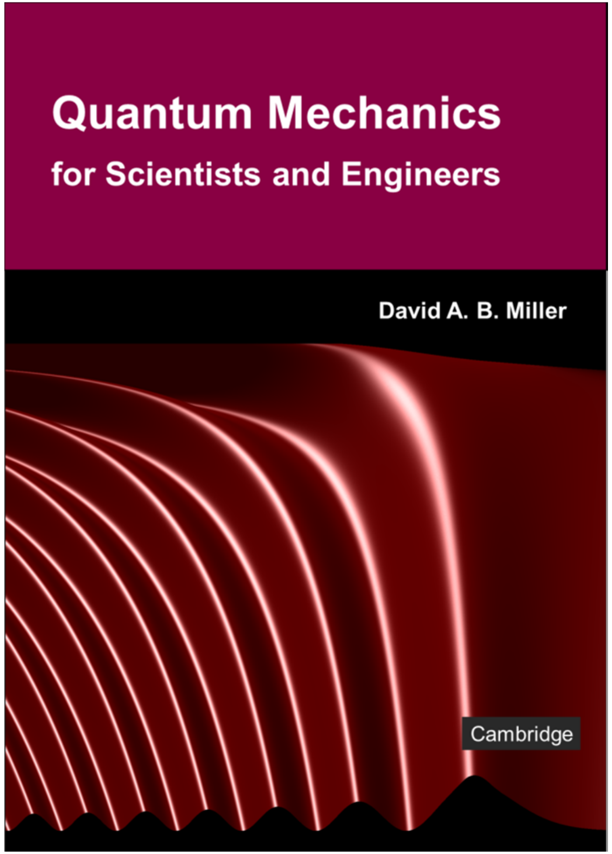
3.1 Particles and barriers

Slides: Video 3.1.1 Sets of functions

Text reference: Quantum Mechanics for Scientists and Engineers

Section 2.7 (“Completeness of sets – Fourier series”)

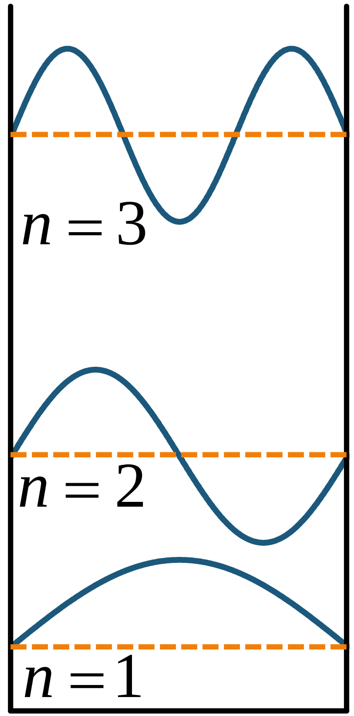


Particles and barriers

Sets of functions

Quantum mechanics for scientists and engineers

David Miller


$n=3$
$n=2$
$n=1$

Fourier series

Suppose we are interested in the behavior of some function

such as a loudspeaker cone displacement

from time 0 to time t_o

presuming it starts and ends at 0 displacement

An appropriate Fourier series would be

$$f(t) = \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi t}{t_o}\right)$$

where a_n are the amplitudes of these frequency components

Fourier series

Similarly, if we had any function $f(z)$

over the distance L_z from $z = 0$ to $z = L_z$

and that started and ended at 0 height

we could similarly write it as

$$f(z) = \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi z}{L_z}\right)$$

for some set of numbers or "amplitudes" a_n

which we would have to work out

Fourier series and eigenfunctions

We remember our set of normalized eigenfunctions

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

With a minor change

we could use these instead of the sines

$$f(z) = \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi z}{L_z}\right) = \sum_{n=1}^{\infty} b_n \psi_n(z)$$

where $b_n = \sqrt{L_z / 2}\; a_n$

Expansion in eigenfunctions

Now we can restate the same mathematics in new words

$$f(z) = \sum_{n=1}^{\infty} b_n \psi_n(z)$$

is now the

expansion of $f(z)$ in the complete set of (normalized) eigenfunctions $\psi_n(z)$

Note that, though we have illustrated this by connecting to Fourier series

this will work for other sets of eigenfunctions also

Basis sets of functions

A set of functions such as the $\psi_n(z)$

that can be used in this way to represent a function such as $f(z)$

is referred to as

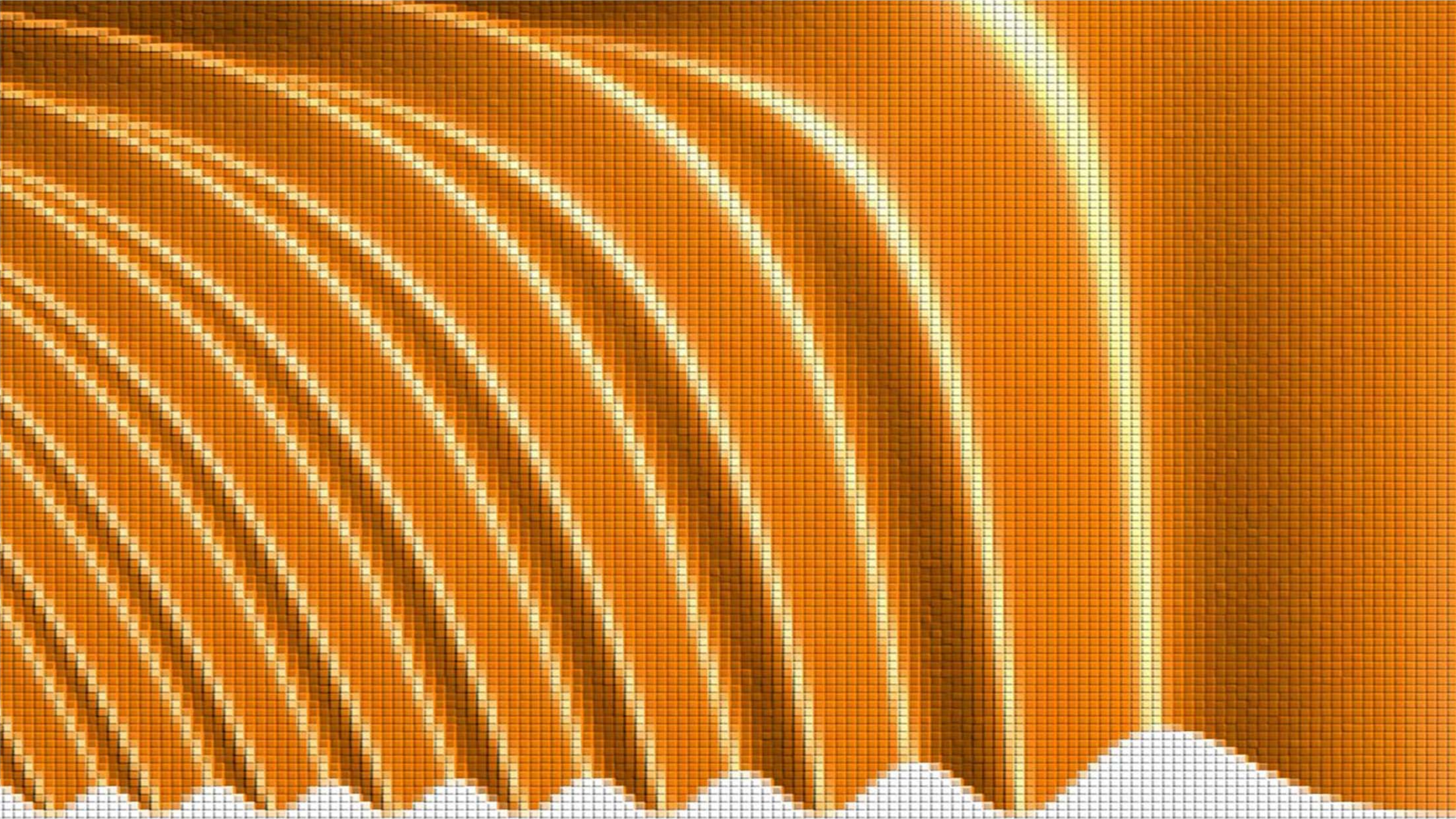
a "basis set of functions"

or, more simply,

a "basis"

The set of "expansion coefficients" (amplitudes) b_n is then

the "representation" of $f(z)$ in the basis $\psi_n(z)$

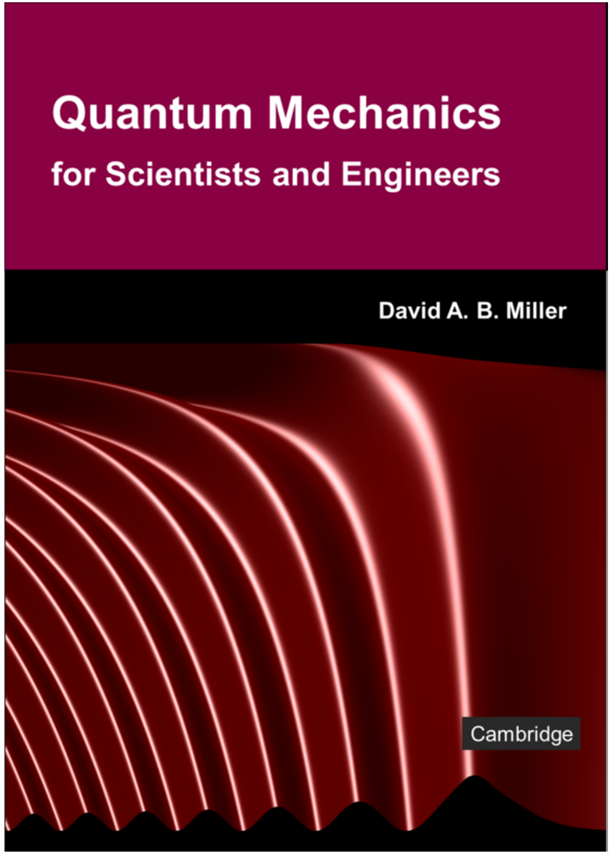


3.1 Particles and barriers

Slides: Video 3.1.3 Orthogonality of functions

Text reference: Quantum Mechanics for Scientists and Engineers

Section 2.7 (“Orthogonality of eigenfunctions” and “Expansion coefficients”)



Particles and barriers

Orthogonality of functions

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Orthogonal functions

In addition to being a complete set

the eigenfunctions

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

are also "orthogonal" to one another

Two non-zero functions $g(z)$ and $h(z)$

defined from 0 to L_z

are said to be orthogonal if

$$\int_0^{L_z} g^*(z)h(z)dz = 0$$

Orthogonal functions

It is easy to show mathematically that the functions

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

are orthogonal to one another

because, as we could prove

$$\int_0^{L_z} \psi_n^*(z)\psi_m(z)\,dz = 0 \text{ for } n \neq m$$

This mutual orthogonality is another common property of the eigenfunctions we will find

Orthogonality and parity

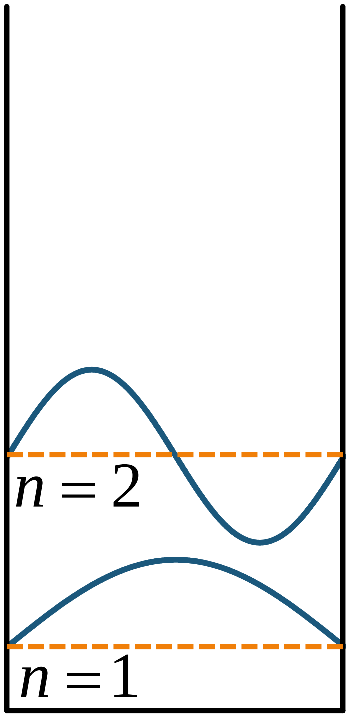
Functions with opposite parity

- such as the first two particle-in-a box eigenfunctions

are always orthogonal

Whatever contribution we get to the integral from the left side

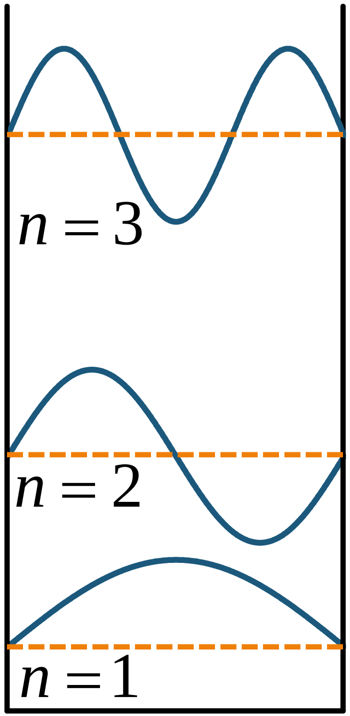
- we get the opposite from the right
  - so they cancel out
    - we do not even need to work out the integral



Orthogonality and parity

With sine functions like this
- even those sine functions of the same parity are also orthogonal
  - which is less obvious but also true

For example
- the n=3 eigenfunction
  - is orthogonal to
- the n=1 eigenfunction



Orthonormality

We can introduce the "Kronecker delta"

For our normalized eigenfunctions

we can therefore write the orthogonality and the normalization as one condition

A set of functions that is both normalized and mutually orthogonal is "orthonormal"

Kronecker delta

$\delta_{nm} = 0$ for $n \neq m$

$\delta_{nn} = 1$

$$\int_0^{L_z} \psi_n^*(z)\psi_m(z)\,dz = \delta_{nm}$$

Orthonormality condition

Expansion coefficients

Suppose we want to write the function $f(x)$

in terms of a complete set of orthonormal functions $\psi_n(x)$

i.e., we want to write

$$f(x) = \sum_n c_n \psi_n(x)$$

To find the "expansion coefficients" c_n

premultiply by $\psi_m^*(x)$

and integrate

Expansion coefficients

Premultiplying by $\psi_m^*(x)$ and integrating gives

$$\int \psi_m^*(x) f(x) dx = \int \psi_m^*(x) \left[\sum_n c_n \psi_n(x) \right] dx$$

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

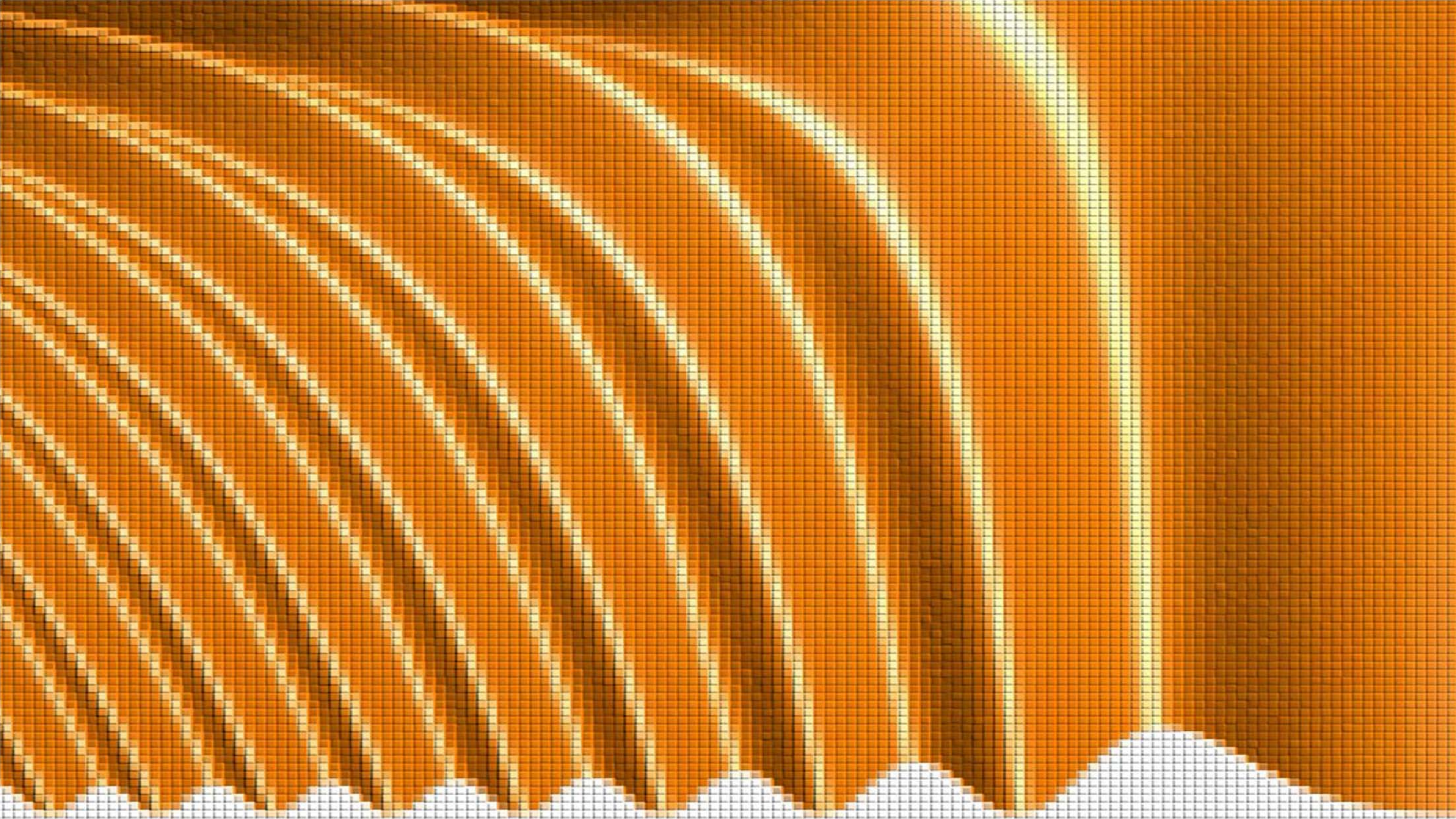
$$= c_m$$

If we have an orthonormal complete set

we can now expand any function in it

Generally an integral like $\int \psi_m^*(x) f(x) dx$

is also called an "overlap integral"

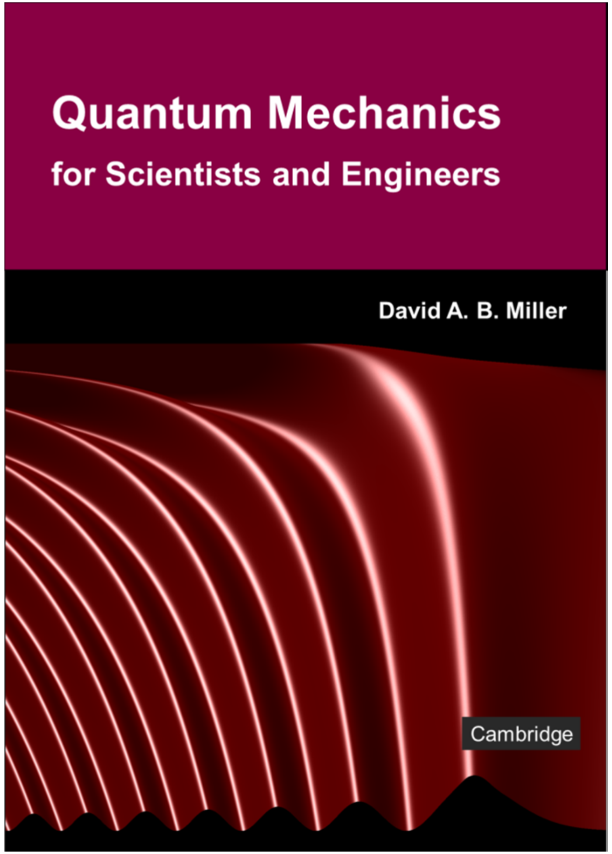


3.1 Particles and barriers

Slides: Video 3.1.5 Barriers and boundary conditions

Text reference: Quantum Mechanics for Scientists and Engineers

Section 2.8



Particles and barriers

Barriers and boundary conditions

Quantum mechanics for scientists and engineers

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Boundary conditions

For our Schrödinger equation

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

if we presume that E, V and ψ are finite

then $d^2\psi/dz^2$ must be finite also, so

$d\psi/dz$ must be continuous

If there was a jump in $d\psi/dz$

then $d^2\psi/dz^2$ would be infinite at that point

Boundary conditions

Also

$d\psi / dz$ must be finite

otherwise $d^2\psi / dz^2$ could be infinite

being the limit of a difference

involving infinite quantities

For $d\psi / dz$ to be finite

ψ must be continuous

Boundary conditions

Now that we have these two boundary conditions

ψ must be continuous

$d\psi / dz$ must be continuous

we can proceed to solve problems with finite "heights" of boundaries

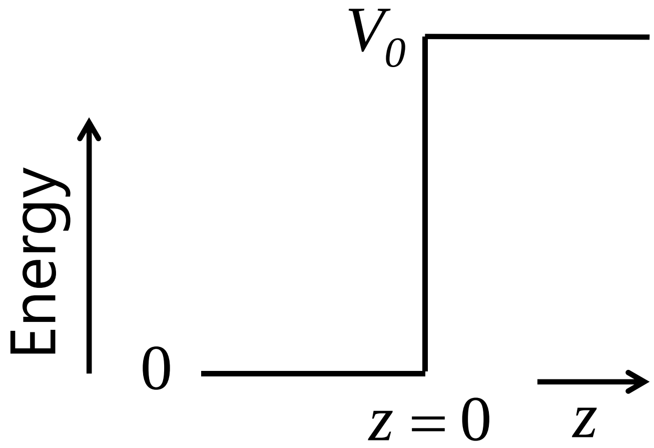
Infinitely thick barrier

Suppose we have a barrier of height V_o

- with potential 0 to the left of the barrier

A quantum mechanical wave is incident from the left

- The energy E of this wave is positive
  - i.e., $E > 0$



Infinitely thick barrier

We allow for reflection from the barrier

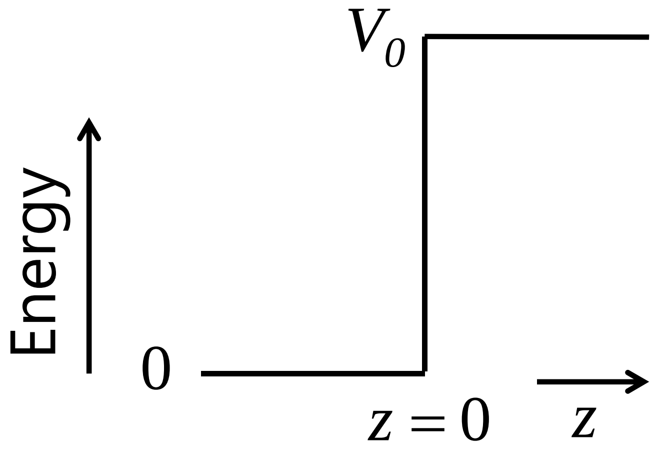
into the region on the left

Using the general solution on the left

with complex exponential waves

$$\psi_{left}(z) = C\exp(ikz) + D\exp(-ikz)$$

where, as before $k = \sqrt{2mE/\hbar^2}$



$C\exp(ikz)$ is the incident wave, going right

$D\exp(-ikz)$ is the reflected wave, going left

Infinitely thick barrier

Presume that $E < V_o$

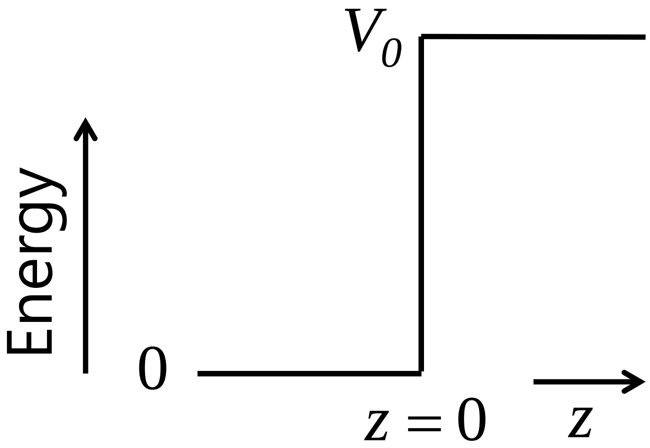
i.e., the incident wave energy is less than the barrier height

Inside the barrier, the wave equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(z)}{dz^2}+V_o\psi(z)=E\psi(z)$$

i.e., mathematically

$$\frac{d^2\psi(z)}{dz^2}=\frac{2m}{\hbar^2}(V_o-E)\psi(z)$$



Infinitely thick barrier

The general solution of

$$\frac{d^2\psi(z)}{dz^2} = \frac{2m}{\hbar^2}(V_o - E)\psi(z)$$

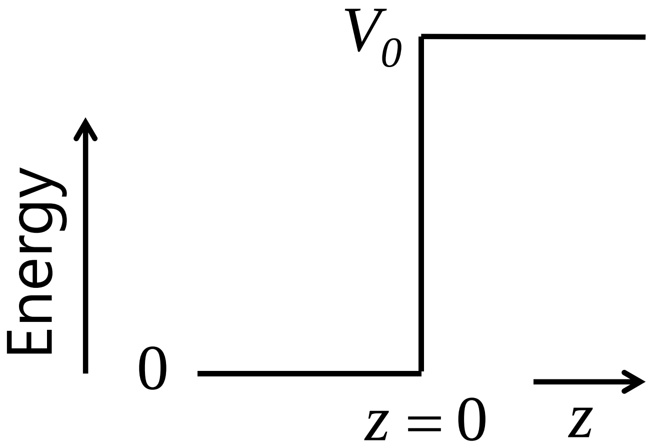
for the wave on the right is

$$\psi_{right}(z) = F\exp(\kappa z) + G\exp(-\kappa z)$$

where $\kappa = \sqrt{2m(V_o - E)/\hbar^2}$

We presume $F = 0$

otherwise the wave increases exponentially to the right for ever



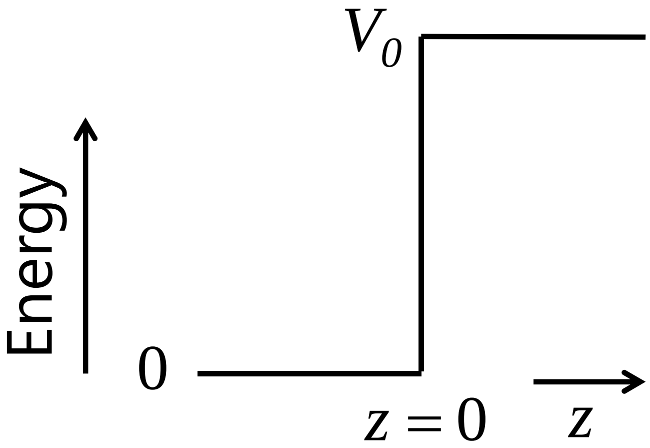
Infinitely thick barrier

Hence the wave on the right

inside the barrier, is

$$\psi_{right}(z) = G\exp(-\kappa z)$$

with $\kappa = \sqrt{2m(V_o - E)/\hbar^2}$



This solution proposes that the wave inside the barrier is not zero

Instead, it falls off exponentially

Infinitely thick barrier

Using the boundary conditions

we complete the solution

On the left, we have $\psi_{left}(z) = C\exp(ikz) + D\exp(-ikz)$

On the right we have $\psi_{right}(z) = G\exp(-\kappa z)$

Continuity of the wavefunction at $z = 0$ gives

$$C + D = G$$

Continuity of the wavefunction derivative at $z = 0$ gives

$$ikC - ikD = -\kappa G$$

i.e.,

$$C - D = \frac{i\kappa}{k}G$$

Infinitely thick barrier

Adding

$$C + D = G$$

$$C - D = \frac{i\kappa}{k} G$$

gives

$$2C = \left(1 + \frac{i\kappa}{k}\right) G = \left(\frac{k + i\kappa}{k}\right) G$$

Equivalently

$$G = \frac{2k}{k + i\kappa} C = \frac{2k\left(k - i\kappa\right)}{k^2 + \kappa^2} C$$

so we have found the amplitude G of the wave in the barrier in terms of the amplitude C of the incident wave

Infinitely thick barrier

Subtracting $$C + D = G$$
$$C - D = \frac{i\kappa}{k} G$$

gives $$2D = \left(1 - \frac{i\kappa}{k}\right) G = \left(\frac{k - i\kappa}{k}\right) G$$

Since we found $G = 2k / (k + i\kappa) C$

then $$D = \frac{k - i\kappa}{k + i\kappa} C$$

so we have found the amplitude D of the reflected wave in terms of the amplitude C of the incident wave

Infinitely thick barrier

We have now formally solved the problem

the wave on the left is $$\psi_{left}(z) = C\exp(ikz) + D\exp(-ikz)$$

with $$D = \frac{k - i\kappa}{k + i\kappa}C$$

the wave on the right is $$\psi_{right}(z) = G\exp(-\kappa z)$$

with $$G = \frac{2k}{k + i\kappa}C$$

where

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

Reflection at an infinitely thick barrier

Note that $$D = \frac{k - i\kappa}{k + i\kappa} C$$

so $$\frac{D}{C} = \frac{k - i\kappa}{k + i\kappa}$$

so $$\left|\frac{D}{C}\right|^2 = \frac{k - i\kappa}{k + i\kappa}\frac{k + i\kappa}{k - i\kappa} = 1$$

so the barrier is 100% reflecting

though there is a phase shift on reflection

an effect with no classical analog

Wavefunction at a barrier

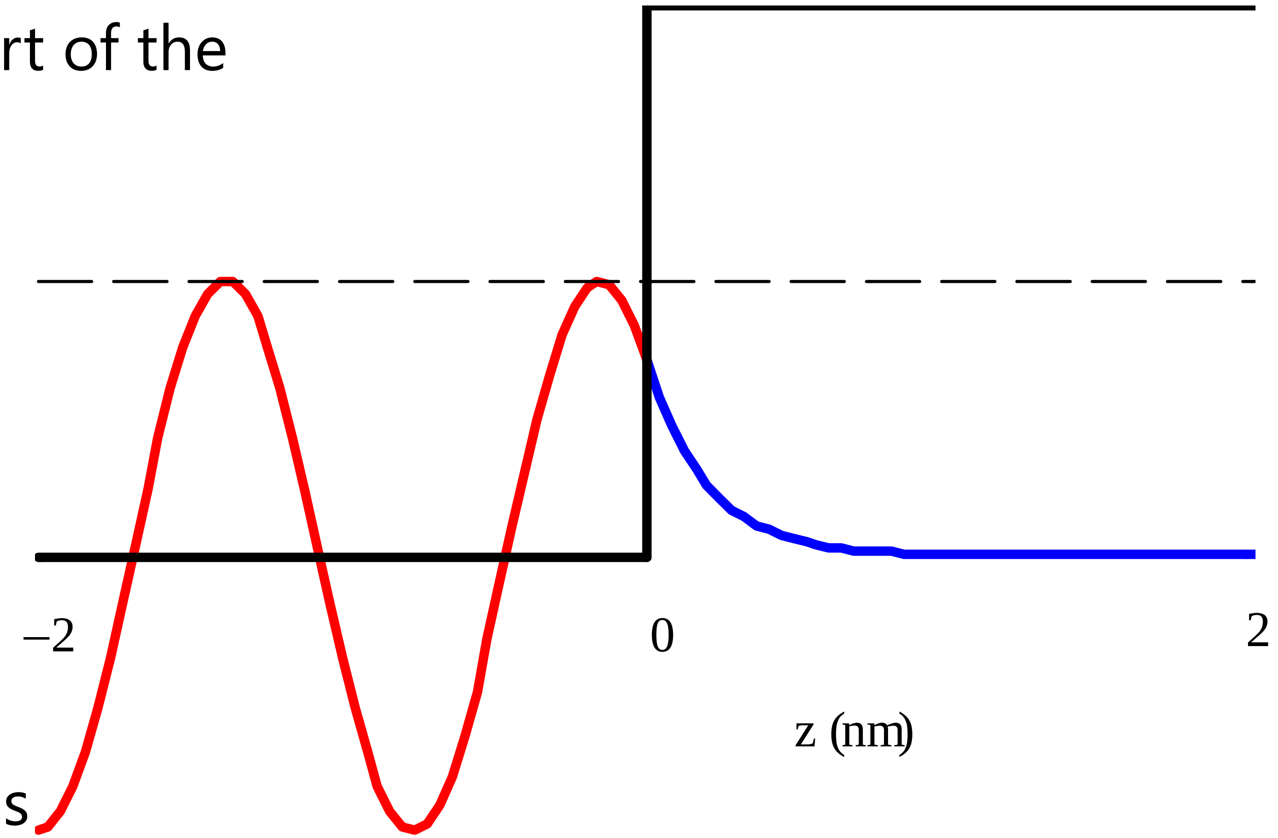
We plot the real part of the wavefunction

- for an electron
  - energy 1 eV
- at a barrier
  - height 2 eV

Note

- the wavefunction
- and its derivative

are both continuous



Tunneling penetration

For a barrier of height V_o= 2 eV

with an electron energy E = 1 eV

$$\kappa = \sqrt{2m\left(V_o - E\right)/\hbar^2}$$

$$\simeq \sqrt{2\times 9.1095\times 10^{-31}\times\left(2-1\right)\times 1.602\times 10^{-19}/\left(1.055\times 10^{-34}\right)^2}$$

$$\simeq 5\times 10^9\,\mathrm{m}^{-1}$$

i.e., the “attenuation length” of the wave amplitude into the barrier

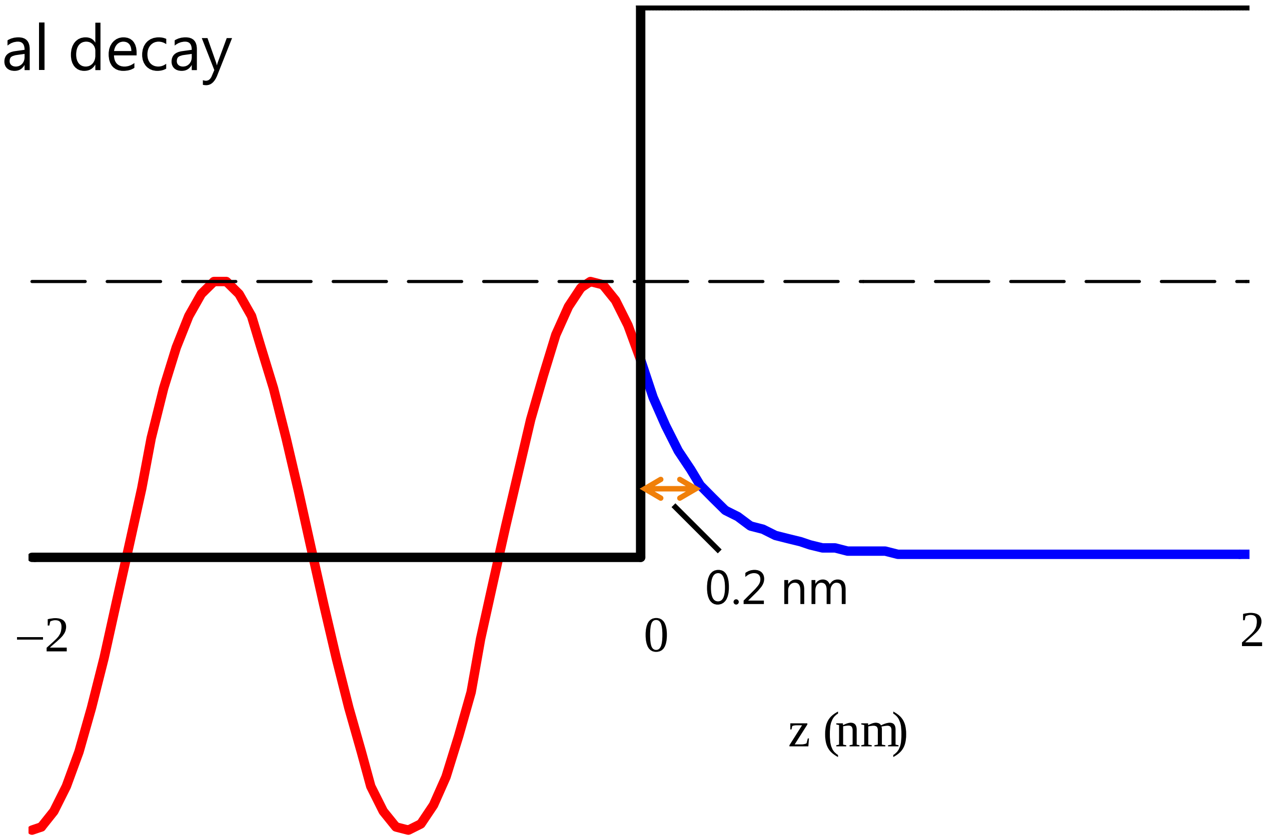
the length to fall to 1/e of its initial value, is

$$1/\kappa \cong 0.2\ \mathrm{nm} \equiv 2\ \text{Å}$$

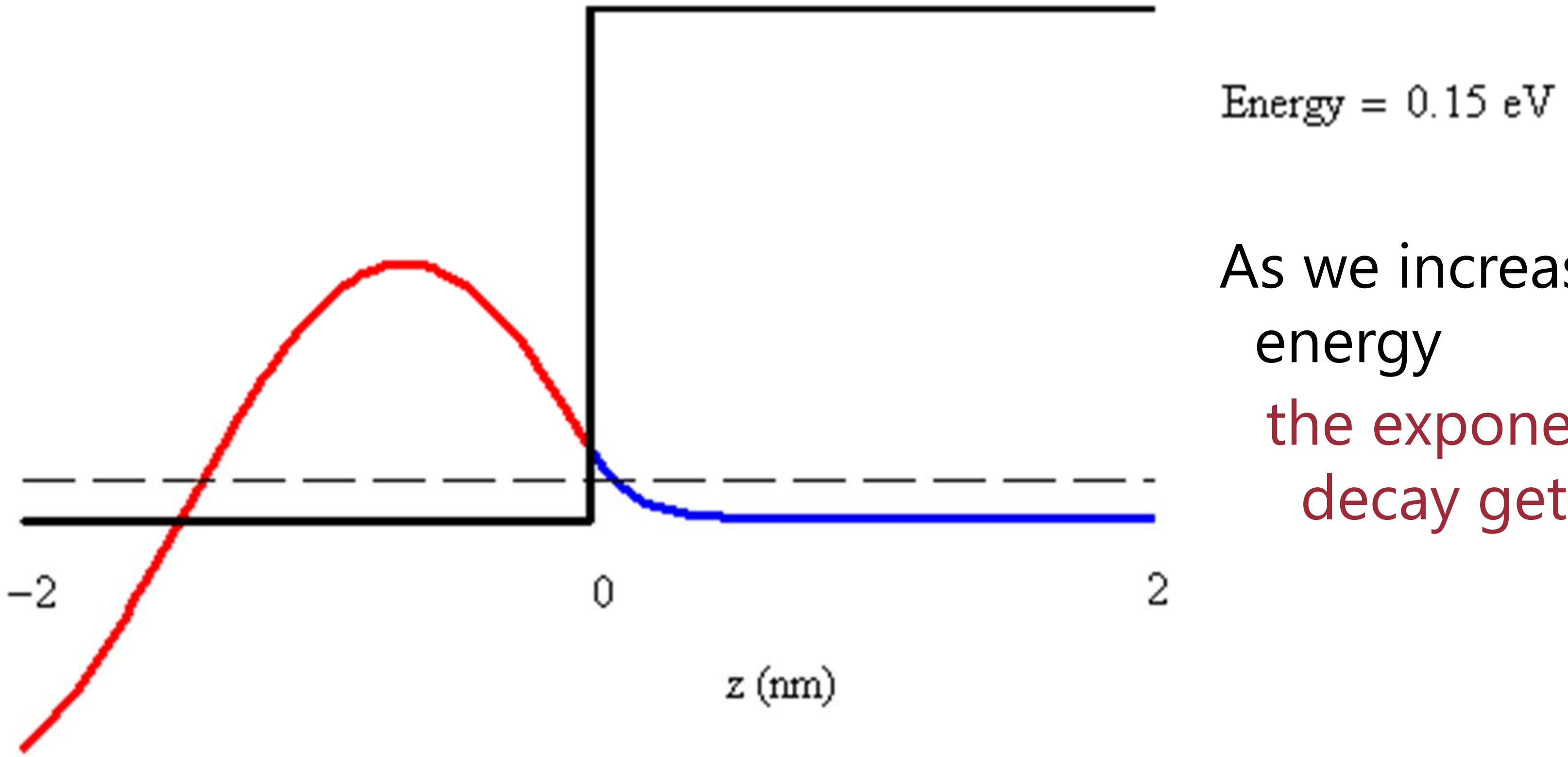
Wavefunction at a barrier

Note the exponential decay length

$1/\kappa \cong 0.2 \text{ nm} \equiv 2 \text{ Å}$



Wavefunction at a barrier



As we increase the energy

the exponential decay gets longer

Probability density at a barrier

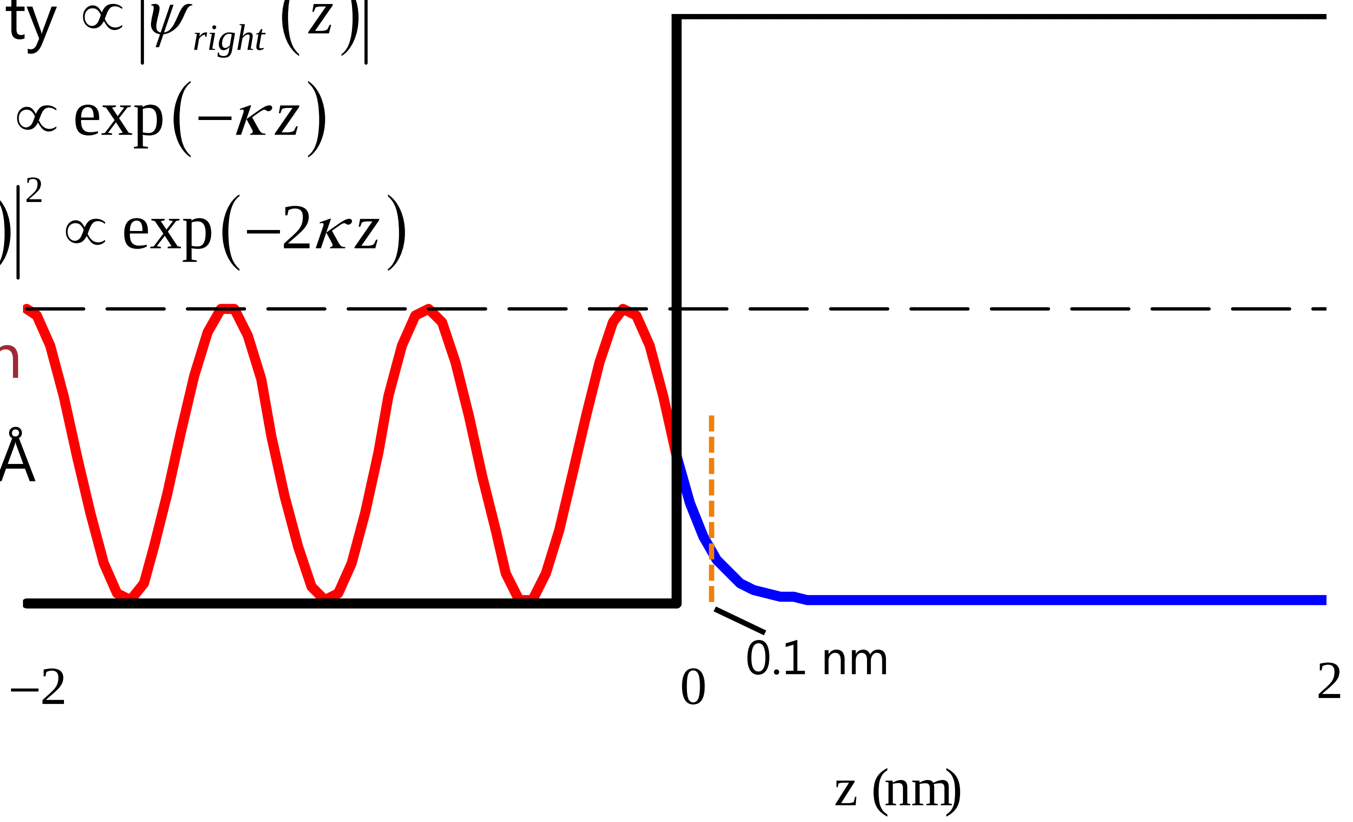
Probability density $\propto \left|\psi_{right}(z)\right|^2$

With $\psi_{right}(z) \propto \exp(-\kappa z)$

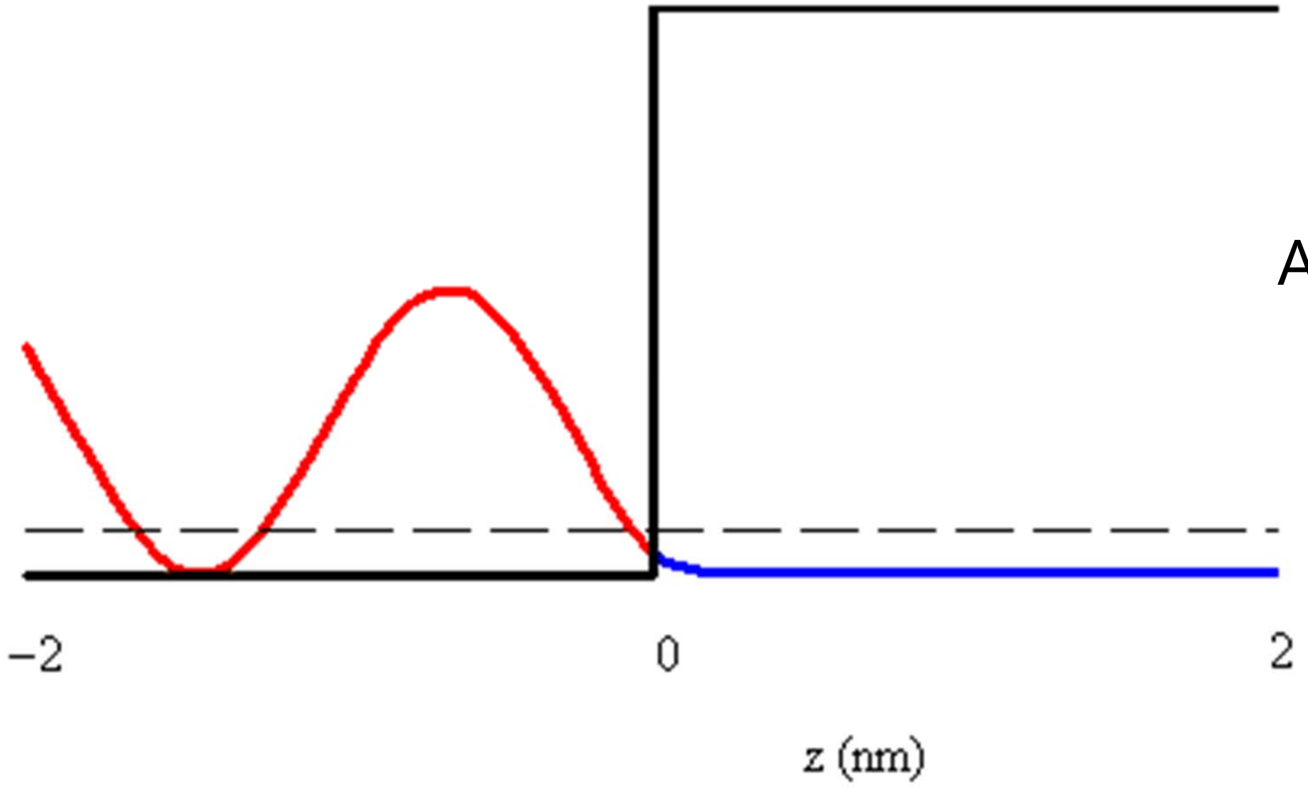
then $\left|\psi_{right}(z)\right|^2 \propto \exp(-2\kappa z)$

falling by 1/e in

$1/2\kappa \simeq 0.1\ \text{nm} \equiv 1\ \text{Å}$



Probability density at a barrier



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