

Quantum Mechanics - Brief Recap

The wavefunction $\psi(x,t)$ (considering 1D) is governed by Schrödinger's equation -

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}\psi(x,t) + V(x,t)\psi$$

For time independent potential V(x), we can use separation of variables - $\psi(x,t) = X(x)T(t)$

Substituting back in Schrödinger's equation -

$$Xi\hbar \frac{dT}{dt} = \frac{-\hbar^2}{2m} T \frac{d^2X}{dx^2} + V(x)XT$$

Quantum Mechanics Brief Recap – Contd.

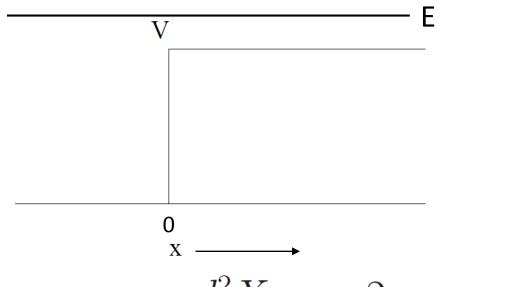
Dividing by $\psi(x,t)$ and setting both sides equal to constant E -

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

$$T(t) = Ae^{-iEt/\hbar}$$

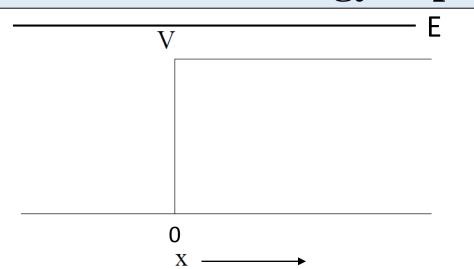
$$\psi(x,t) = Ae^{-iEt/\hbar}X(x)$$

To obtain X(x), we need to solve - $\frac{\hbar^2}{2m}\frac{d^2X}{dx^2} = -[E-V(x)]X$



We have to solve for -

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



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For right-side, the momentum is - $p' = \sqrt{2m(E - V)}$

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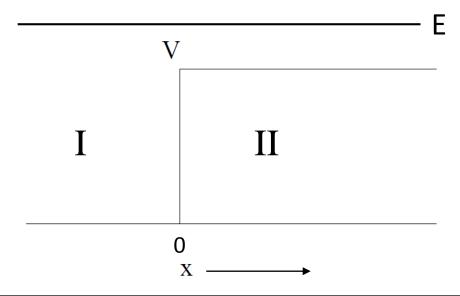
$$\frac{d^2X}{dx^2} = \frac{-p'^2}{\hbar^2}X$$

$$X(x) = A_1' e^{ip'x/\hbar} + A_2' e^{-ip'x/\hbar}$$

Solution:
$$\psi_{II}(x,t) = e^{-iEt/\hbar} \left[A_1' e^{ip'x/\hbar} + A_2' e^{-ip'x/\hbar} \right]$$

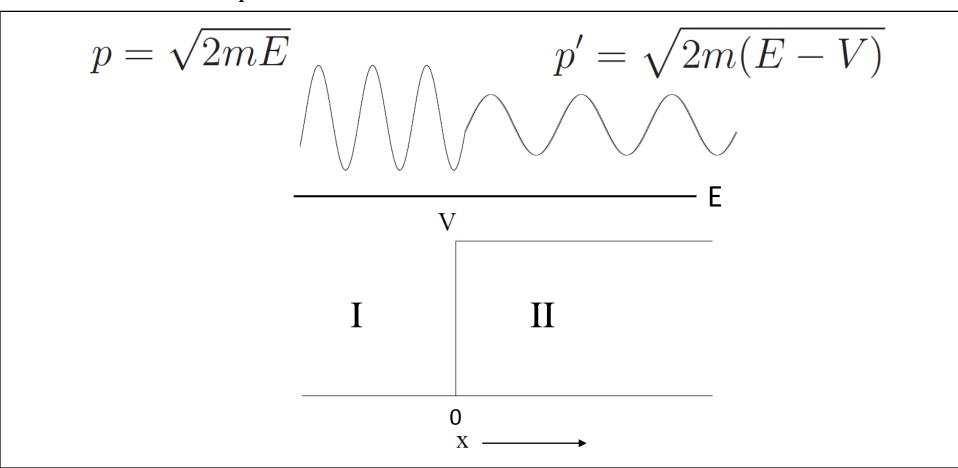
$$\psi_{I}(x,t) = e^{-iEt/\hbar} \left[A_1 e^{ipx/\hbar} + A_2 e^{-ipx/\hbar} \right]$$

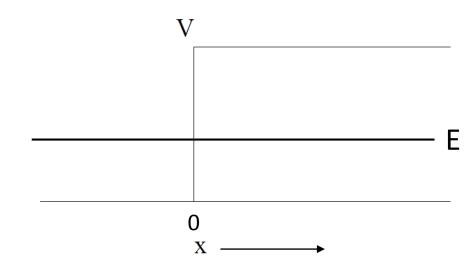
$$p = \sqrt{2mE} \qquad \qquad p' = \sqrt{2m(E - V)}$$



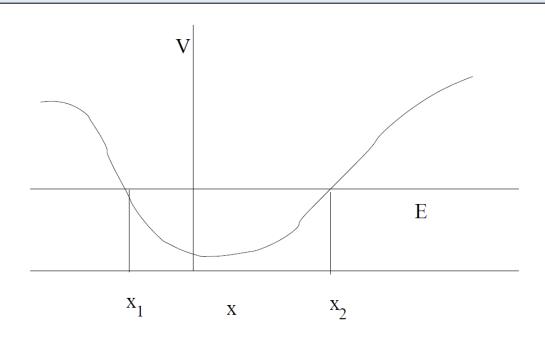
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$$\psi_{I}(x,t) = e^{-iEt/\hbar} \left[A_1 e^{ipx/\hbar} + A_2 e^{-ipx/\hbar} \right]$$





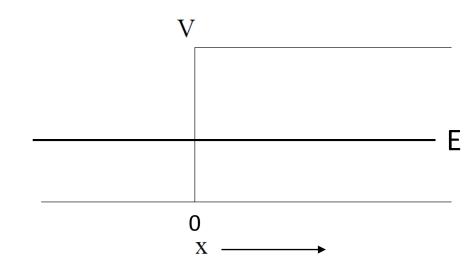
In Classical Mechanics



$$\frac{p^2}{2m} + V(x) = E \qquad p = \pm \sqrt{2m(E - V(x))}$$

In Classical Mechanics, the particle's motion is restricted between x_1 and x_2 , as otherwise p becomes imaginary

What happens in Quantum Mechanics?



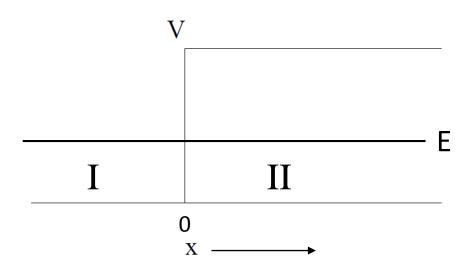
Defining -
$$\sqrt{2m(E-V)} = \sqrt{-1}\sqrt{2m(V-E)} = iq$$

$$\frac{d^2X}{dx^2} = \frac{q^2}{\hbar^2}X$$

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$$X(x) = A_1 e^{-qx/\hbar} + A_2 e^{qx/\hbar}$$



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To ensure wavefunction remains finite as $x \to +\infty$, $A_2 = 0$

$$X_{\mu}(x) = A_1 e^{-qx/\hbar}$$

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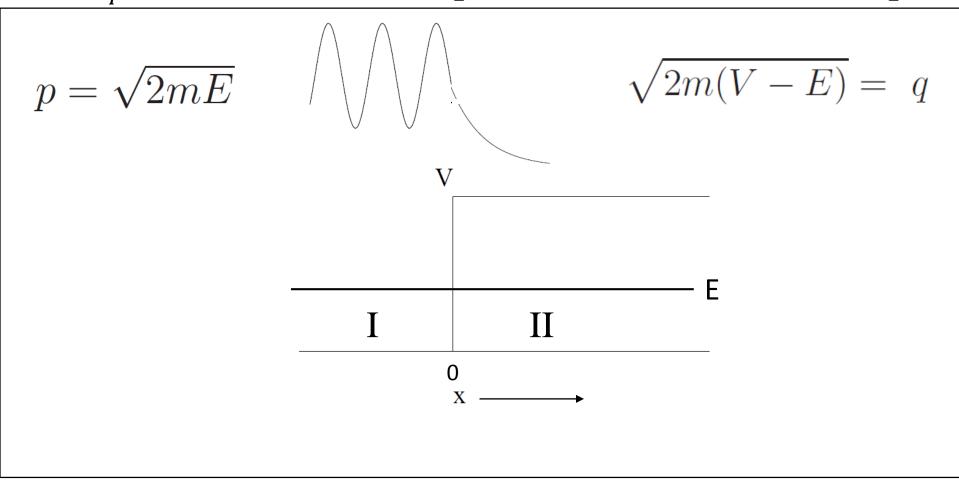
To ensure wavefunction remains finite as $x \to +\infty$, $A_2 = 0$

$$X_{n}(x) = A_{1}e^{-qx/\hbar}$$

Total solution for within the potential step - $\psi_{_{\! I\! I}}(x,t)=A_1e^{-iEt/\hbar}e^{-qx/\hbar}$

$$\psi_{II}(x,t) = A_1 e^{-iEt/\hbar} e^{-qx/\hbar}$$

$$\psi_{I}(x,t) = e^{-iEt/\hbar} \left[A_1 e^{ipx/\hbar} + A_2 e^{-ipx/\hbar} \right]$$



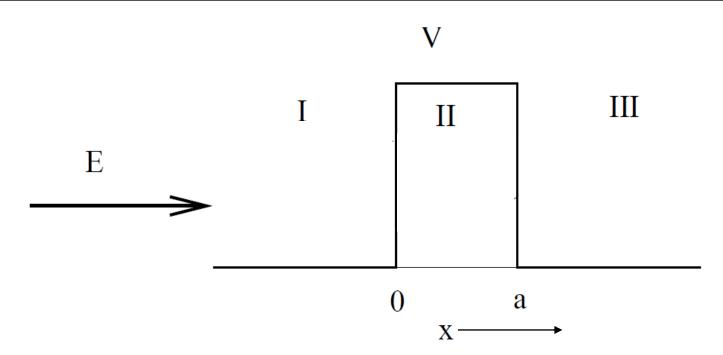
$$\psi_{I}(x,t) = A_1 e^{-iEt/\hbar} e^{-qx/\hbar}$$

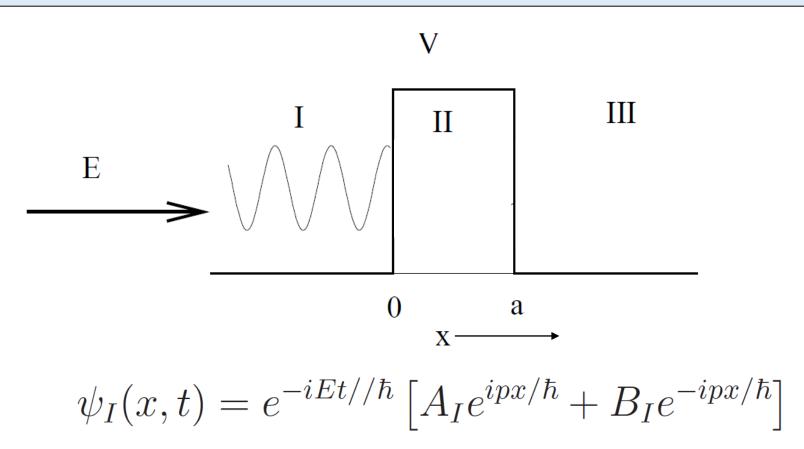
$$\psi_{I}(x,t) = e^{-iEt/\hbar} \left[A_1 e^{ipx/\hbar} + A_2 e^{-ipx/\hbar} \right]$$

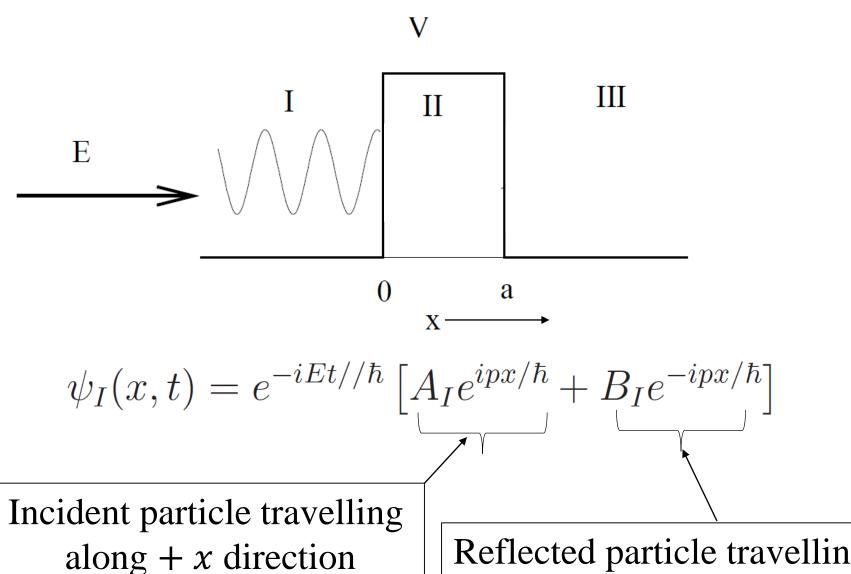
$$p = \sqrt{2mE}$$

$$\sqrt{2m(V-E)} = q$$

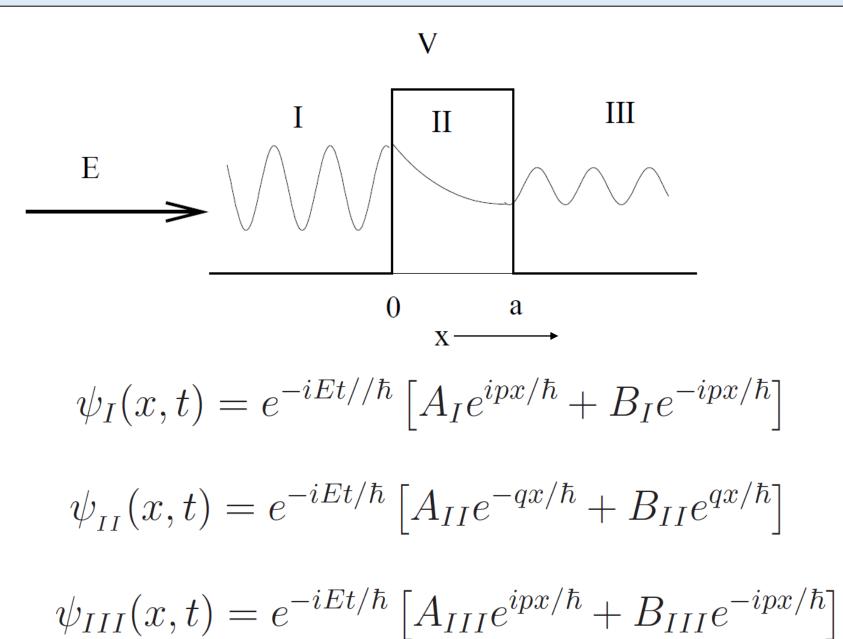
$$\sqrt{2m(V-E)} = q$$
 So finite probability of finding particle within barrier for E

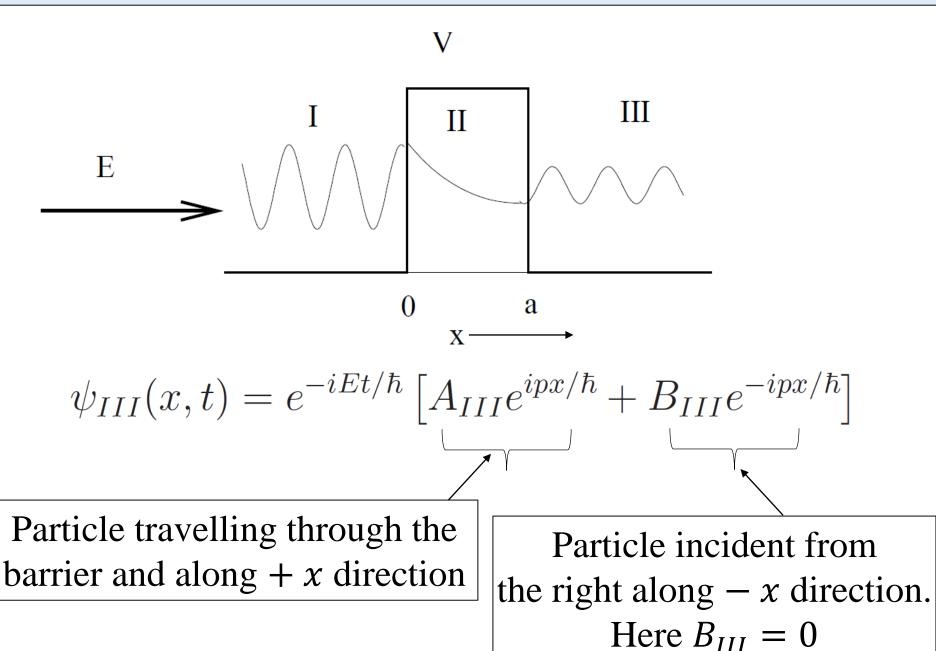


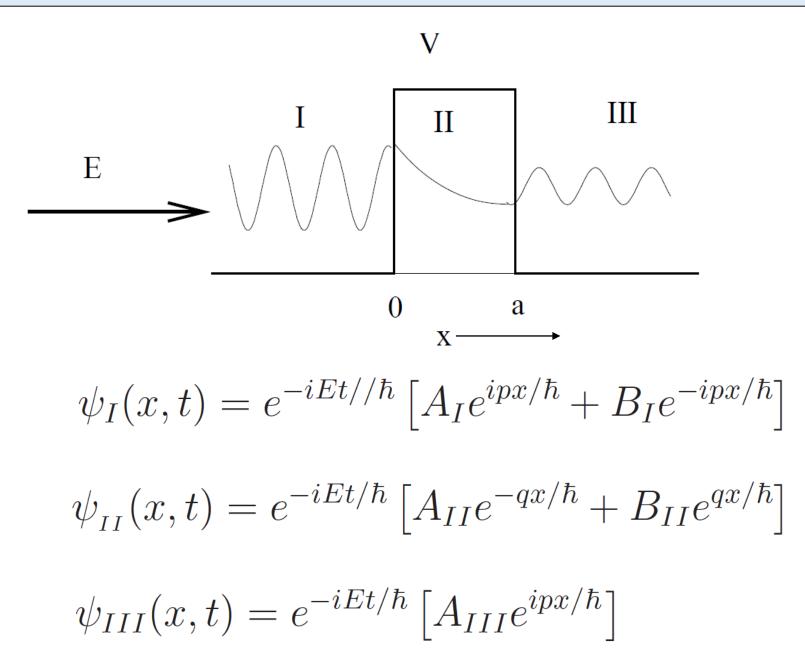


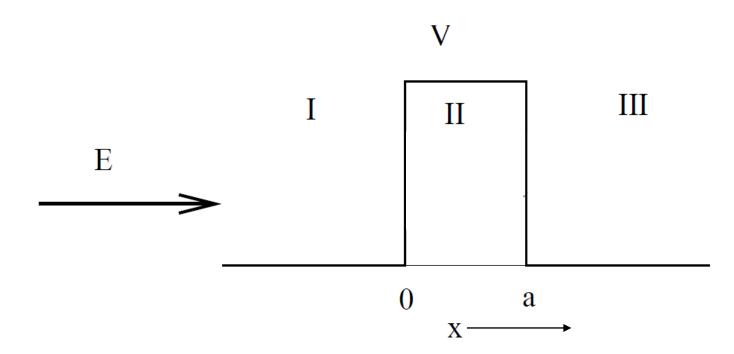


Reflected particle travelling along -x direction









Boundary conditions to be satisfied at x = 0 –

$$\psi_I(0,t) = \psi_{II}(0,t)$$

$$\left(\frac{\partial \psi_I}{\partial x}\right)_{x=0} = \left(\frac{\partial \psi_{II}}{\partial x}\right)_{x=0}$$

Origin of boundary conditions

The wavefunction $\psi(x,t)$ (considering 1D) is governed by Schrödinger's equation -

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Further assumption for ease of calculation

Let us assume that the potential step is very high, i.e. $V\gg E$

$$q = \sqrt{2m(V - E)} \approx \sqrt{2mV}$$

$$p = \sqrt{2mE}$$

$$\frac{p}{a} = \sqrt{\frac{E}{V}} \ll 1$$

$$\psi_{I}(x,t) = e^{-iEt//\hbar} \left[A_{I} e^{ipx/\hbar} + B_{I} e^{-ipx/\hbar} \right]$$

$$\psi_{II}(x,t) = e^{-iEt/\hbar} \left[A_{II} e^{-qx/\hbar} + B_{II} e^{qx/\hbar} \right]$$

Applying boundary conditions at x = 0

$$\psi_I(0,t) = \psi_{II}(0,t) \implies A_I + B_I = A_{II} + B_{II}$$

$$\left(\frac{\partial \psi_I}{\partial x}\right)_{x=0} = \left(\frac{\partial \psi_{II}}{\partial x}\right)_{x=0} \Rightarrow ip\left(A_I - B_I\right) = -q\left(A_{II} - B_{II}\right)$$
$$A_I - B_I = \frac{iq}{n}\left(A_{II} - B_{II}\right)$$

$$\psi_{II}(x,t) = e^{-iEt/\hbar} \left[A_{II} e^{-qx/\hbar} + B_{II} e^{qx/\hbar} \right]$$

$$\psi_{III}(x,t) = e^{-iEt/\hbar} \left[A_{III} e^{ipx/\hbar} \right]$$

Applying boundary conditions at x = a

Wavefunction continuity -

$$A_{II}e^{-qa/\hbar} + B_{II}e^{qa/\hbar} = A_{III}e^{ipa/\hbar}$$

First deriavative continuity -

$$-q\left[A_{II}e^{-qa/\hbar} - B_{II}e^{qa/\hbar}\right] = ipA_{III}e^{ipa/\hbar}$$

$$A_{II}e^{-qa/\hbar} - B_{II}e^{qa/\hbar} = \frac{-ip}{q}A_{III}e^{ipa/\hbar}$$

Applying boundary conditions at x = a

First deriavative continuity -

$$A_{II}e^{-qa/\hbar} - B_{II}e^{qa/\hbar} = \frac{-\imath p}{q}A_{III}e^{ipa/\hbar}$$

Since - $p/q \ll 1$

$$A_{II}e^{-qa/\hbar} - B_{II}e^{qa/\hbar} = 0$$

$$B_{II} = e^{-2qa/\hbar} A_{II} \ll A_{II}$$

Small

$$\psi_{II}(x,t) = e^{-iEt/\hbar} \left[A_{II} e^{-qx/\hbar} + B_{II} e^{qx/\hbar} \right]$$

Wavefunction continuity at x = a

$$A_{II}e^{-qa/\hbar} + B_{II}e^{qa/\hbar} = A_{III}e^{ipa/\hbar}$$

Also from last slide - $A_{II}e^{-qa/\hbar} - B_{II}e^{qa/\hbar} = 0$

$$A_{III} = 2e^{-ipa/\hbar}e^{-qa/\hbar}A_{II}$$

Wavefunction continuity at x = a

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$$A_{III} = 2e^{-ipa/\hbar}e^{-qa/\hbar}A_{II}$$

Recalling boundary conditions at x = 0

$$A_I + B_I = A_{II} + B_{II} \quad \& \quad A_I - B_I = \frac{iq}{p} \left(A_{II} - B_{II} \right)$$

$$\left(1 + \frac{iq}{p} \right) A_{II} = 2A_I$$

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Since $q/p \gg 1$

$$A_{II} = -\frac{ip}{q} 2A_I$$

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Since $q/p \gg 1$

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Also from last slide -

$$A_{III} = 2e^{-ipa/\hbar}e^{-qa/\hbar}A_{II}$$

$$A_{III} = -4i\frac{p}{q} e^{-ipa/\hbar} e^{-qa/\hbar} A_I$$

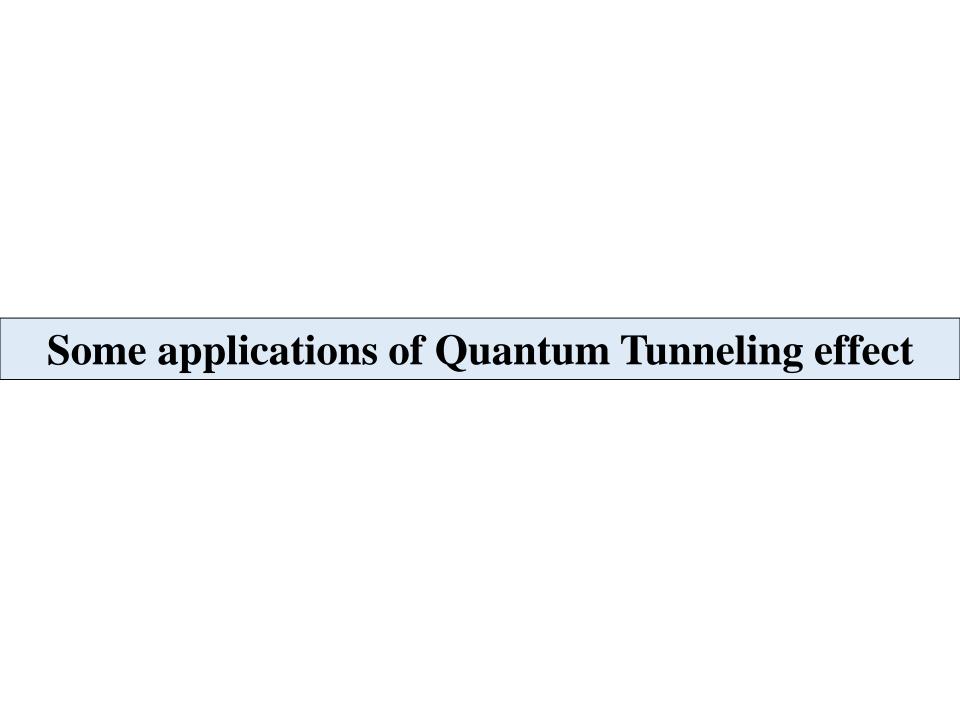
$$A_{III} = -4i\frac{p}{q} e^{-ipa/\hbar} e^{-qa/\hbar} A_I$$

The transmission coefficient T is -

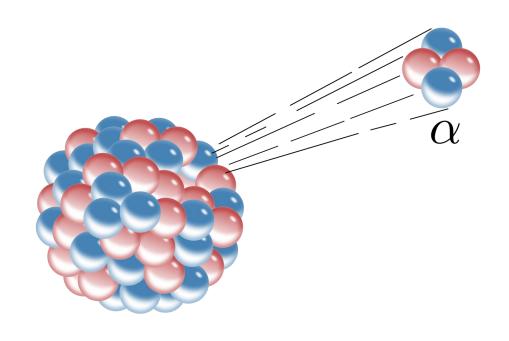
$$T = \frac{|A_{III}|^2}{|A_I|^2} = 16\frac{p^2}{q^2}e^{-2qa/\hbar}$$

Since -
$$\frac{p}{q} = \sqrt{\frac{E}{V}} \ll 1$$

$$T = 16 \frac{E}{V} e^{-2a\sqrt{2mV}/\hbar}$$



Alpha Decay



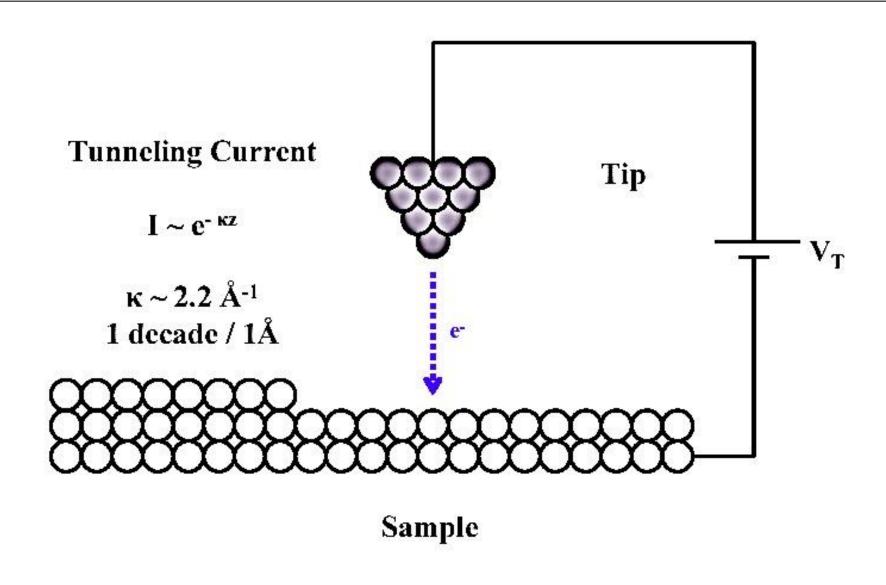
Alpha particle (a Helium-4 nucleus) is held within nucleus by nuclear forces.

It experiences a potential barrier to come outside the nucleus.

Still Alpha particles can come outside nucleus because of tunneling

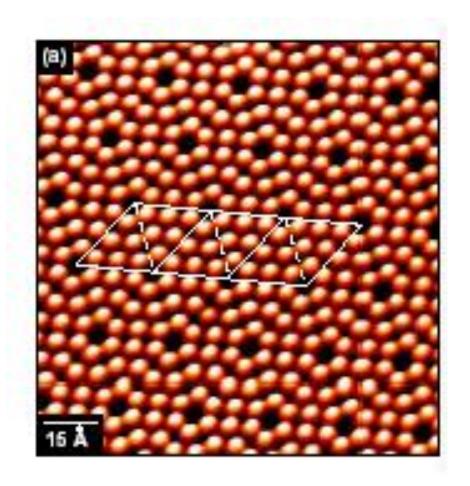
Source of image: Wikipedia

Scanning Tunneling Microscope



Electron tunneling across the air gap

Scanning Tunneling Microscope



STM scan of a Si sample Each bright spot indicates a Si atom