

Topic 9: Quantum propagation

Outline:

- wavepacket propagation
- quantum mechanical currents
- potential step
- potential barrier
- quantum mechanical tunnelling
- the HUP for time and energy
- QM tunnelling in nature

Wavepacket propagation

Wavepacket propagation

Recall

- a wavepacket consisting of a **continuous** spectrum of momenta p

e.g., unbound (free) states, or bound states in x -dependent potential $V(x)$

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp \phi(p) \exp\left(\frac{i}{\hbar} px\right)$$

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Below we will consider some simplified cases.

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Below we will consider some simplified cases.

First let's introduce some useful and general language.

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$$j(x, t) = -i\frac{\hbar}{2m} \left[\Psi^*(x, t) \frac{\partial \Psi(x, t)}{\partial x} - \Psi(x, t) \frac{\partial \Psi^*(x, t)}{\partial x} \right]$$

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- if $\Psi(x, t)$ is a solution of the TDSE, then $P(x, t)$ and $j(x, t)$ satisfy a continuity equation

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- Physical interpretation: conservation of probability.
The change of the probability density at x is equal to its “outflow” from there.
- Analogous to: electric charge current, gas density and flow, etc.

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- take $\psi(x)$ to be a real function (like in bound states)

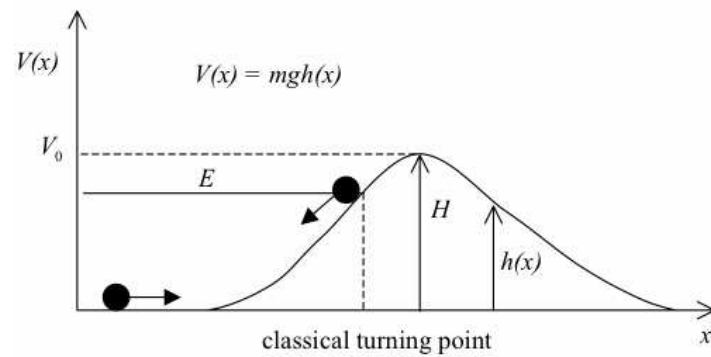
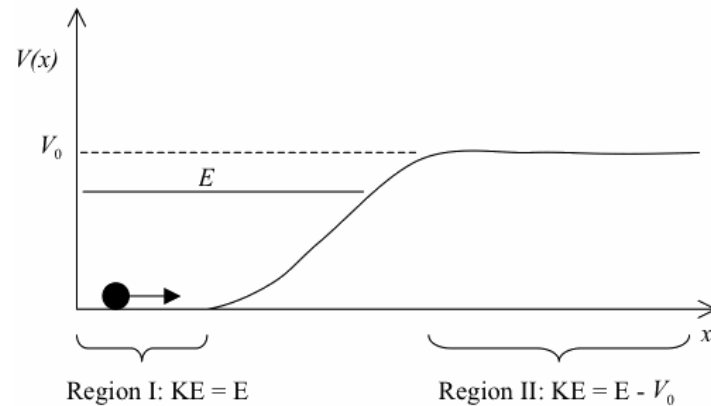
$$j(x, t) = 0$$

Interpretation: a bound state of definite energy is a standing wave.

Classical Potential Steps and Barriers

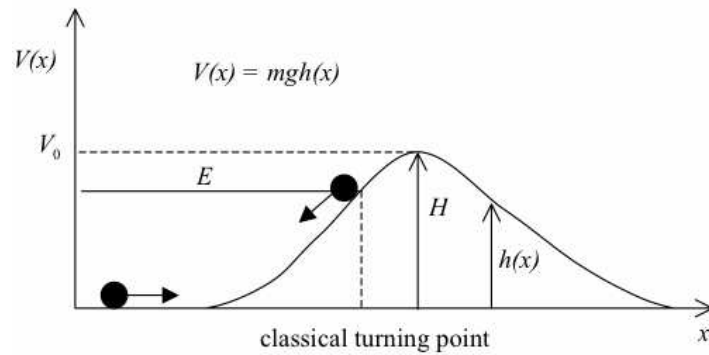
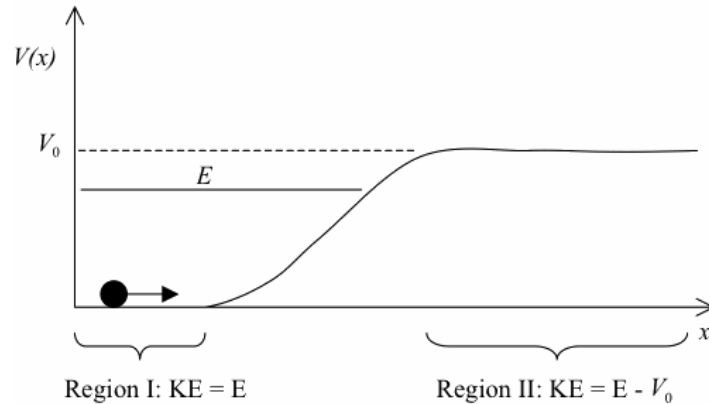
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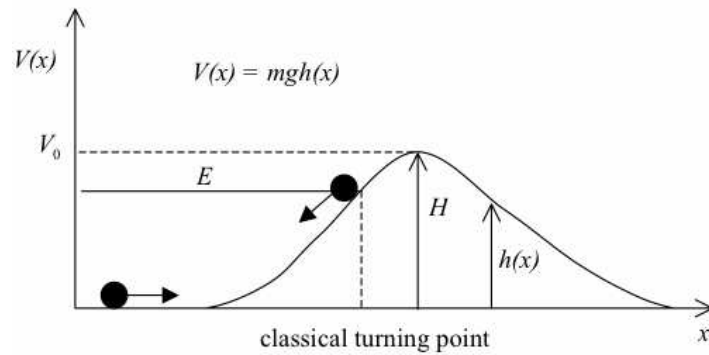
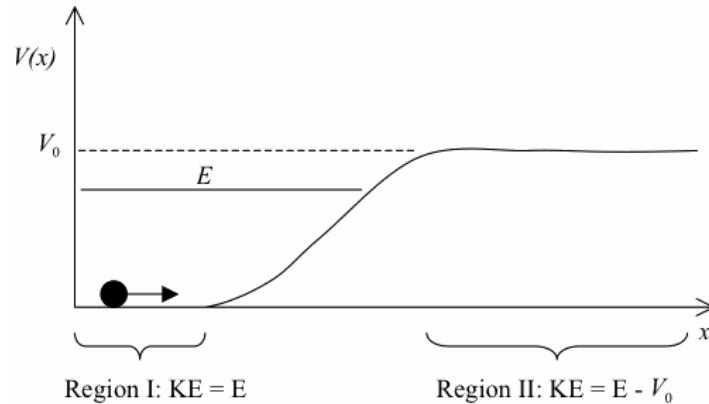


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- if $E > V_0$, all the particles will pass over the step/barrier (they are transmitted)
- they will slow down (smaller momentum)
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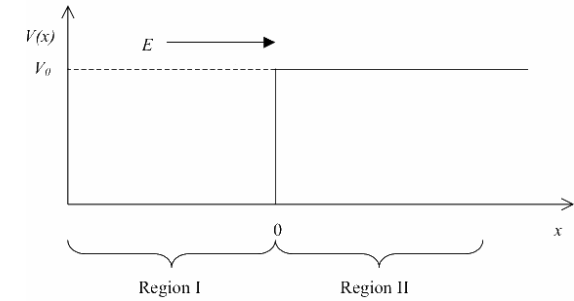
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In both cases the flux of particles must be the same. (They don't sink anywhere.)

Quantum mechanical potential step

Quantum mechanical potential step

Consider a flux of particles with total energy E incident from the left on a square potential step. Assume $E > V_0$.



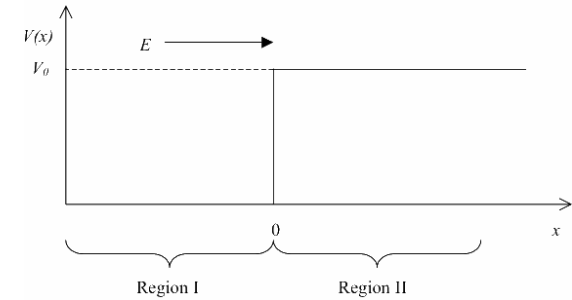
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$$\Rightarrow \psi''(x) = -k_1^2 \psi(x) \quad k_1^2 = \frac{2mE}{\hbar^2} > 0$$



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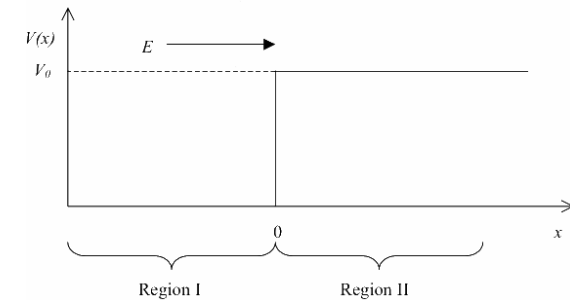
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The physical solutions are

$$\psi_I(x) = \underbrace{A \exp(ik_1 x)}_{\text{incident}}$$



$$\text{KE: } T_1 = \frac{\hbar^2 k_1^2}{2m} = E$$

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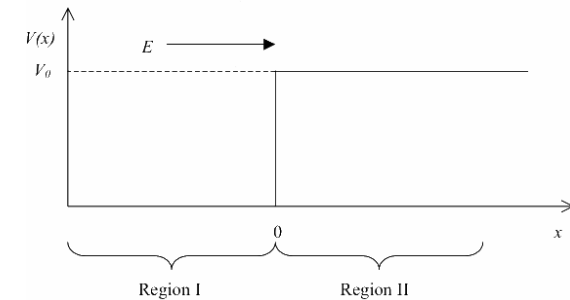
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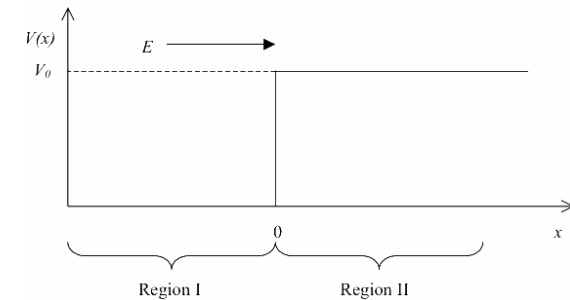
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A, R – (complex) amplitudes

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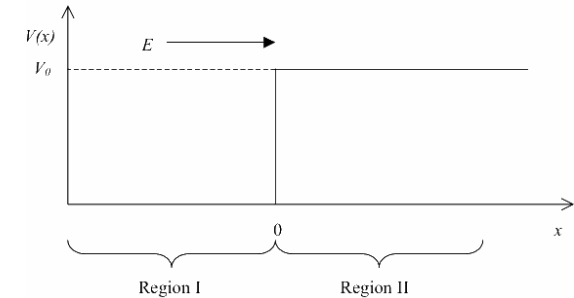
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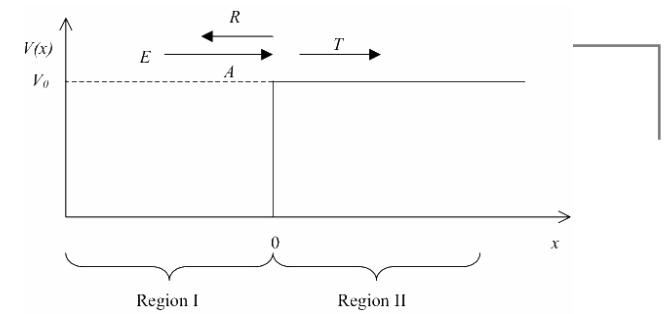
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$$\psi_{II}(x) = \underbrace{T \exp(ik_2 x)}_{\text{transmitted}}$$

T – (complex) amplitude

Reflection and transmission

Compute the currents:



Reflection and transmission

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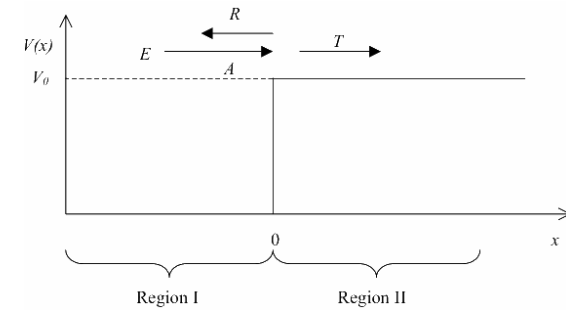
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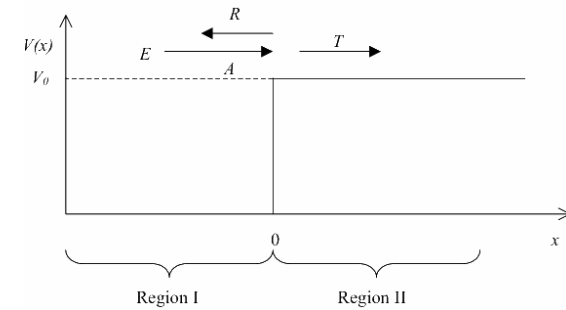
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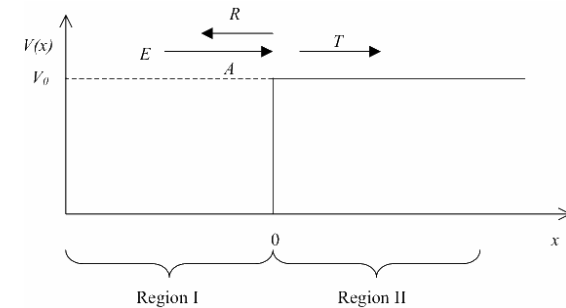
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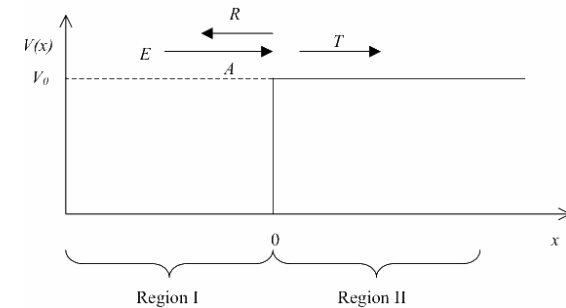
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$$P_R = \frac{|j_R|}{|j_I|} = \frac{|R|^2 k_1 \hbar / m}{|A|^2 k_1 \hbar / m} = \frac{|R|^2}{|A|^2} = \left| \frac{R}{A} \right|^2$$

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• the probability of transmission P_T

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Note:

$$P_R + P_T = 1$$

This is a reflection of the fact that the current is conserved,

$$j_I + j_R = j_T$$

(proof)

QM potential step

Comments:

$$k_1^2 = \frac{2mE}{\hbar^2}, k_2^2 = \frac{2m(E - V_0)}{\hbar^2}$$

• in the limit of a vanishing step, $V_0 \searrow 0$ or large energy, $E \gg V_0$:

$$k_2 \nearrow k_1 \quad \Rightarrow \quad P_R \searrow 0 \quad P_T \nearrow 1$$

QM potential step - cont.

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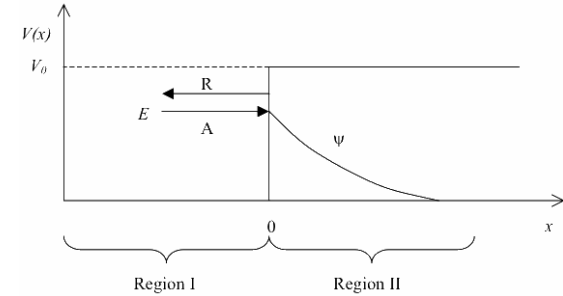
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$$\Rightarrow \psi''(x) = \alpha^2 \psi(x) \quad \alpha^2 = \frac{2m(V_0 - E)}{\hbar^2} > 0$$

The solution is

$$\psi_{II}(x) = \underbrace{T \exp(-\alpha x)}_{\text{tunnelling}}$$

KE: $T_2 = E - V_0 < 0!$

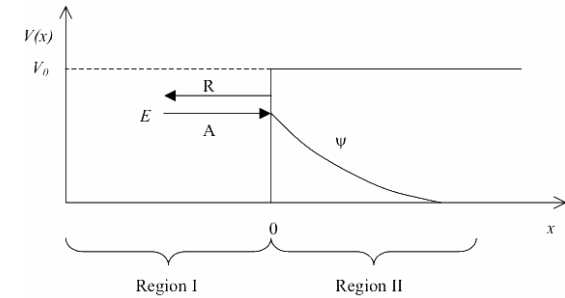
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$$\Rightarrow \psi''(x) = \alpha^2 \psi(x) \quad \alpha^2 = \frac{2m(V_0 - E)}{\hbar^2} > 0$$

The solution is

$$\psi_{II}(x) = \underbrace{T \exp(-\alpha x)}_{\text{tunnelling}}$$

KE: $T_2 = E - V_0 < 0!$

● the wavef'n $\psi_{II}(x)$ is real \Rightarrow the current $j_T = 0$

\Rightarrow the probability of transmission $P_T = 0 \Rightarrow P_R = 1 - P_T = 1$

The whole beam is reflected.

as expected

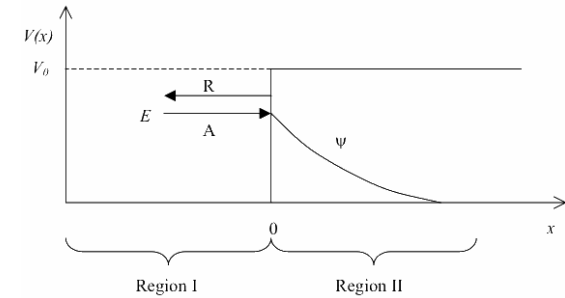
QM potential step - cont.

Consider next $E < V_0$

- $x < 0$ (Region I): $k_1^2 = \frac{2mE}{\hbar^2} > 0$

The solutions are the same as for $E > V_0$,

$$\psi_I(x) = \underbrace{A \exp(ik_1x)}_{\text{incident}} + \underbrace{R \exp(-ik_1x)}_{\text{reflected}}$$



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- the penetration (tunneling) depth is $1/\alpha = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$

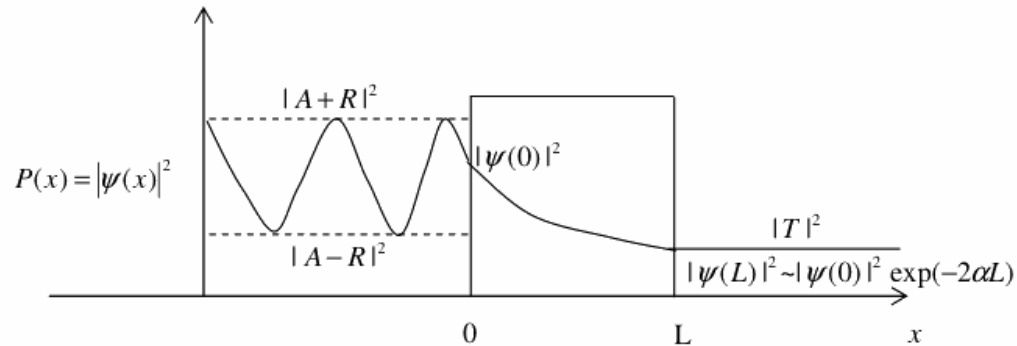
Tunnelling through a barrier

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- If the step has a finite length L

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See also <http://yepes.rice.edu/PhysicsApplets/WavePacket.html>

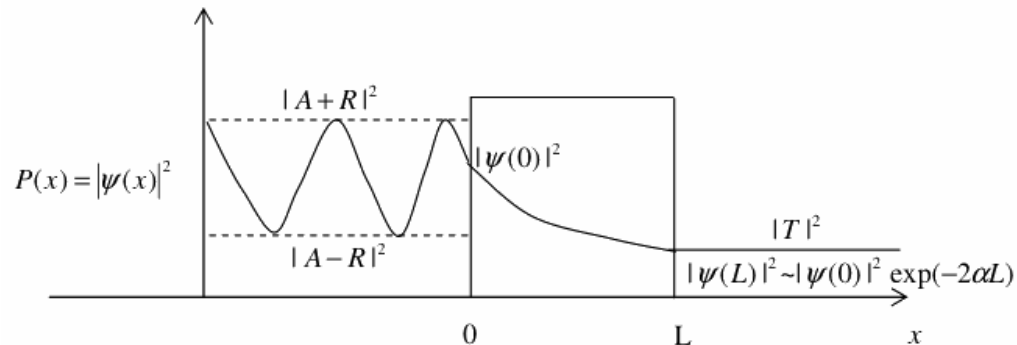
- particle tunnelling between classically allowed regions can take place

$$P_T \simeq |\psi(L)|^2 \simeq |\psi(0)|^2 \exp(-2\alpha L)$$

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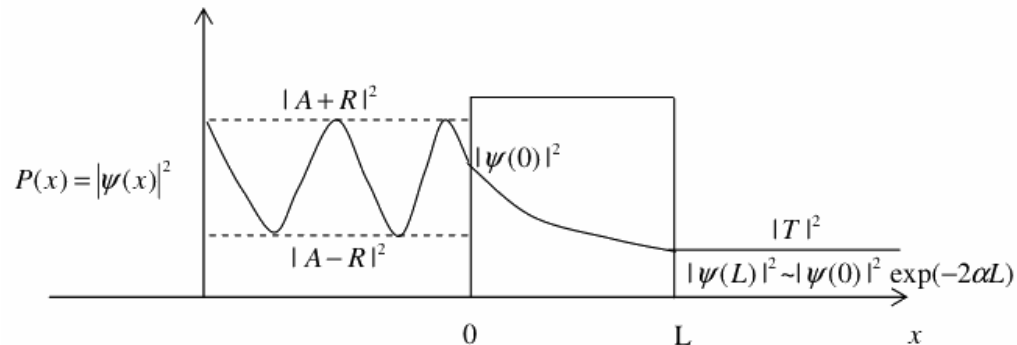
- The HUP for time and energy:

let ΔE denote the uncertainty in the energy of the particle as it tunnels through the barrier and Δt the time needed to pass through it. Then

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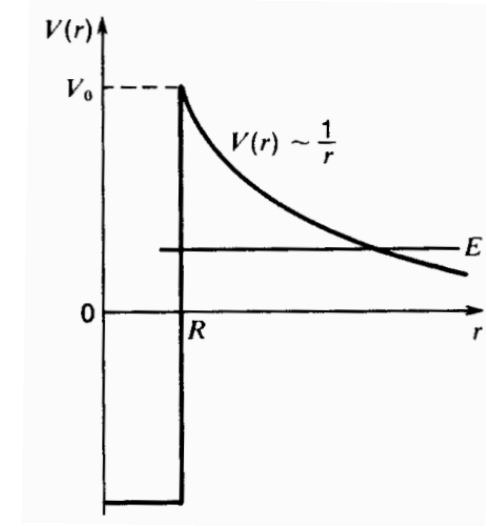
- during tunnelling the conservation of energy is violated but the HUP prevents us from observing it experimentally

Tunnelling in nature - examples

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α particles (${}^4\text{He}$) tunnel through a nuclear potential barrier arising from the Coulomb repulsion



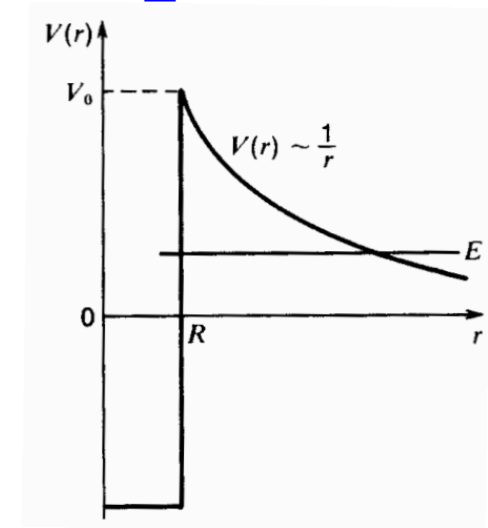
Tunnelling in nature - examples

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Nuclear fusion is essentially the inverse of α -decay. Here light nuclei tunnel through the Coulomb barrier to form a strongly bound state. Quantum mechanical tunnelling is necessary to explain nuclear fusion in stars.



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- **covalent bonding**

Chemical bonding occurs via the tunnelling of electrons between nuclei. The electrons “resonate” between nuclei, thus lowering their energy and forming a bond.

