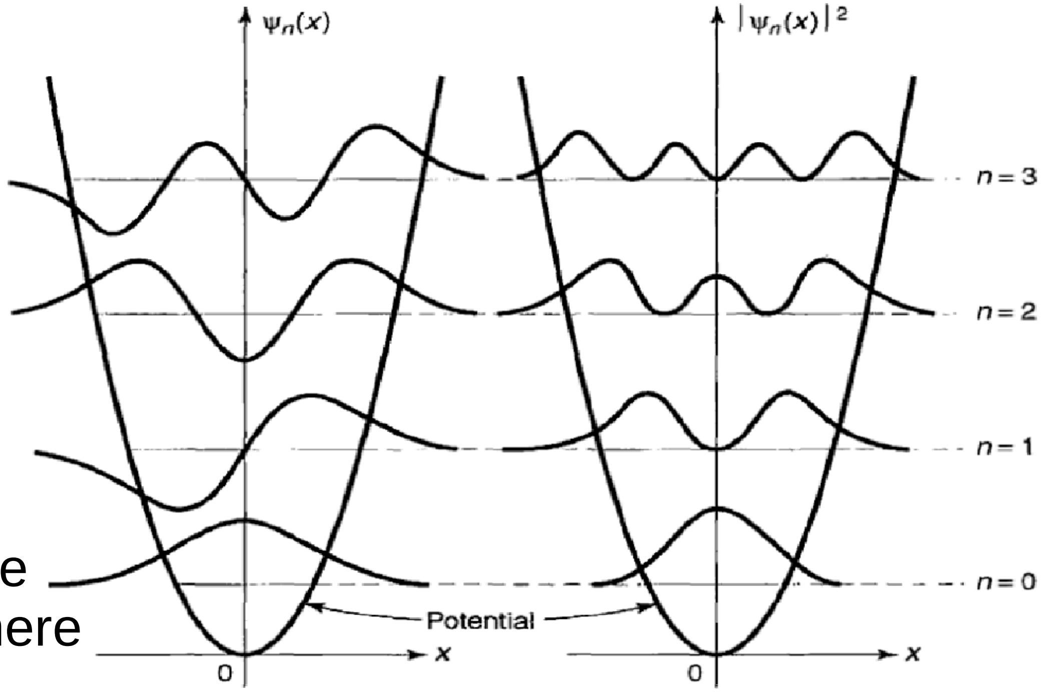
(c)

A quantum scattering state

In QUANTUM mechanics, a particle can exist in a region where *E* > *V*, because |Ψ(*x*,*t*)|2 could be non-zero in such a classically forbidden region.

Features of the QM solutions for the harmonic oscillator I

1. $|\psi_n|^2 \neq 0$ outside the harmonic well



The particle has non zero probability to be found in classically forbidden regions, where $E < V$

Quantum Tunelling effect

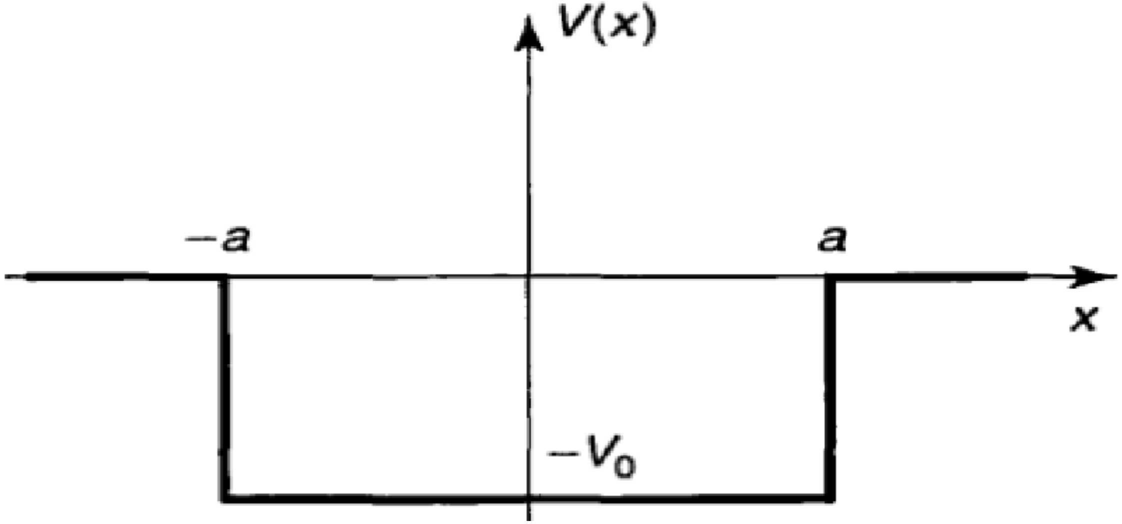
Classifying bound or scattering states in QM

$$\begin{cases} E < [V(-\infty) \text{ and } V(+\infty)] \Rightarrow \ \text{bound state.} \\ E > [V(-\infty) \text{ or } V(+\infty)] \Rightarrow \ \text{scattering state} \end{cases}$$

Use the criteria to determine which state Ψ is in a given potential

QHO is a bound state
Infinite quantum well is a bound state
Free particle is a scattering state

Finite quantum well

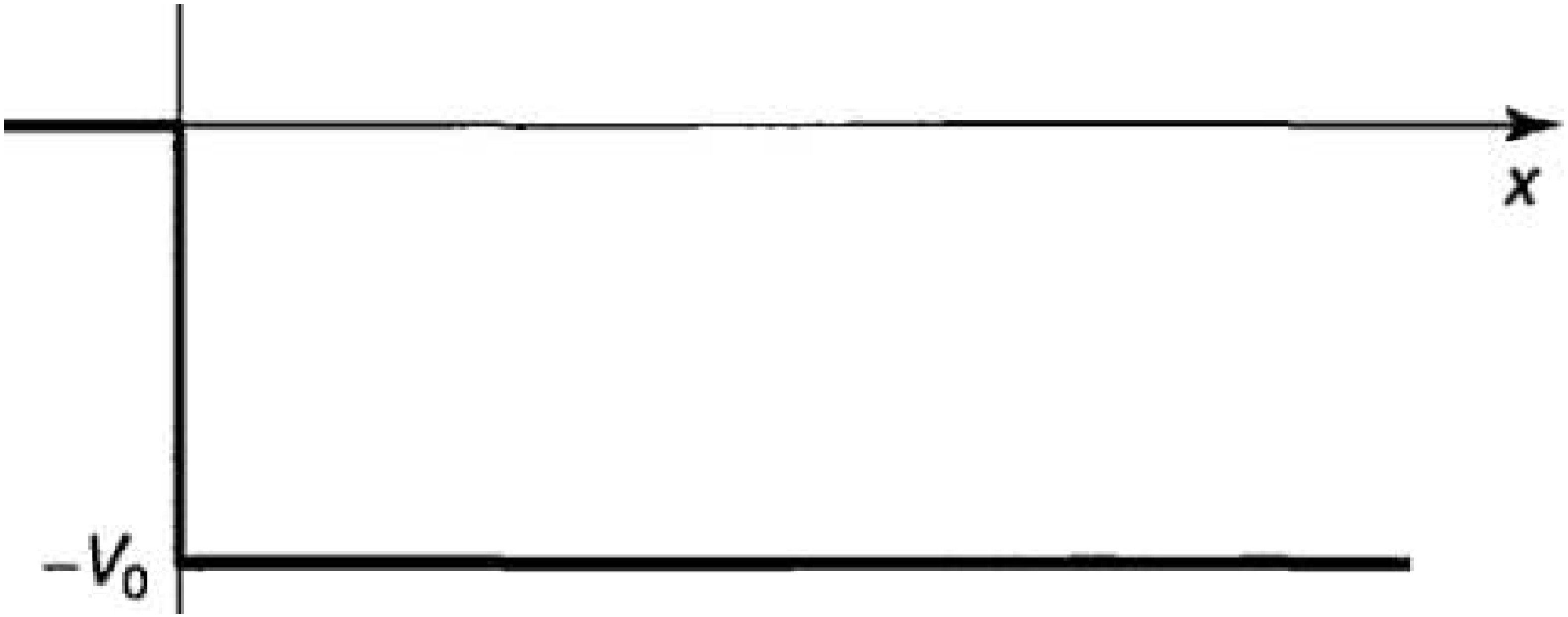


Ψ_n a bound state if $-V_0 < E < 0$

Ψ a scattered state if $E > 0$

What state Ψ is if $E < -V_0$?

Step potential

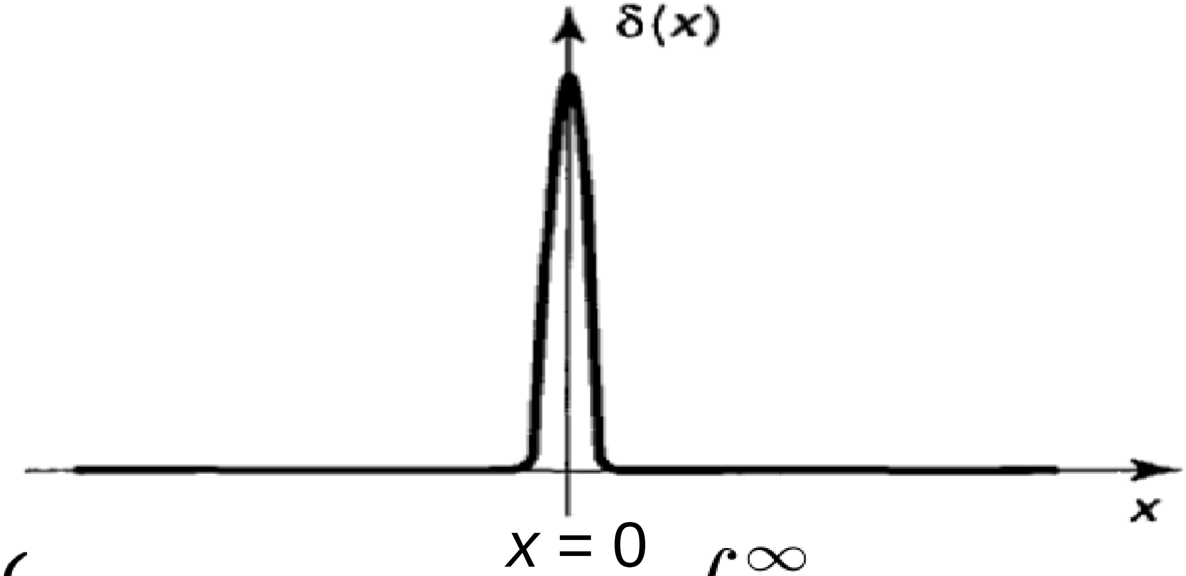


Ψ a scattered state for all allowed *E.*

Can you tell why?

What state Ψ is if $E < -V_0$?

Dirac Delta function, δ(*x*)



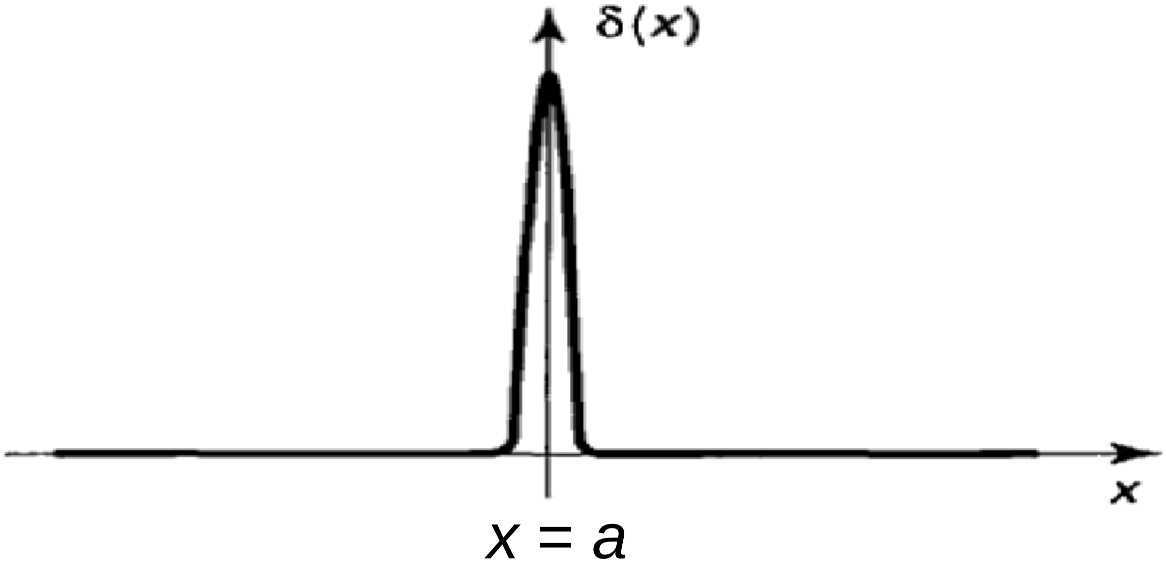
$$\delta(x) = \begin{cases} 0, & \text{if } x \neq 0 \\ \infty, & \text{if } x = 0, \end{cases} \qquad \int_{-\infty}^{\infty} \delta(x)\,dx = 1$$

$$\int_{-\infty}^{\infty} e^{i(p'-p)y}\,dy = 2\pi\delta(p'-p)$$

Exercise: What is the dimension of the Dirac delta function?

Hint: refer to the normalisation equation of it.

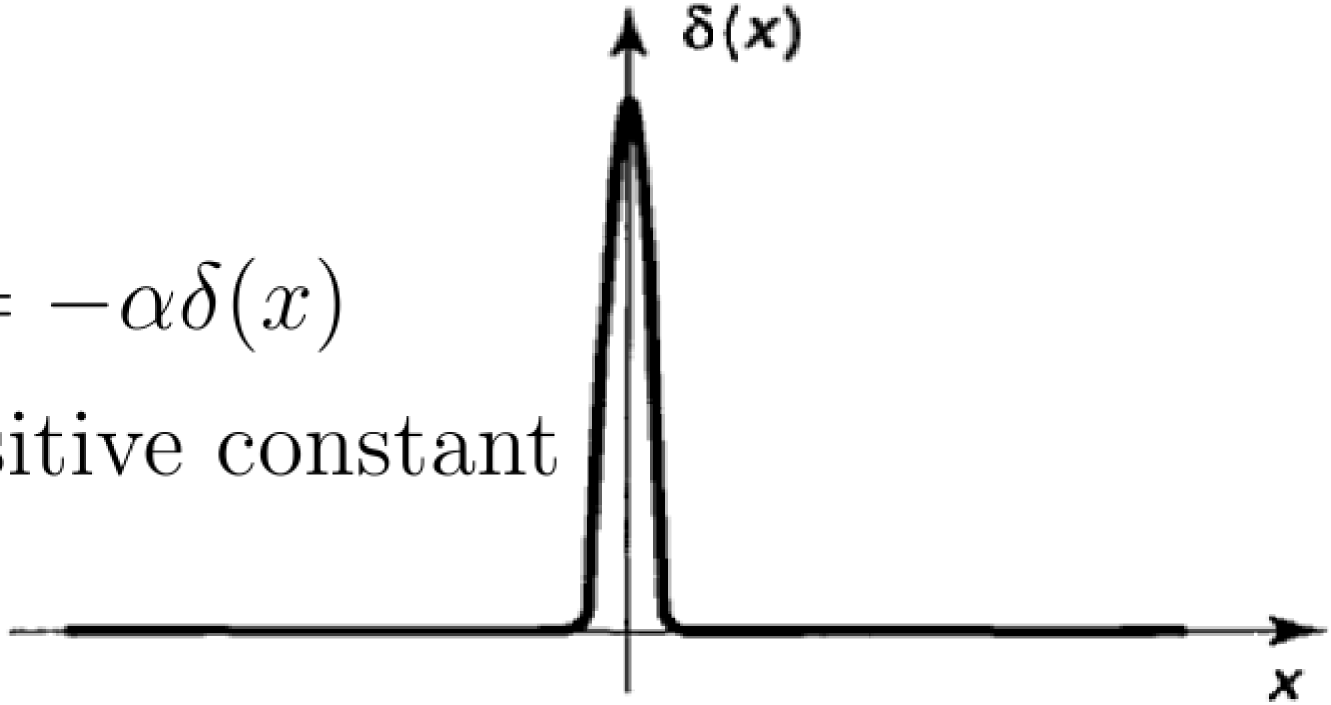
δ(*x*-*a*)



$\delta(x-a)$ is a sharp spike at $x = a$

$$\int_{-\infty}^{\infty} \delta(x-a) f(x) dx = f(a)$$

Dirac delta potential



$$V(x) = -\alpha\delta(x)$$

α a positive constant

Can Ψ in a bound state?

Can Ψ in scattered state?

Bound or scattering state?

- If $E > 0$: scattering state
- If $E < 0$: bound state
- Convince yourself that these are true

Solving SE in Dirac delta potential

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

- The solution depends on whether $E > 0$ or $E < 0$
- We will consider only the case with $E < 0$ in ZCT 205

Solving SE in Dirac delta potential

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

To solve the TISE for three different regions:

- $$-\infty < x < 0$$
  $$0 > x > \infty$$
  $$x = 0$$

$X \neq 0$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \equiv \kappa^2\psi$$

$$\kappa \equiv \sqrt{\frac{-2mE}{\hbar^2}}$$

κ is real and positive (since $E < 0$ by assumption)

The general solution for the left of x=0 region $-\infty < x < 0$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \equiv \kappa^2\psi$$

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}$$

A has to be set to zero so that $\psi(x)$ remains finite as $x \to -\infty$

$$\psi(x) = Be^{\kappa x}, \;\; x < 0$$

The general solution for the right of x=0 region $0 < x < \infty$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \equiv \kappa^2\psi$$

$$\psi(x) = Fe^{-\kappa x}, \; x > 0$$

Solution at *x*=0

- The solution to the TISE must obey the following boundary conditions strictly:

1. ψ is always continuous
2. $\frac{d\psi}{dx}$ is continuous except at points where the potential is infinite

- BD1: solutions left to *x*=0 and right to *x*=0 have to match at *x* = 0:

Solution at *x*=0

1. ψ is always continuous

solutions left to *x*=0 and right to *x*=0 have to matched at *x* = 0:

$$\lim_{x\to 0^-} \psi(x) = \lim_{x\to 0^+} \psi(x)$$

$$\psi(x=0) = F = B$$

$$\psi(x) = \begin{cases} Be^{\kappa x}, x \leq 0 \\ Be^{-\kappa x}, x \geq 0. \end{cases}$$

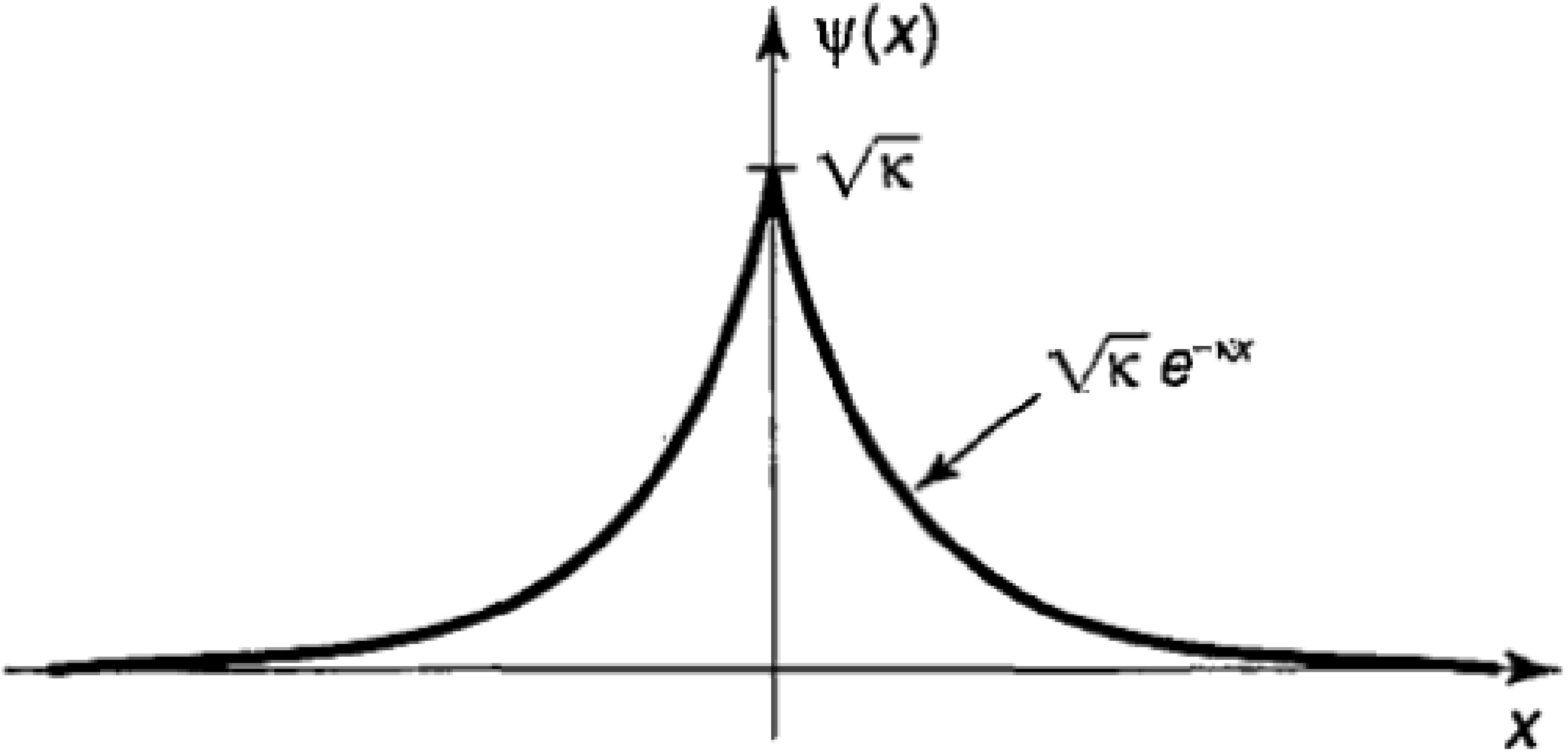
Normalisation

$$\psi(x) = \begin{cases} Be^{\kappa x}, x \leq 0 \\ Be^{-\kappa x}, x \geq 0. \end{cases}$$

Normalisation gives the value of $B = \sqrt{\kappa}$

SHOW THIS

$$\psi(x) = \begin{cases} Be^{\kappa x}, x \le 0 \\ Be^{-\kappa x}, x \ge 0. \end{cases}$$



This is a bound state. Can you see why?

BD II, at the vicinity of *x* = 0, -*ε* ≤ *x* ≤ *ε*

2. $\frac{d\psi}{dx}$ is continuous except at points where the potential is infinite

This BD gives rise to energy quantisation

$$\lim_{\epsilon\longrightarrow 0} -\frac{\hbar^2}{2m}\int_{-\epsilon}^{+\epsilon}\frac{d^2\psi}{dx^2}dx + \lim_{\epsilon\longrightarrow 0}\int_{-\epsilon}^{+\epsilon}V(x)\psi(x)dx$$

$$= \lim_{\epsilon\longrightarrow 0} E\int_{-\epsilon}^{+\epsilon}\psi(x)dx$$

The first term in the LHS

$$\lim_{\epsilon \to 0} \int_{-\epsilon}^{+\epsilon} \frac{d^2\psi}{dx^2} dx$$

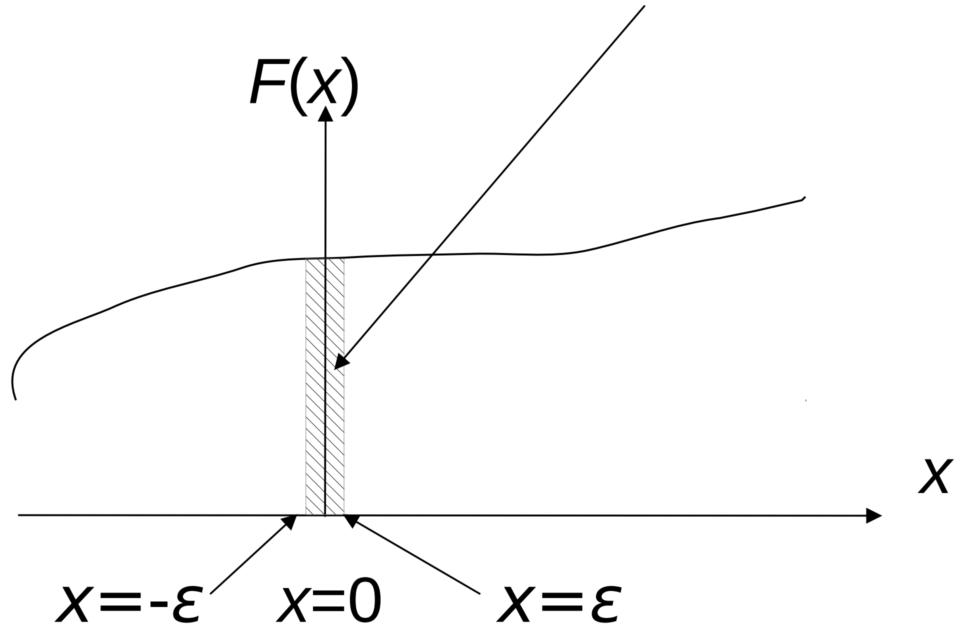
$$= \lim_{\epsilon \to 0} \left(\left. \frac{d\psi(x)}{dx} \right|_{\epsilon} - \left. \frac{d\psi(x)}{dx} \right|_{-\epsilon} \right) \equiv \Delta$$

DO YOU SEE HOW TO GO FROM LINE 1 TO LINE 2?

NEED TO RECALL ZCA 110 !

Show $\displaystyle\int_{-\epsilon}^{+\epsilon} \frac{d^2\psi}{dx^2}dx = \left(\left.\frac{d\psi(x)}{dx}\right|_{\epsilon} - \left.\frac{d\psi(x)}{dx}\right|_{-\epsilon} \right)$

$$\int F(x)\,dx = [F(x)\,dx]_{-\epsilon}^{\epsilon} = (F(\epsilon) - F(-\epsilon))\,dx$$



$$\int F(x)\,dx = \big(F(\epsilon) - F(-\epsilon)\big)\,dx$$

Now, let

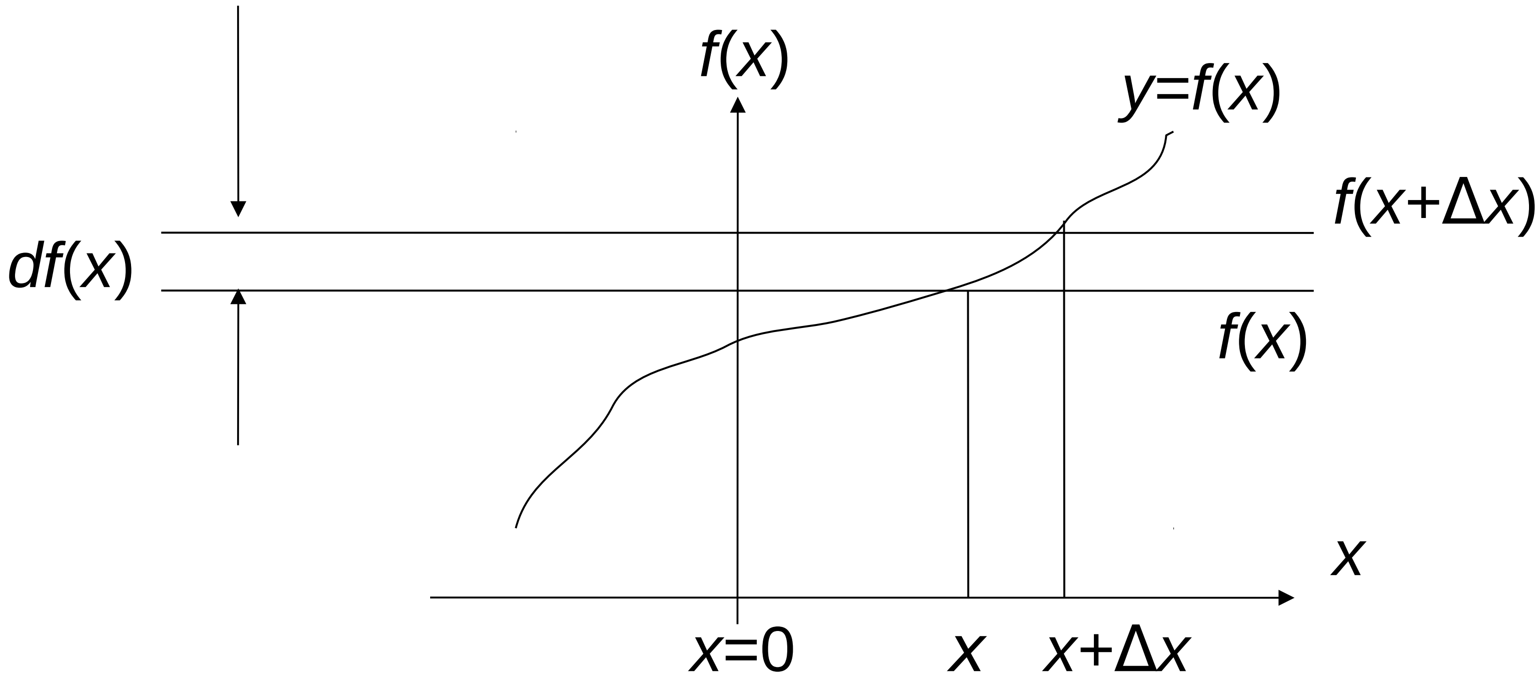
$$F(x) = \frac{df(x)}{dx}$$

$$\int \left(\frac{df(x)}{dx}\right) dx = \left(\frac{df}{dx}(\epsilon) - \frac{df}{dx}(-\epsilon)\right) dx$$

By definition, the differential d*f*(*x*) is

$$df(x) = \frac{df(x)}{dx} \cdot dx$$

Geometrical interpretation of differential, d*f*(x)



$$df(x) = \lim\ f(x+\Delta x) - f(x) = \frac{df(x)}{dx} \cdot dx$$

$$\int \left(\frac{df(x)}{dx} \right) dx = \left(\frac{df}{dx}(\epsilon) - \frac{df}{dx}(-\epsilon) \right) dx = [df(x)]_{-\epsilon}^{\epsilon}$$

$$= f(\epsilon) - f(-\epsilon)$$

Now, let $f(x) = \frac{d\psi(x)}{dx}$

$$\int \frac{d}{dx} \left(\frac{d\psi(x)}{dx} \right) dx = \frac{d\psi}{dx}(\epsilon) - \frac{d\psi}{dx}(-\epsilon)$$

$$\Delta = \left(\left. \frac{d\psi(x)}{dx} \right|_{\epsilon} - \left. \frac{d\psi(x)}{dx} \right|_{-\epsilon} \right)$$

The second term

$$\lim_{\epsilon \longrightarrow 0} \int_{-\epsilon}^{+\epsilon} V(x)\psi(x)dx$$

$$= \lim_{\epsilon \longrightarrow 0} \int_{-\epsilon}^{+\epsilon} -\alpha\delta(x)\psi(x)dx = -\alpha\psi(0)$$

The last term

$$\lim_{\epsilon \longrightarrow 0} \int_{-\epsilon}^{\epsilon} \psi(x)dx = 0$$

Putting everything together

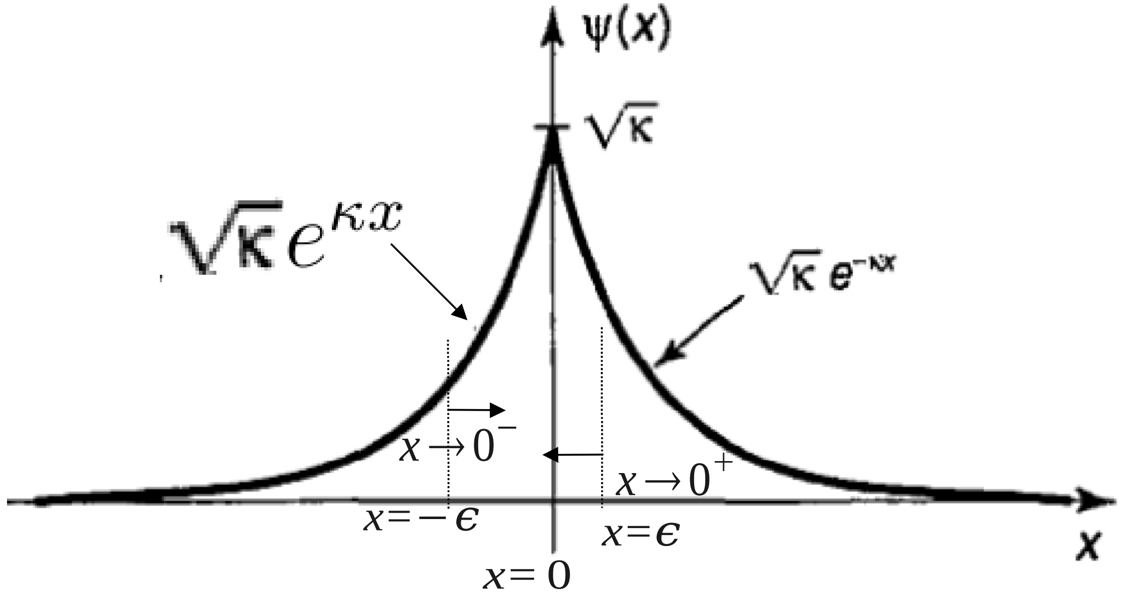
$$\lim_{\epsilon \to 0} -\frac{\hbar^2}{2m}\int_{-\epsilon}^{+\epsilon}\frac{d^2\psi}{dx^2}dx + \lim_{\epsilon \to 0}\int_{-\epsilon}^{+\epsilon}V(x)\psi(x)dx$$

$$= \lim_{\epsilon \to 0} E\int_{-\epsilon}^{+\epsilon}\psi(x)dx$$

$$-\frac{\hbar^2}{2m}\Delta \quad + \quad (-\alpha\psi(0)) = 0$$

$$\frac{\hbar^2}{2m}\Delta = \alpha\sqrt{\kappa}$$

Look closer at Δ



$$\Delta = \left(\frac{d\psi(x)}{dx}\bigg|_{\epsilon} - \frac{d\psi(x)}{dx}\bigg|_{-\epsilon} \right)$$

$$\lim_{x\to 0^+} \frac{d\psi(x)}{dx} - \lim_{x\to 0^-} \frac{d\psi(x)}{dx} = -2\kappa B$$

$$= -2\kappa^{3/2}$$

κB $-\kappa B$

$$B = \sqrt{\kappa}.$$

Quantisation of E shown, finally

$$\frac{\hbar^2}{2m}\Delta = \alpha\sqrt{\kappa}$$

$$\frac{\hbar^2}{2m}\Delta = -\frac{\hbar^2}{2m}\cdot -2\kappa^{3/2} = \alpha\sqrt{\kappa}$$

$$\kappa^2 = \frac{m^2}{\hbar^4}\alpha^2 = -2\frac{mE}{\hbar^2} \qquad \kappa \equiv \sqrt{\frac{-2mE}{\hbar^2}}$$

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

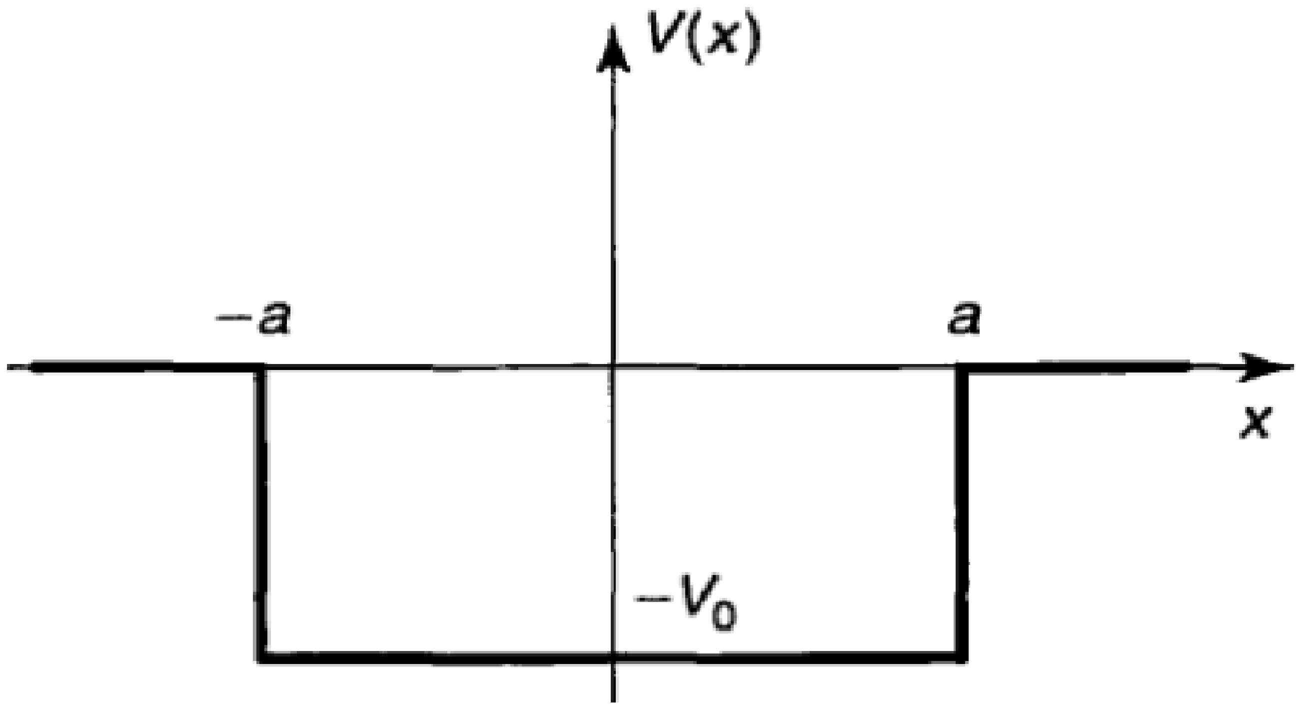
No higher energy states like in the case of QHO or infinite quantum well

Only a single bounded state

The Finite Square Well

$$V(x) = \begin{cases} -V_0, & \text{for } -a \le x \le a, \\ 0, & \text{for } |x| > a, \end{cases}$$

V_0 is a positive constant



Bound state solution, $-V_0 < E < 0$

Three regions: $x \leq -a$, $-a < x < a$, $x \geq a$

$x < -a$

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi$$

$$\kappa = \sqrt{-\frac{2mE}{\hbar^2}}$$

$-a < x < a$

$$\frac{d^2\psi}{dx^2} = -l^2\psi$$

$$l = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

$x \geq a$

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi$$

$$\kappa = \sqrt{-\frac{2mE}{\hbar^2}}$$

Bound state solutions

$x < -a$

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi$$

$$\psi(x) = A\exp(-\kappa x) + B\exp(\kappa x)$$

$A = 0$

$$\psi(x) = B\exp(\kappa x)$$

$-a < x < a$

$$\frac{d^2\psi}{dx^2} = -l^2\psi$$

$x \geq a$

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi$$

$$\psi(x) = F\exp(-\kappa x) - G\exp(\kappa x)$$

$G = 0$

$$\psi(x) = F\exp(-\kappa x)$$

$$\psi(x) = C\sin(lx) + D\cos(lx)$$

Symmetric potential

- Since the potential is even, *V*(*x*) = *V*(-*x*),
- the solutions must be either even or odd

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

To prove this statement, first we have to show that Ψ(-*x*) is a solution to the TISE if *V*(-*x*) = *V*(-*x*) with energy *E*

To show Ψ(-*x*) is a solution to the TISE with energy *E*, the following must be true:

$$-\frac{\hbar}{2\mathrm{m}}\frac{d^2}{dx^2}(ANYTHING)+V(x)(ANYTHING)=E\cdot(ANYTHING);$$

$$where ANYTHING \equiv \psi(-x)$$

$$-\frac{\hbar}{2m}\frac{d^2}{dx^2}(ANYTHING)+V(x)(ANYTHING)=E\cdot(ANYTHING);$$

$$where ANYTHING \equiv \psi(-x)$$

EQ. (1)

- To prove EQ. (1), begin from an TISE

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

$x \to x' = -x$

$$\frac{d}{dx}=\frac{dx'}{dx}\frac{d}{dx'}=(-1)\frac{d}{dx'}$$

$$\frac{d^2}{dx^2}=\ldots=(-1)^2\frac{d^2}{dx'^2}=\frac{d^2}{dx'^2}$$

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

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

Since $V(-x) \to V(x)$

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

EQ. (1) is hence proven, and we says $\Psi(-x)$ is a solution to the TISE with energy E

Both Ψ(*x*) and Ψ(-*x*) are solutions to the TISE with energy *E*, hence so is the linear combination

$$\psi_{\pm}(x) = \psi(x) \pm \psi(-x)$$

$$\psi_{+}(x) = \psi(x) + \psi(-x)$$ is an even solution

$$\psi_{+}(-x) = \psi(-x) + \psi(x) = \psi_{+}(x)$$

$$\psi_{-}(x) = \psi(x) - \psi(-x)$$ is an odd solution

$$\psi_{-}(-x) = \psi(-x) - \psi(x) = -\left(\psi(x) - \psi(-x)\right) = -\psi_{-}(x)$$

Conclusion: If *V*(*x*) = *V*(-*x*), the solutions to the TISE are made up of odd and even ones, $\psi_{+}(x), \psi_{-}(x)$

Assume the solution is of even parity

$$\psi(x) = \begin{cases} Fe^{-\kappa x}, \text{ for } x \leq -a, \\ D\cos(lx), \text{ for } -a < x < +a, \\ \psi(-x), \text{ for } x \geq a \end{cases}$$

$$(1)\ \psi(x) \text{ continuous; } (2)\ \frac{d\psi}{dx} \text{ continuous}$$

at the point $x = a$:

BD (1): $$Fe^{-\kappa a} = D\cos la$$

BD (2): $$-\kappa Fe^{-\kappa a} = -lD\sin la$$

$$Fe^{-\kappa a} = D\cos la$$

$$-\kappa F e^{-\kappa a} = -lD\sin la$$

↓

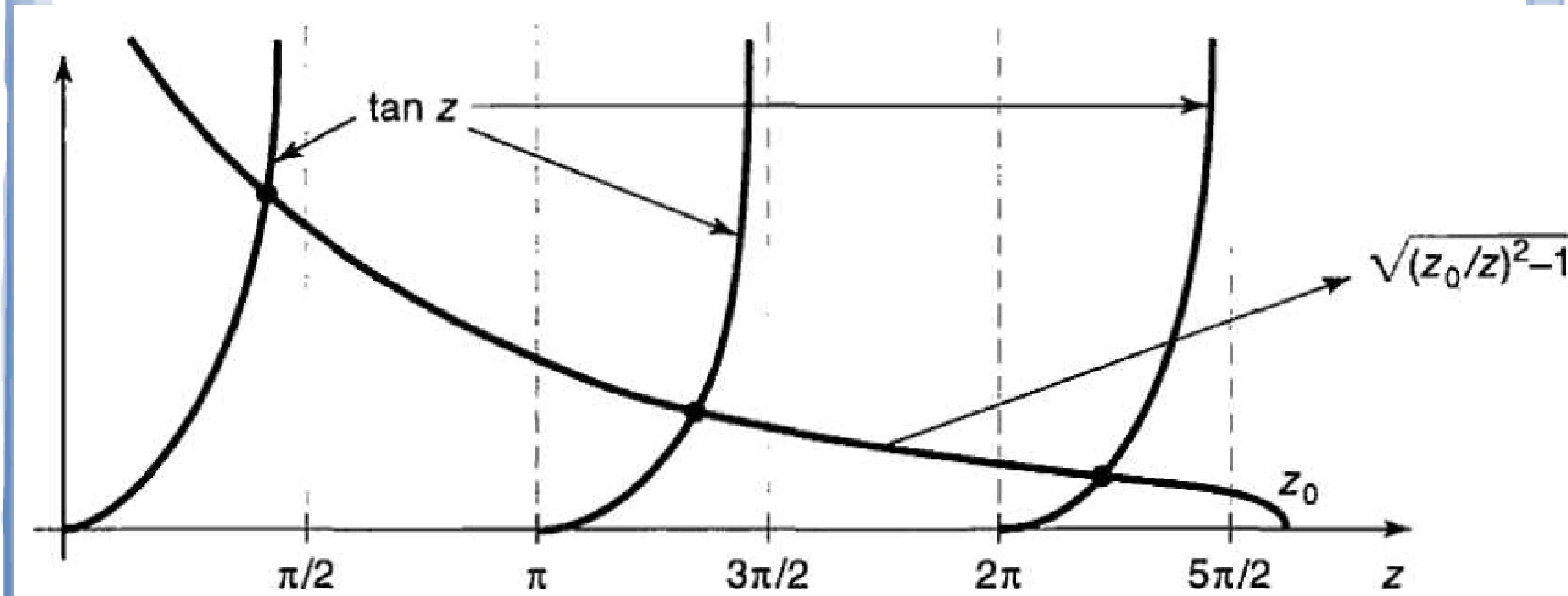
$$\kappa = l\tan(la)$$

Show this ↓ Let $z \equiv la$ and $z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}$

$$\tan z = \sqrt{(z_0/z)^2 - 1}$$

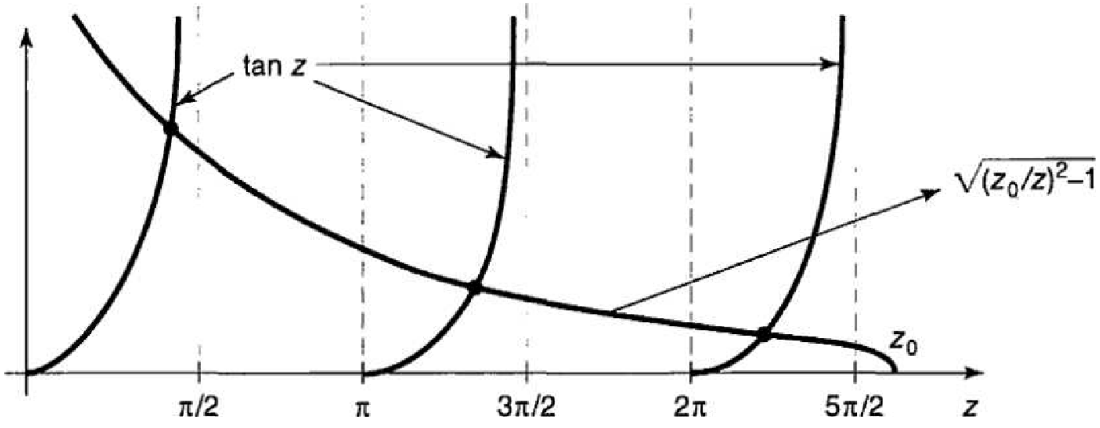
z_0 a dimensionless parameter that describes how deep is the well

Graphical solution to $\tan z = \sqrt{(z_0/z)^2 - 1}$, for $z_0 = 8$ (*even states*)



$$z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}.$$

Quantisation of energy



$$E_n = z_n^2 \frac{\hbar^2}{2ma^2} - V_0$$

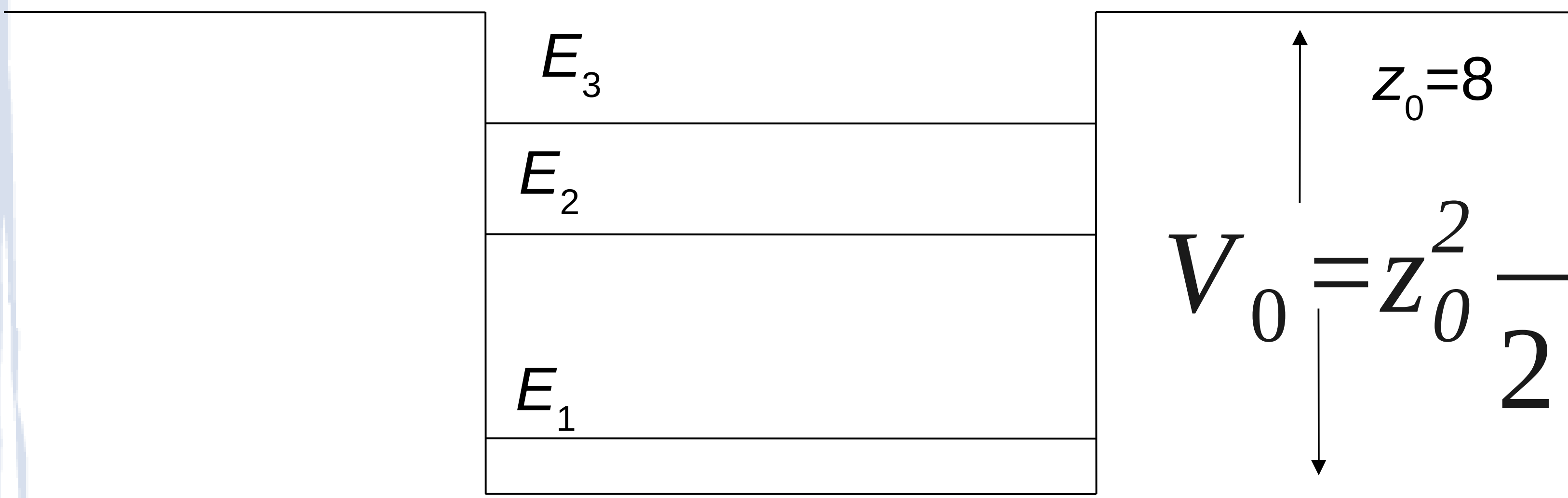
z_n values of z for the intersections in the curves

z_n are to be obtained numerically.

Only three solutions exist. This means only three quantised energies exists for the potential value with z_0=8.

Three allowed energy levels in a well with finite depth z_0=8

$$E_n = \frac{z_n^2 \hbar^2}{2ma^2} - V_0$$

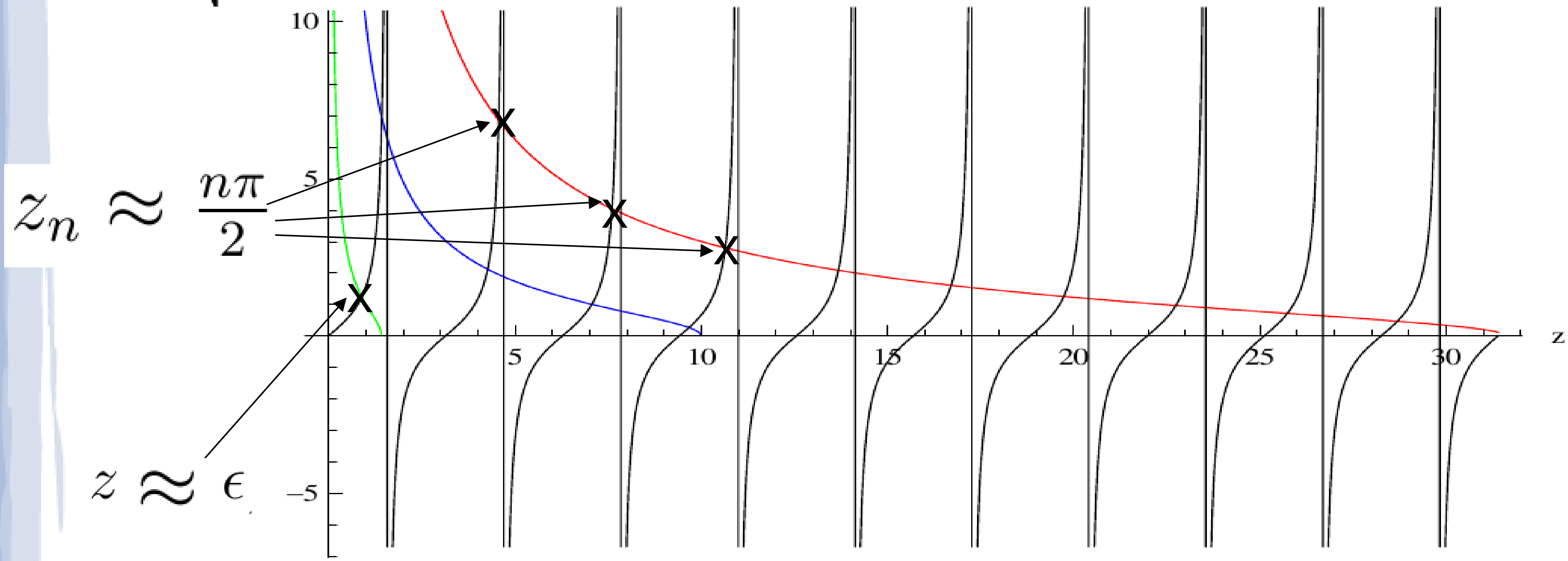


$$V_0 = z_0^2 \frac{\hbar^2}{2ma^2}$$

Solution to $\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$ for V_0=500, 50, 5 unit.

Note that as $V_0 \rightarrow \infty$, there is only one solution left. It is located in the range of $0 < z < \pi/2$. For small z, the roots tend to occur near to the values of nπ/2.

$y = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$; $y = \tan z$ {Red: V_0=500; Blue: V_0=50; Green: V_0=1}



Limiting expressions for E_n, z_n

$$z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}. \qquad \tan z = \sqrt{(z_0/z)^2 - 1}$$

For wide, deep well, $z_0 \gg 1$

$$z_n \approx \frac{n\pi}{2} \qquad E_n \approx \frac{n^2\pi^2\hbar^2}{2m(2a)^2} - V_0.$$

(for low odd *n*)

For shallow, narrow well, z_0 is tiny

$$z \approx \epsilon \qquad E = \frac{\hbar^2\epsilon^2}{2ma^2} - V_0$$

SHOW THIS

Odd parity solution

- We have shown the solutions and allowed energies for even parity case.

$$\psi(x) = \begin{cases} Fe^{-\kappa x}, & \text{for } x \leq -a, \\ D\cos(lx), & \text{for } -a < x < +a, \\ \psi(-x), & \text{for } x \geq a \end{cases}$$

$$E_n = z_n^2 \frac{\hbar^2}{2ma^2} - V_0$$

- But don't forget there is still the odd parity solutions.

$$\psi(x) = \begin{cases} Fe^{-\kappa x}, & \text{for } x \leq -a, \\ C\sin(lx), & \text{for } -a < x < +a, \\ \psi(-x), & \text{for } x \geq a. \end{cases}$$

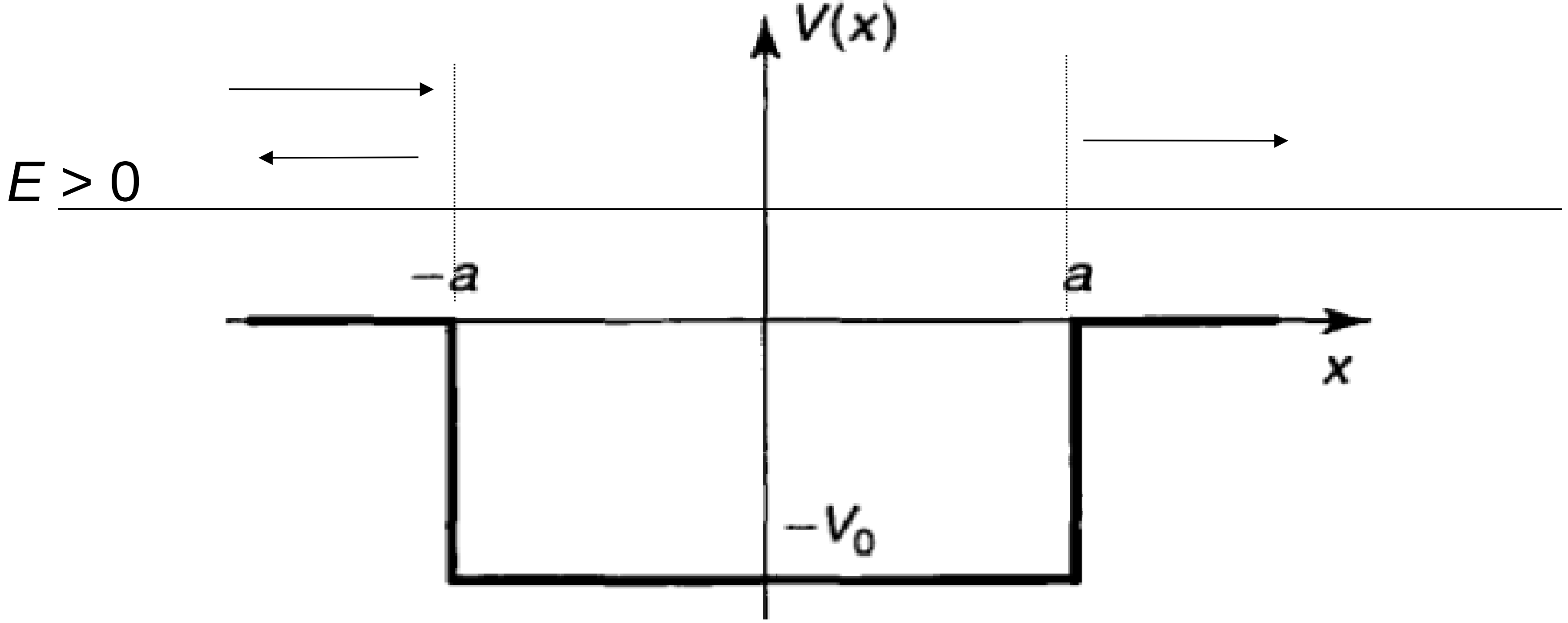
Energy for the odd parity solution

- What is the allowed energies for the odd parity solution, $E_n = ?$
- To do so, simply repeat the steps using $C\sin(lx)$ instead of $D\cos(lx)$

Scattering state solutions

- $E > 0$
- Consider a particle incident upon the potential from the left, and there is no particle incident

or reflected from the right.



$x \leq -a$

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{real and positive}$$

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

For $-a < x < a$

$$\frac{d^2\psi}{dx^2} = -l^2\psi$$

$$l = \sqrt{\frac{2m}{\hbar^2}(E + V_0)}$$ real and positive

$$\psi(x) = C\sin(lx) + D\cos(lx)$$

For $x \geq a$

$$\psi(x) = Fe^{ikx} + Ge^{-ikx}$$

No reflected wave
from the far right

$$\psi(x) = Fe^{ikx}, \quad x \geq a.$$

Compactly

Traveling wave

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

$$\text{For } x \leq -a,$$

standing wave

$$\psi(x) = C\sin(lx) + D\cos(lx)$$

$$\text{For } -a < x < a$$

Traveling wave

$$\psi(x) = Fe^{ikx}, \quad x \geq a.$$

$$\text{For } x \geq a$$

$$l = \sqrt{\frac{2m}{\hbar^2}(E + V_0)}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

Can you tell whether the wavelength in the well is larger or smaller than outside the well?

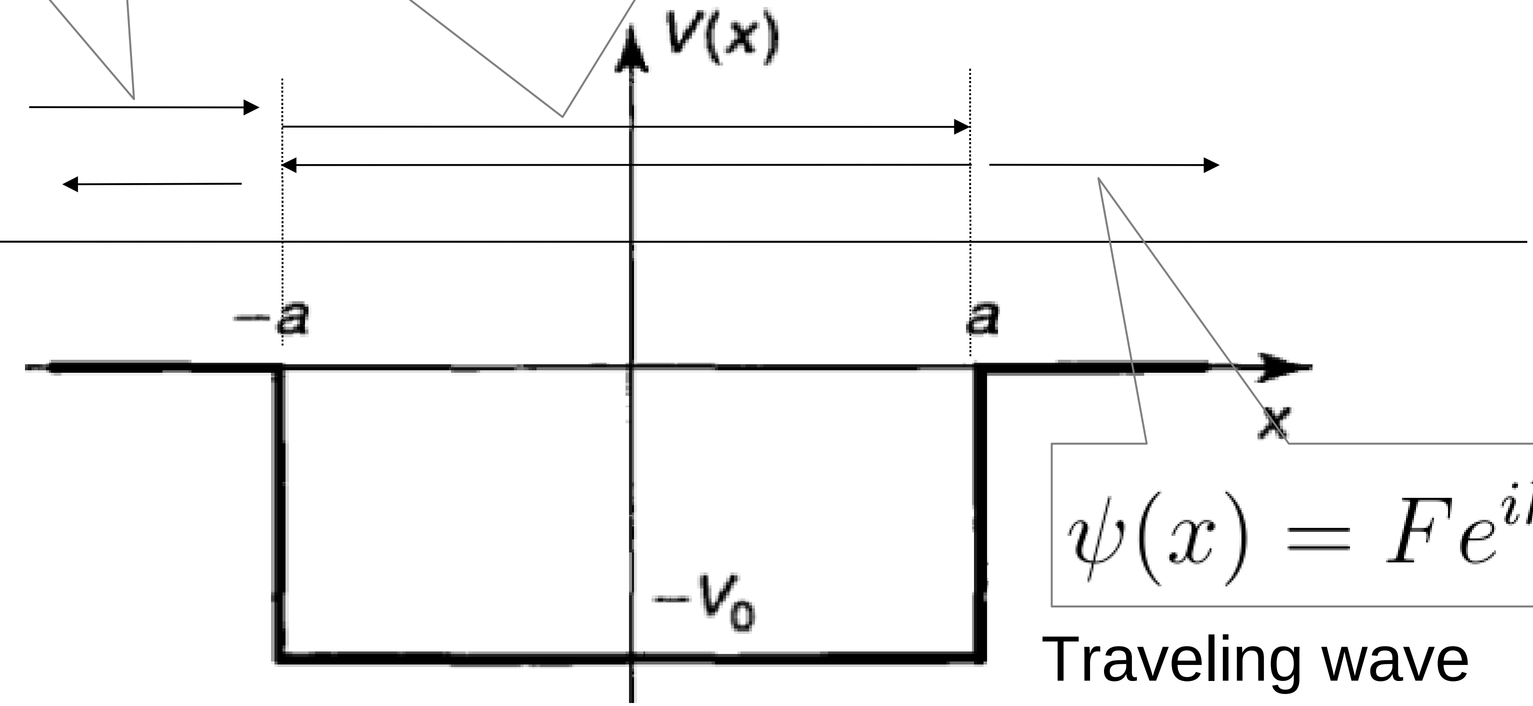
$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

Traveling wave

$$\psi(x) = C\sin(lx) + D\cos(lx)$$

standing wave

$E > 0$



$$\psi(x) = Fe^{ikx}$$

Traveling wave

Imposing BC at x = -a

$$(\text{BC})\ \#1 \text{ at } x = -a$$

$$\psi(x) \text{ continuous at } x = -a$$

$$\begin{aligned} Ae^{-ika} + Be^{ika} &= C\sin(-la) + D\cos(-la) \\ &= -C\sin(la) + D\cos(la) \end{aligned}$$

$$\text{boundary condition (BC) \#2 at } x = -a$$

$$\frac{d\psi}{dx} \text{ continuous at } x = -a$$

$$ik\left[Ae^{-ika} - Be^{ika}\right] = l\left[C\cos(la) + D\sin(la)\right]$$

Imposing BC at *x* = *a*

boundary condition (BC) #1 at $x = a$

$$Fe^{ika} = C\sin(la) + D\cos(la)$$

boundary condition (BC) #2 at $x = a$

$$ikFe^{ika} = l\left[C\cos(la) - D\sin(la)\right]$$

Tidying up

$$Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la)$$

$$ik\left[Ae^{-ika} - Be^{ika}\right] = l\left[C\cos(la) + D\sin(la)\right]$$

$$Fe^{ika} = C\sin(la) + D\cos(la)$$

$$ikFe^{ika} = l\left[C\cos(la) - D\sin(la)\right]$$

- The BC results in a total of 4 algebraic equations with 5 unknowns (*A*, *B*, *C*, *D*, *F*).

A as an independent unknown

express B, C, D, F in terms of A

$$B = i\frac{\sin(2la)}{2kl}(l^2 - k^2)F$$

$$F = \frac{e^{-2ika}A}{\cos(2la) - i\frac{(k^2+l^2)}{2kl}\sin(2la)}$$

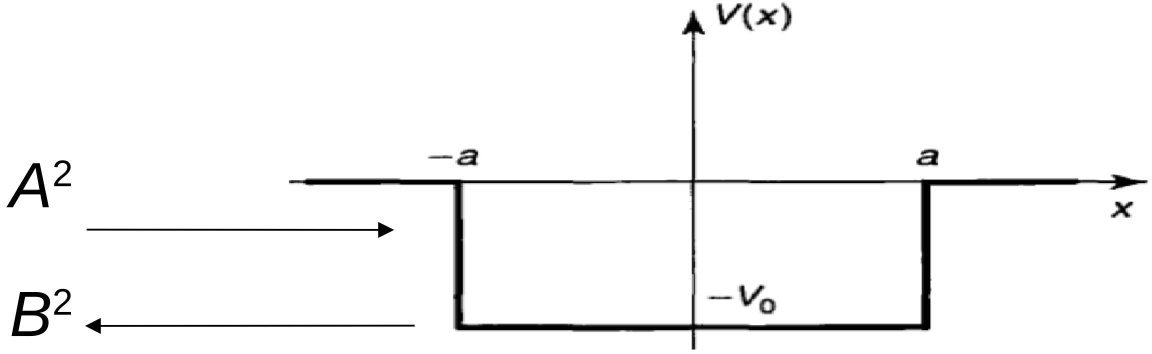
Exercise: Derive this

Reflection coefficient

$$R = \frac{|B|^2}{|A|^2}$$

The fraction of the incoming number (from the left) that will bounce back.

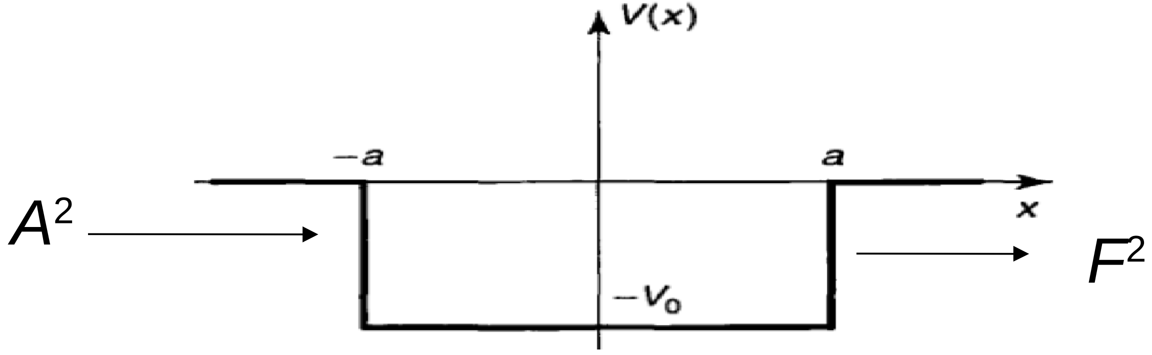
- Of relevance only in region x < −a.



Transmission coefficient

$$T = \frac{\left|F\right|^2}{\left|A\right|^2}$$

How much of the incident number has transmitted through the potential to come out to the other side.



To conserve probability, $T + R = 1$

Transmission coefficient

$$T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)$$

Exercise: Show this.

Hint: use these relations

$$T = \frac{|F|^2}{|A|^2} \qquad R = \frac{|B|^2}{|A|^2} \qquad T + R = 1.$$

$$B = i\frac{\sin(2la)}{2kl}(l^2 - k^2)F$$

$$F = \frac{e^{-2ika}A}{\cos(2la) - i\frac{(k^2+l^2)}{2kl}\sin(2la)}$$

"Transparent potential"

- If $\dfrac{2a}{\hbar}\sqrt{2m(E+V_0)} = n\pi$ so that

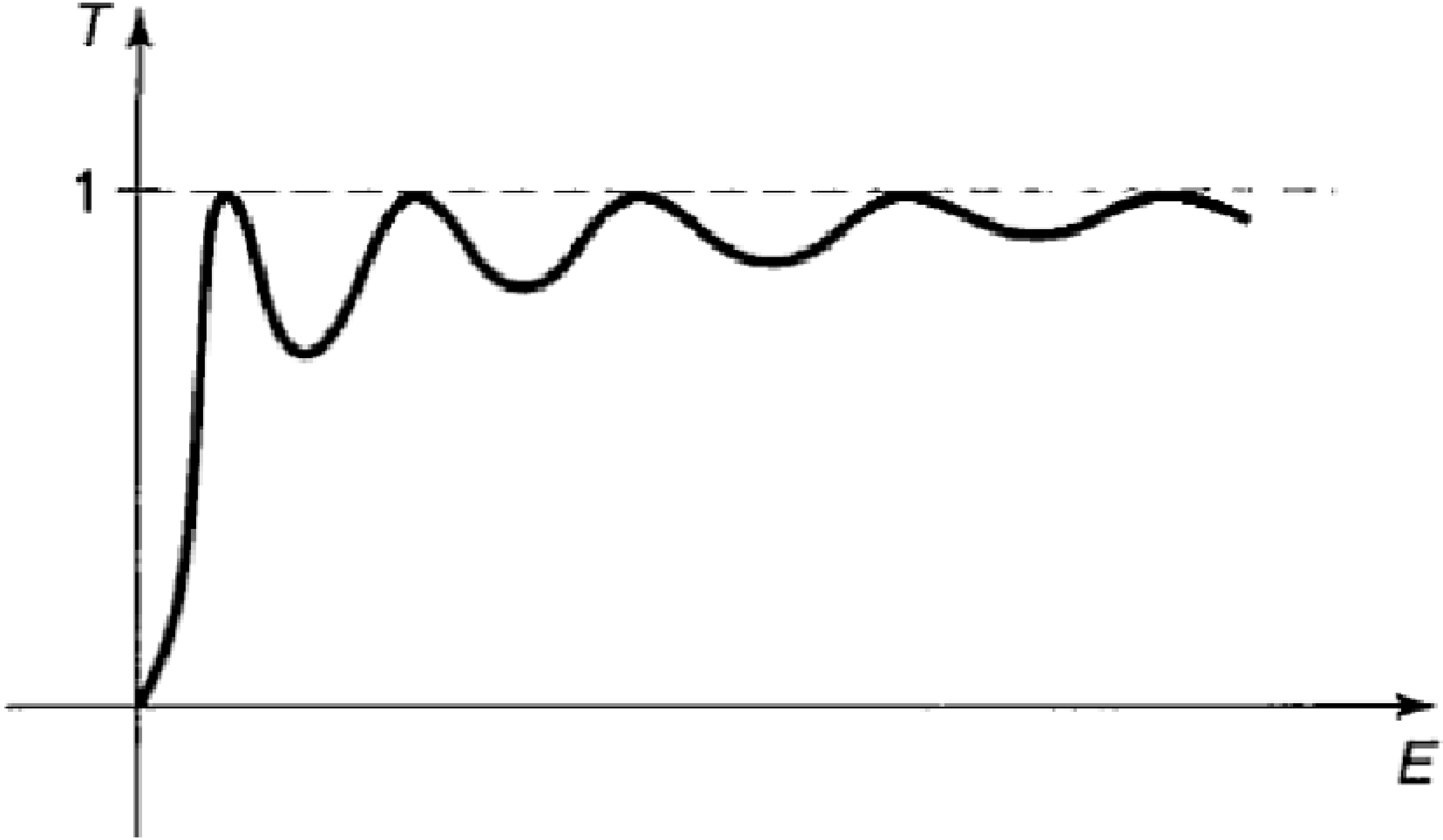
$$T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)$$

- $T = 1$
- No reflection, $R = 0$.

$$E_n = n^2\frac{\pi^2\hbar^2}{2m(2a)^2} - V_0.$$

This is exactly the same set of discrete energies as that of an infinite square well.

Ramsauer-Townsend effect



Tutorial 2.2

Q1

Solution to the Dirac potential is given by

$$\psi(x) = \begin{cases} Be^{\kappa x}, x \leq 0 \\ Be^{-\kappa x}, x \geq 0, \end{cases}$$

Normalisation gives the value of $B = \sqrt{\kappa}$

SHOW THIS

Q2

$$\kappa = l\tan(la)$$

Show this ↓ Let $z \equiv la$ and $z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}$

$$\tan z = \sqrt{(z_0/z)^2 - 1}$$

Q3

Given the four algebraic equations

$$Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la)$$

$$ik\left[Ae^{-ika} - Be^{ika}\right] = l\left[C\cos(la) + D\sin(la)\right]$$

$$Fe^{ika} = C\sin(la) + D\cos(la)$$

$$ikFe^{ika} = l\left[C\cos(la) - D\sin(la)\right]$$

Show

$$B = i\frac{\sin(2la)}{2kl}(l^2 - k^2)F$$

$$F = \frac{e^{-2ika}A}{\cos(2la) - i\frac{(k^2+l^2)}{2kl}\sin(2la)}$$

Q4

Given

$$R = \frac{|B|^2}{|A|^2} \qquad T = \frac{|F|^2}{|A|^2} \qquad T + R = 1$$

$$B = i\frac{\sin(2la)}{2kl}(l^2 - k^2)F$$

$$F = \frac{e^{-2ika}A}{\cos(2la) - i\frac{(k^2+l^2)}{2kl}\sin(2la)}$$

Show

$$T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)$$

TUTORIAL QUESTION

∗Problem 2.34 Consider the "step" potential:

$$V(x) = \begin{cases} 0, & \text{if } x \le 0, \\ V_0, & \text{if } x > 0. \end{cases}$$

(a) Calculate the reflection coefficient, for the case $E < V_0$, and comment on the answer.

(b) Calculate the reflection coefficient for the case $E > V_0$.

(c) For a potential such as this, which does not go back to zero to the right of the barrier, the transmission coefficient is *not* simply $|F|^2/|A|^2$ (with A the

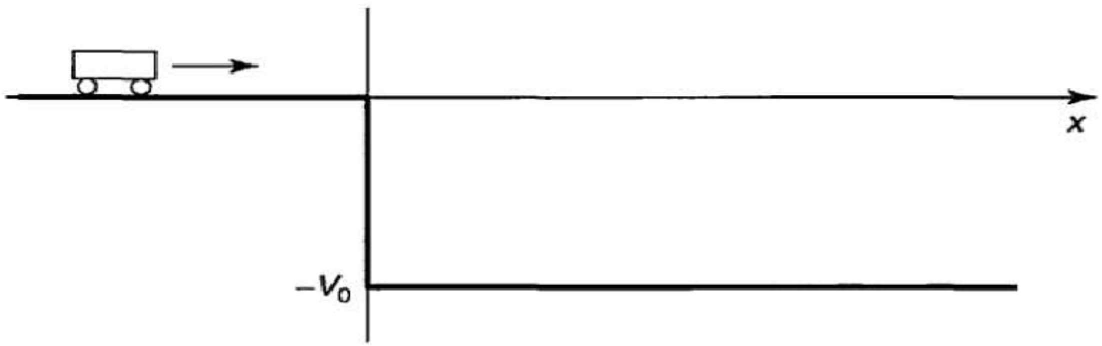


FIGURE 2.20: Scattering from a "cliff" (Problem 2.35).

incident amplitude and F the transmitted amplitude), because the transmitted wave travels at a different *speed*. Show that

$$T = \sqrt{\frac{E - V_0}{E}} \frac{|F|^2}{|A|^2}, \qquad [2.172]$$

for $E > V_0$. *Hint:* You can figure it out using Equation 2.98, or—more elegantly, but less informatively—from the probability current (Problem 2.19). What is T, for $E < V_0$?

(d) For $E > V_0$, calculate the transmission coefficient for the step potential, and check that $T + R = 1$.