

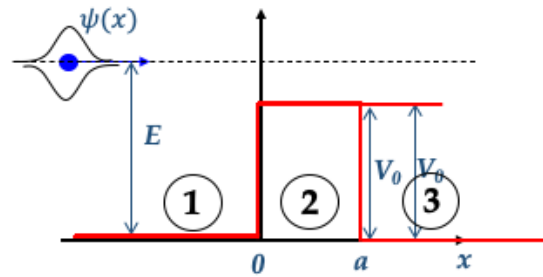
Part-2

Potential Barriers

Potential barrier : $E > V_0$

- define potential :

$$\begin{aligned} V(x) &= 0 & \text{if } x < 0 & : \text{Region 1} \\ &= V_0 < E & \text{if } 0 < x < a & : \text{Region 2} \\ &= 0 & \text{if } x > a & : \text{Region 3} \end{aligned}$$



Region 1

Region 2

Region 3

- write down T.I.S.E :

$$\frac{\hbar^2}{2m} \frac{d^2 \psi_1(x)}{dx^2} + E \psi_1(x) = 0$$

$$\frac{\hbar^2}{2m} \frac{d^2 \psi_2(x)}{dx^2} + [E - V_0] \psi_2(x) = 0$$

$$\frac{\hbar^2}{2m} \frac{d^2 \psi_3(x)}{dx^2} + E \psi_3(x) = 0$$

- define general expression for the eigen function :

$$\psi_1(x) = A \underbrace{\exp(ik_1 x)}_{\text{moving along: } +x} + B \underbrace{\exp(-ik_1 x)}_{-x}$$

$$\psi_2(x) = C \underbrace{\exp(ik_2 x)}_{+x} + D \underbrace{\exp(-ik_2 x)}_{-x}$$

$$\psi_3(x) = F \underbrace{\exp(ik_3 x)}_{+x} + G \underbrace{\exp(-ik_3 x)}_{-x}$$

$$\text{where, } k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\text{where, } k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

$$\text{where, } k_3 = \sqrt{\frac{2mE}{\hbar^2}} = k_1$$

A & B are amplitudes (constants)

C & D are amplitudes (constants)

F & G are amplitudes (constants); $G = 0$

- This is almost similar problem, except that we have 3 regions and 2 boundaries.
- So we proceed with the same template recipe, with a mindful of the subscripts 1,2 and 3
- Same as before, we can neglect the reflected part in region 3 and k_2 is lower than $k_1 = k_3$, i.e the wavelength of the matter wave inside the region 2 will be longer than both sides.

- **apply boundary conditions to find A, B, C, D & F :**

$$\begin{aligned}
 \checkmark \quad \psi_1(x)|_{x=0} &= \psi_2(x)|_{x=0} \Rightarrow A + B = C + D \\
 \checkmark \quad \frac{d\psi_1(x)}{dx}|_{x=0} &= \frac{d\psi_2(x)}{dx}|_{x=0} \Rightarrow k_1(A - B) = k_2(C - D) \\
 \checkmark \quad \psi_2(x)|_{x=a} &= \psi_3(x)|_{x=a} \Rightarrow C \exp(ik_2a) + D \exp(-ik_2a) = F \exp(ik_1a) \quad (\text{note, } k_3 = k_1 = \sqrt{2mE}/\hbar) \\
 \checkmark \quad \frac{d\psi_2(x)}{dx}|_{x=a} &= \frac{d\psi_3(x)}{dx}|_{x=a} \Rightarrow k_2 [C \exp(ik_2a) - D \exp(-ik_2a)] = k_1 F \exp(ik_1a)
 \end{aligned}$$

- **with some algebra (rather messy ☹), you can find**

$$T = \frac{J_T}{J_I} = \frac{F^2}{A^2} = \left[1 + \frac{\sin^2(k_2a)}{4 \frac{E}{V_0} \left(\frac{E}{V_0} - 1 \right)} \right]^{-1} \quad \text{where, } k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

- **now, let's try to make some sense of this...**

Classically $T = 1$ and $R = 0$ for all $E/V_0 > 1$.

But Quantum mechanically, this is not always the case, even if $E \gg V_0$

However, there are some energies for which the barrier has no effect, and $T = 1$!

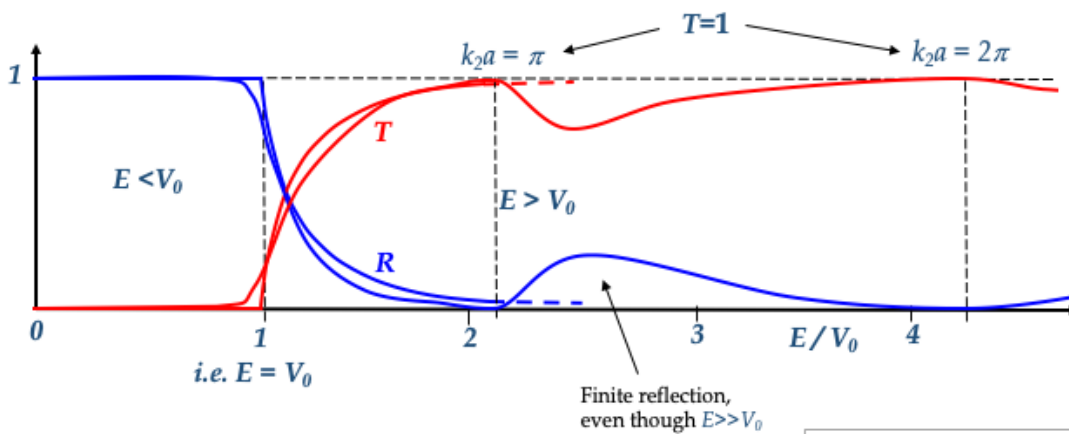
This happens when (from the expression of T above), $\sin(k_2a) = 0 \Rightarrow k_2a = m\pi$, where $m = 1, 2, \dots$

i.e. when the de-Broglie wavelength in the region 2 (inside the barrier) $= \lambda_2 = \frac{2\pi}{k_2} = \frac{2a}{m}$

i.e. when the width of the barrier, $a = m \frac{\lambda_2}{2}$, which leads to destructive interference between the reflections from the boundaries at $x=0$ and $x=a$

- Since we have two boundaries, we need to apply 4 boundary conditions. This is also useful as we have so many unknowns – A, B, C, D and E
- Note that the derivation for T is not necessary for the assessment. But you can try using the same procedure as we did for the step.
- The important point to note from the expression of T is that, it has a \sin^2 term, which tells that the transmission is kind of oscillating. We knew from the potential step that the transmission drops monotonically as we increase the V , but here we see that it can be 100% in some special cases, even if the V is close to E . This is another interesting effect (as experimentally proved, called Ramsauer-Townsend effect, next slide) that can be explained by the wave nature of particles. The transmission in these special situation becomes 100% as the reflected waves from the both boundaries destructively interfere as they are exactly out of phase.
- So if you fix the V , the transmission will fluctuate by changing the width – a weird thing if we think from a classical mechanics point of view, isn't it?

Plotting the reflection and transmission coefficient in this case,

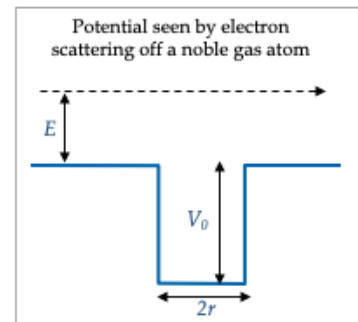


Ramsauer-Townsend Effect

When electrons scatter off atoms with tightly bound closed shells, the potential can be approximated by the potential well shown on right. The probability of the electron scattering reduces to zero when $k_2 a = \pi$ (note in this case k_2 is different from the expression above).

This effect was discovered by Ramsauer and Townsend in the early 1920s : they saw electrons of few eV energies pass through atoms as if there were not there.

This was probably the first experimental evidence for the wave nature of particles, although it was not interpreted as such at the time.

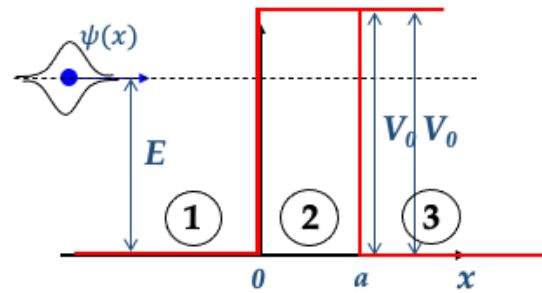


- Another example of this phenomenon we found in our day-to-day life is the use of anti-reflection coatings used in the glasses to minimize reflection – the thickness of the coating is such that there is a destructive interference of the light reflected from the both sides of the coating.
- See the section of the text book for more information.
- As you see in the graph, the curve around $E=V$ is not the same that we saw in the case of potential step. Here it is shown that there is a non-zero T even for the case $E < V \Rightarrow$ its called tunneling, we will look at it now – basically saying that particles can tunnel through a barrier, even if they don't have enough energy to go over it. Interesting, isn't it?

Potential barrier : $E < V_0$

- define potential :

$$\begin{aligned} V(x) &= 0 & \text{if } x < 0 & : \text{Region 1} \\ &= V_0 > E & \text{if } 0 < x < a & : \text{Region 2} \\ &= 0 & \text{if } x > a & : \text{Region 3} \end{aligned}$$



Region 1

- write down T.I.S.E :

$$\frac{\hbar^2}{2m} \frac{d^2 \psi_1(x)}{dx^2} + E \psi_1(x) = 0$$

Region 2

Note, $[E - V_0]$ is -ve

$$\frac{\hbar^2}{2m} \frac{d^2 \psi_2(x)}{dx^2} + [E - V_0] \psi_2(x) = 0$$

Region 3

$$\frac{\hbar^2}{2m} \frac{d^2 \psi_3(x)}{dx^2} + E \psi_3(x) = 0$$

- define general expression for the eigen function :

$$\psi_1(x) = A \exp(ik_1x) + B \exp(-ik_1x)$$

moving along: $+x$ $-x$

$$\psi_2(x) = C \exp(ik_2x) + D \exp(-ik_2x)$$

$+x$ $-x$

$$\psi_3(x) = F \exp(ik_3x) + G \exp(-ik_3x)$$

$+x$ $-x$

$$\text{where, } k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

A & B are amplitudes (constants)

$$\text{where, } k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} = i \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = ik'_2$$

C & D are amplitudes (constants)

$$\text{where, } k_3 = \sqrt{\frac{2mE}{\hbar^2}} = k_1$$

F & G are amplitudes (constants); $G = 0$

- So nothing so fancy about this problem, all same except that the k_2 is imaginary. Hence we can substitute $k_2 = ik'_2$. This immediately tells us that wavefunction inside the barrier is an exponential decay, instead of an oscillating profile. So if the width of the barrier is not wide enough, the amplitude of the exponential decaying wavefunction could be high enough to leak a part of the wavefunction into region 3. That's the tunneling effect.
- So we proceed with the derivation as before, defining TISE for each region, defining wavefunctions in each region (only considering the valid terms, for instance, taking $G=0$) and the corresponding wavenumbers.

Hence the general expressions of the eigen functions would be

$$\psi_1(x) = A \exp(ik_1x) + B \exp(-ik_1x) \quad \psi_2(x) = C \exp(-k'_2x) + D \exp(k'_2x) \quad \psi_3(x) = F \exp(ik_1x)$$

(note, $k_3 = k_1 = \sqrt{2mE}/\hbar$, $k_2 = ik'_2$)

- **apply boundary conditions to find A, B, C, D & F:**

$$\begin{aligned} \checkmark \quad \psi_1(x)|_{x=0} &= \psi_2(x)|_{x=0} \Rightarrow A + B = C + D \\ \checkmark \quad \frac{d\psi_1(x)}{dx}|_{x=0} &= \frac{d\psi_2(x)}{dx}|_{x=0} \Rightarrow k_1(A - B) = ik'_2(C - D) \\ \checkmark \quad \psi_2(x)|_{x=a} &= \psi_3(x)|_{x=a} \Rightarrow C \exp(-k'_2a) + D \exp(k'_2a) = F \exp(ik_1a) \\ \checkmark \quad \frac{d\psi_2(x)}{dx}|_{x=a} &= \frac{d\psi_3(x)}{dx}|_{x=a} \Rightarrow k'_2 [C \exp(-k'_2a) - D \exp(k'_2a)] = ik_1 F \exp(ik_1a) \end{aligned}$$

- **with some algebra (rather messy ☹), you can find**

$$T \approx 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0}\right) e^{-2k'_2a} \quad \text{when } k'_2a \gg 1$$

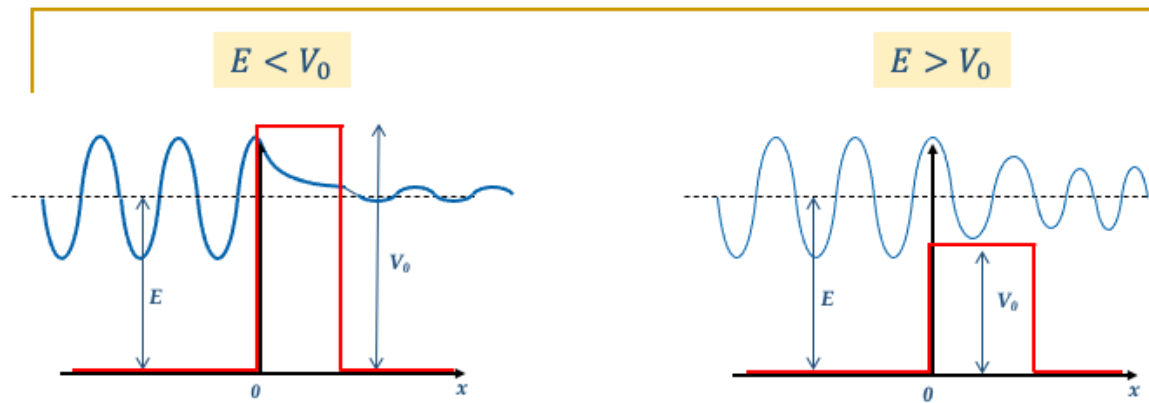
i.e. there is a finite probability of finding the particle at the other side of the barrier !!!

“ QUANTUM TUNNELLING ”

- The transmission coefficient is a function of E, V_0, a and m .
- But most importantly, the expression is dominated by the exponential term $e^{-2k'_2a}$, where, $k'_2 = \sqrt{2m(V_0 - E)}/\hbar$
i.e. a small change in $(V_0 - E)$ and m can change the tunnelling probability significantly!

- Next step would be to apply the boundary conditions and then some algebra to find the transmission coefficient.
- Note the algebra for getting the expression for T is not for assessment, but one can try.
- So, as you see from the expression for T, the transmission depends strongly on the E and V values, but the main factor is the exponential term, which is a function of k'_2a , i.e. even for a given k_2 , depends strongly on the thickness of the barrier. This is not very unexpected as we knew before that the wavefunction inside the barrier is exponentially decaying, hence the transmission will depend on the amplitude of the wavefunction at the end of the barrier.
- Of course, the transmission also depends on the difference between E and V. Both due to the k'_2 in the exponent, as well as the terms outside the exponential. But still the change due to the change in k'_2 controls the transmission predominantly, due to the exponential term.
- So in summary, we see that we can have finite transmission (and can be very significant as well depending on the product k'_2a , for instance an ultra-thin barrier even with a very high V) through a barrier, that can be controlled by varying the barrier height or width. This knowledge simply

transformed the world around us – we'll now see some implications of quantum tunneling.



A fun problem!

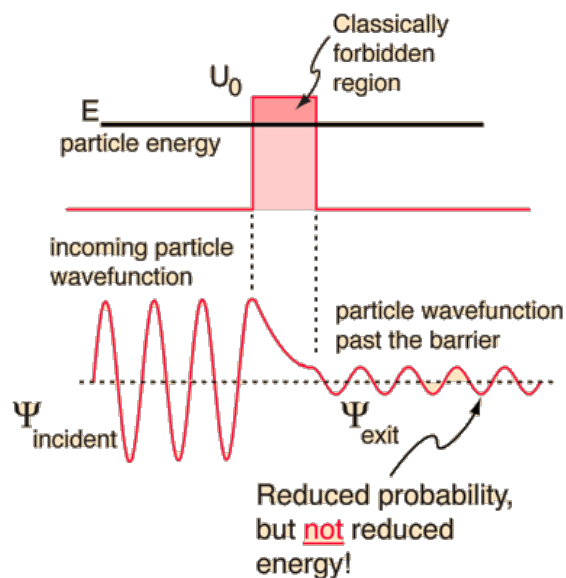
What is the probability of you running through a wall? Let's assume mass of 50 kg and the wall of 5 cm thick representing an effective barrier height of 10^4 J

$$T \approx 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0}\right) e^{-2k_2' a} \quad e^{-2k_2' a} = \exp\left(\frac{-2a\sqrt{2m(V_0 - E)}}{\hbar}\right) \approx \exp\left(\frac{-2 \times 0.05 \sqrt{2 \times 50 \times 10^4}}{10^{-34}}\right) = \exp(-10^{32})$$

Not even a atom of my body will go through!

So, tunnelling occurs for very small particles, and thin, small barriers.

- Note the amplitude, profile and wavelength of the wave in different region in both cases.

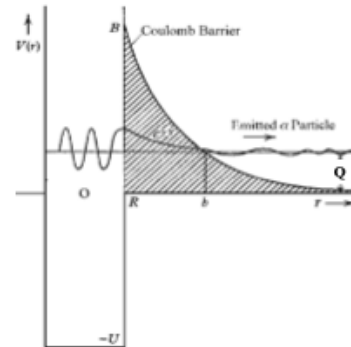


Some examples of Quantum tunnelling ...

Alpha decay of a nucleus

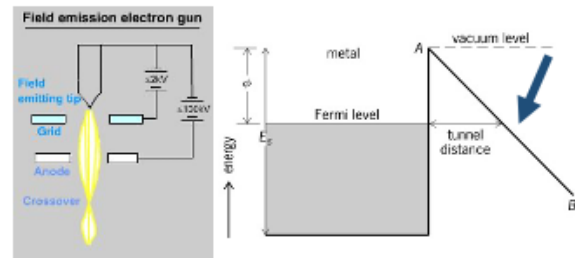
- If 2 protons and 2 neutrons form an alpha particle, it experiences a potential with distance r as shown
- Alphas can tunnel through the coulomb barrier
- Probability (and thus half-life $t_{1/2}$) very dependent on energy of emitted alpha Q .

Nuclide	Half-life (years)	Decay Q-value (MeV)
$^{241}_{95}\text{Am}$	432	5.84
$^{238}_{92}\text{U}$	4.5×10^9	4.27
$^{234}_{92}\text{Pu}$	1.4×10^{17}	1.97



Field Emission

- In this type of electron gun, very strong ($>10^9$ V/m) is used to extract the electrons from a metal filament
- Works by suppressing the potential barrier by the applied voltage, so that electrons can tunnel through.
- This gives much brighter source than guns operated via thermionic emission process, but needs a very good vacuum.

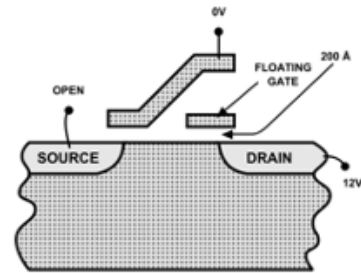


- A detailed theory of these application areas are not needed for assessment.
- Alpha decay, one of the hot topic in early era of quantum mechanics, is one of the classic examples of quantum tunneling. More details on the Eisberg book.
- Also see the videos and websites linked in the canvas page.

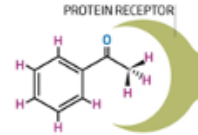
Some examples of Quantum tunnelling ...

Flash Memory

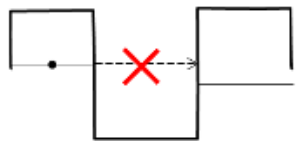
- Based on "floating gate" transistor
- If charged, the Floating Gate suppresses current from flowing from the Source to the Drain, i.e. a "0". If uncharged then stores a "1"
- But how do you remove charge from the floating gate if it has no electrical connections?



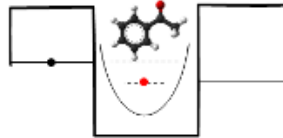
How does a nose generate the signals that the brain registers as smell ?



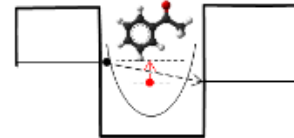
The fragrant molecules fits into the protein receptor like a key in a lock.



Electron has no state to tunnel across to



Molecule moves into receptor.
Molecule in ground vibrational level.



Electron excites a transition in the molecule and loses enough energy to tunnel to lower level.

<http://www.newscientist.com/article/dn20130-fly-sniffs-molecules-quantum-vibrations.html>

- See the youtube video for the floating gate.

<https://www.youtube.com/watch?v=s7JLXs5es7I&list=PLcvD3t93938OqujvgiPyZFioO9V2A2liZ&index=1>

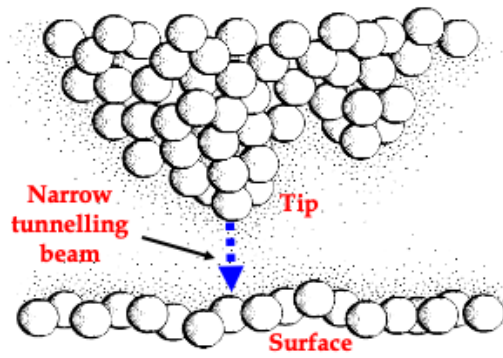
from 3.45 – 5 min, then 7-9 min.

- See the newscientist page for this interesting concept of how tunneling is responsible for the smell.

Some examples of Quantum tunnelling ...

■ Scanning Tunnelling Microscope (STM)

- In a STM, a fine tip (only a few atoms wide at its point) is controlled with $< 1 \text{ \AA}$ precision.
- Electrons at the top of the conduction band in the tip require an energy equal to the work function to escape. If the tip is close enough to a surface there is a barrier and when a potential difference U is applied, electrons can tunnel into empty states in the surface.
- Let us approximate this by a square barrier with height $\phi - eU$, where ϕ is the work function ($\approx 5 \text{ eV}$ for tungsten) and distance from the surface d in \AA (10^{-10} m).



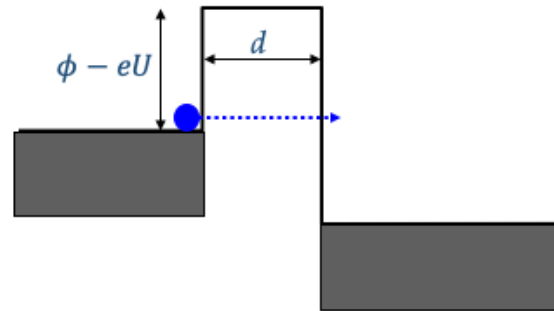
$$T \approx 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0}\right) e^{-2k_2' a}$$

$$e^{-2k_2' a} = \exp\left(\frac{-2a\sqrt{2m(V_0 - E)}}{\hbar}\right)$$

$$= \exp\left(\frac{-2d\sqrt{2m_e(\phi - eU)}}{\hbar}\right) \approx \exp(-1.03d\sqrt{5 - U})$$

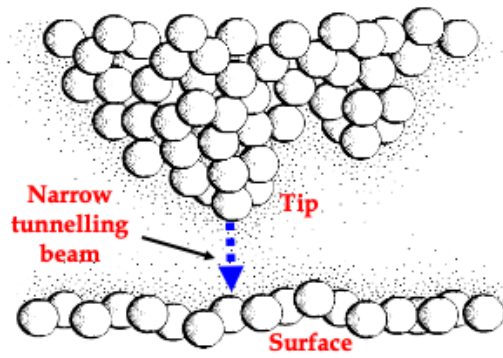
If $U = 0.1 \text{ V}$,

$$\begin{array}{ll} d = 10 \text{ \AA} & \text{gives } T = 1.25 \times 10^{-10} \\ d = 10.1 \text{ \AA} & \text{gives } T = 1.0 \times 10^{-10} \end{array}$$



- Very interesting example, and the perfect one, which tells how sensitive tunneling is to the barrier height and width.
- Note the conversion of ‘volt’ to ‘electron volt’ (which is the unit of energy)

- Due to the exponential dependence, the electron tunnelling current is very sensitive to the surface roughness giving very high resolution.
($0.1\text{\AA} \sim 1/10^{\text{th}}$ of the width of one atom!)
- In scanning the surface, the tunnelling current is kept constant by moving the tip in and out.
- Although it is impossible to get a perfectly sharp tip, the lateral resolution is also very high. Again as tunnelling is sensitive to distance, electrons tunnel from only one atom!



This image is from the Nobel Physics prize winning lecture by Gerd Binnig who won in 1986 "for the design of the scanning tunneling microscope"

http://nobelprize.org/nobel_prizes/physics/laureates/1986/index.html

http://virtual.itg.uiuc.edu/training/AFM_tutorial/