Quantum Physics
PY1T20/PYU11P20

Paul Eastham

Quantum Physics Lecture 12

Particle at a potential step

Step up potential with E<U

Step up potential with E>U

Step down potential

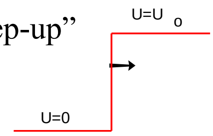
Potential barrier of finite width

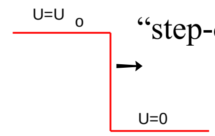
$E < U_o$ Tunnelling

Example: Scanning Tunelling Microscope

Particle meeting step potential

2 types: “step-up”



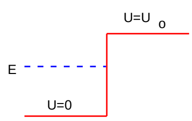


“step-down”

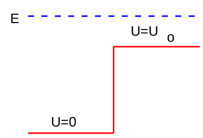
Particle direction “left-to-right”; potential flat apart from step region;

Particle energy E and step size U_o; 3 distinct situations:

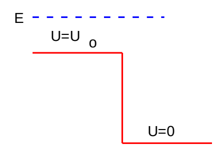
“up” $E < U_o$



“up” $E > U_o$



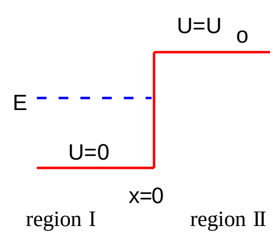
“down” $E > U_o$



Find elements of “propagating” and “decaying” wavefunctions;
Solutions may not be standing waves (as previously)
cannot draw *($\because$ complex ψ)* but can always draw $|\psi|^2$ (real).

Apply SSSE to step-up potential ($E < U_o$)

Classically, particle is reflected!



$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - U)\,\psi = 0$$

For region I, solution is <u>complex</u> exponentials:

$$\boxed{\psi_I = A\exp(ik_1 x) + B\exp(-ik_1 x)}$$

where $k_1 = \sqrt{2mE}/\hbar$

For region II, solutions are <u>real</u> exponentials:

$$\psi_{II} = C\exp(k_2 x) + D\exp(-k_2 x)$$

where $k_2 = \sqrt{2m(U_0 - E)}/\hbar$

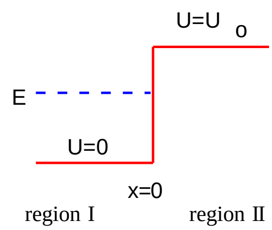
Also, require $C = 0$, to keep ψ finite at large +ve x:

$$\boxed{\psi_{II} = D\exp(-k_2 x)}$$

Apply boundary matching

$\psi_{II} = \psi_I$ at $x = 0$
$D\exp(0) = A\exp(0) + B\exp(0)$
$D = A + B$

$d\psi_{II}/dx = d\psi_I/dx$ at $x = 0$
$-k_2 D\exp(0) = ik_1 A\exp(0) - ik_1 B\exp(0)$
$(ik_2/k_1)D = A - B$



Convenient to write A and B in terms of D:

$$\psi_I = \frac{D}{2}\left(1 + \frac{ik_2}{k_1}\right)\exp(ik_1 x) + \frac{D}{2}\left(1 - \frac{ik_2}{k_1}\right)\exp(-ik_1 x)$$

meaning? *incident particle(s)* *reflected particle(s)*

$$\psi_{II} = D\exp(-k_2 x)$$

particle(s) probability decays into wall!

Particle reflection

Reflection Coefficient $R = B^*B/A^*A$

$$R = \frac{\left(1 - i\frac{k_2}{k_1}\right)^*\left(1 - i\frac{k_2}{k_1}\right)}{\left(1 + i\frac{k_2}{k_1}\right)^*\left(1 + i\frac{k_2}{k_1}\right)} = \frac{\left(1 + i\frac{k_2}{k_1}\right)\left(1 - i\frac{k_2}{k_1}\right)}{\left(1 - i\frac{k_2}{k_1}\right)\left(1 + i\frac{k_2}{k_1}\right)} = 1$$

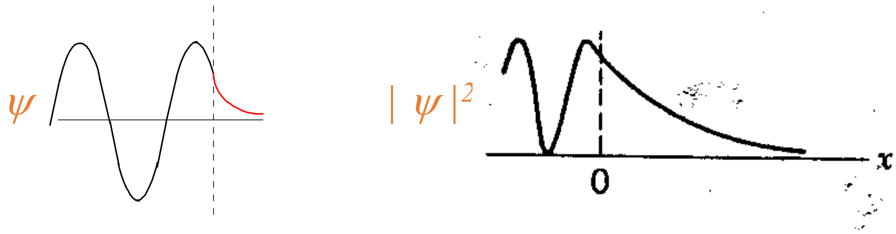
As expected, in agreement with classical picture!

Exercise: use [$\exp(i\theta) = \cos\theta + i\sin\theta$] to show

$$\psi_I = D\cos(k_1 x) - D\left(\frac{k_2}{k_1}\right)\sin(k_1 x)$$

can be rewritten as $\sin(k_1 x + \phi)$ i.e. standing wave!
(combination of equal incident and reflected waves)

Plotting ψ and $|\psi|^2$



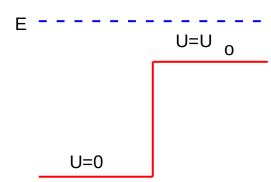
Because in this case ψ_I is a pure standing wave, it can still be plotted; note how ψ_I matches onto ψ_{II} (red)
As U_o increases, k_2 increases (less penetration of wall) and ψ_I moves closer to simple $\sin(k_1 x)$.

Plot of $|\psi|^2$ always possible
Signature of perfect reflection ($R = 1$):
minimum value of $|\psi|^2 = 0$

Apply SSSE to step-up potential ($E > U_o$)

Classically: kinetic energy decrease and particle *not* reflected!

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - U)\psi = 0$$



For region I, solution is complex exponentials as before:

$$\boxed{\psi_I = A\exp(ik_1 x) + B\exp(-ik_1 x)} \quad \text{where} \quad k_1 = \sqrt{2mE}/\hbar$$

For region II, solution is also complex exponentials:

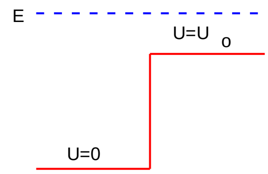
$$\psi_{II} = C\exp(ik_2 x) + D\exp(-ik_2 x) \quad \text{where} \quad k_2 = \sqrt{2m(E - U_0)}/\hbar$$

Require $D = 0$, no negative-going wave for $x > 0$, as all particles are incident in +ve x direction!

Not so for $x < 0$, there is some reflection!

$$\boxed{\psi_{II} = C\exp(ik_2 x)}$$

Apply boundary matching



$\psi_{II} = \psi_I$ at $x = 0$
$C\exp(0) = A\exp(0) + B\exp(0)$
$C = A + B$

$d\psi_{II}/dx = d\psi_I/dx$ at $x = 0$
$ik_2 C\exp(0) = ik_1 A\exp(0) - ik_1 B\exp(0)$
$(k_2/k_1)C = A - B$
Convenient to write B and C in terms of A:

$$\psi_I = A\exp(ik_1 x) + A\frac{k_1 - k_2}{k_1 + k_2}\exp(-ik_1 x)$$

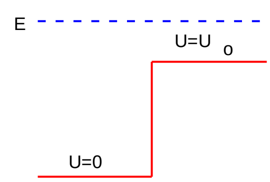
meaning? incident particle(s) reflected particle(s)

$$\psi_{II} = A\frac{2k_1}{k_1 + k_2}\exp(ik_2 x)$$ particle(s) with reduced energy!

Particle reflection

Recall Reflection Coefficient $R = B^*B/A^*A$

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

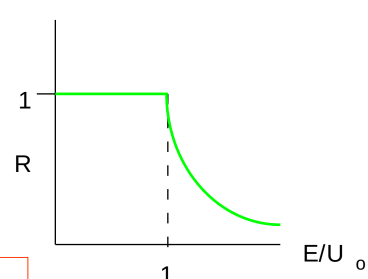


Recall the equations for k_1 and k_2

$$k_2/k_1 = \sqrt{2m(E - U_0)}\Big/\sqrt{2mE} = \sqrt{1 - U_0/E}$$

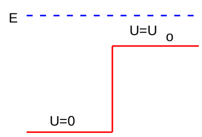
$$R = \left(\frac{1 - \sqrt{1 - U_0/E}}{1 + \sqrt{1 - U_0/E}}\right)^2$$

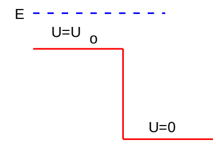
for $E > U_o$ and $R = 1$ for $E < U_o$



Particle meeting step-down potential

compare: “step-up” with “step-down”





Reverse situations, simply exchange k_1 and k_2:

$$\psi_I = A\exp\left(ik_2 x\right) + B\exp\left(-ik_2 x\right)$$

$$\psi_{II} = C\exp\left(ik_1 x\right)$$

Proceed to determine matching etc.

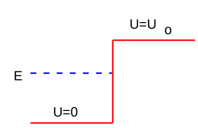
Significant point is that some reflection occurs here too;

Origin of reflectivity is “change in potential U”

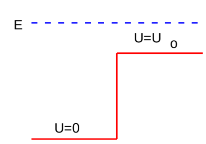
For quantum ‘lemmings’, some reflect from cliff edge….

General conclusions

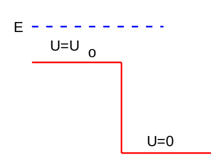
Step-up, where $E < U_o$
- total reflection
- but can exist *in* wall!



Step-up, where $E > U_o$
- decreased kinetic energy
- and partial reflection!

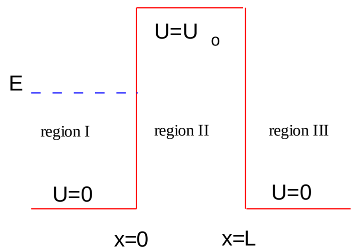


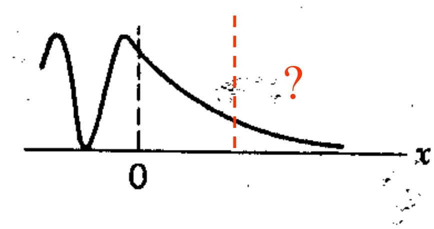
Step-down, where $E > U_o$
- increased kinetic energy
- also partial reflection!



“solve, match, R and plot”

potential barrier ($E < U_o$)





Recall step-up potential, $E < U_o$: particle penetrates into wall. But if the wall is finite width L….?

Solve SSSE:

For region I, solution is <u>complex</u> k_1x exponentials: (A→, B←)
For region II, solution is <u>real</u> k_2x exponentials: (C→, D←)
For region III, solution is <u>complex</u> k_1x exponentials: (F→, G←)

Particle <u>transmission</u> through barrier! *More parameters in solution*

Particle transmission

Recall Reflection Coefficient $R = B^*B/A^*A$
Transmission Coefficient $T = F^*F/A^*A$ *(for $k_I = k_{III}$)*

If assume that $E << U_o$ *(i.e. D very small)* then maths simplifies and

$$T \approx \left[\frac{16}{4 + \left(k_2 / k_1 \right)^2} \right] \exp\left(-2k_2 L\right) \quad or \quad \boxed{T \approx \exp\left(-2k_2 L\right)}$$

Square bracket is of order unity, and *NOTE: strong dependence on L!*

Decay constant k_2 related to height of <u>barrier</u> $(U_o - E)$

$$k_2 = \frac{\sqrt{2m\left(U_o - E\right)}}{h}$$

Examples: Radioactive decay, scanning tunneling microscope…..

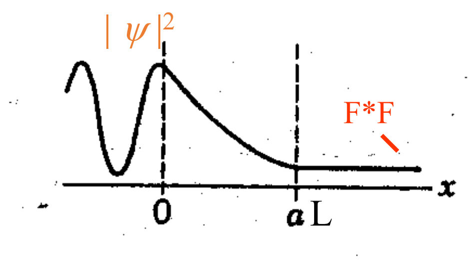
boundary matching and $|\psi|^2$ plot

(1) exclude $G\exp(-k_1 x)$ - no movement in -ve x in region III (G=0)

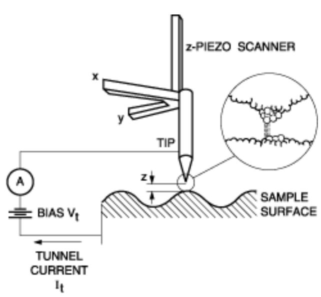
(2) <u>two</u> boundaries $x = 0$ and $x = L$

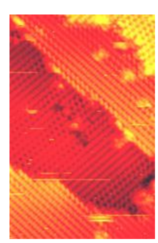
(3) $|\psi|^2$ plot

region I: mix of travelling/standing - partial reflection
region II: exponential decay profile
region III: pure travelling wave (transmitted particles)

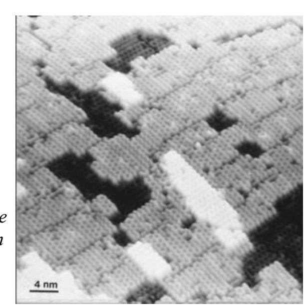


Scanning Tunneling Microscope (STM)





Ge on Si



Sharp point (tip) close (~ 1 nm) to surface; under bias electrons tunnel across the gap (barrier potential width z)

Because of exponential dependence on z (factor of ~10 for 1Å change when U_o ~ 4 eV), tunnel current is very sensitive to variations in z as tip is scanned across surface.

Keep current constant ⇒ z const. ⇒ tip height = image

Also, exponential dependence restricts to narrow <u>region</u> of tunneling, giving "atomic" resolution. ⇒ Imaging atoms…