Chapter 6 – 1D Problems: Unbound States

UM-SJTU Joint Institute
Modern Physics (Summer 2020)
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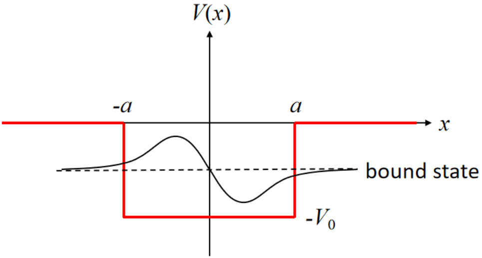
Agenda

Introduction

Introduction



⋆ **Bound States**

If $-V_0 < E < 0$, then the particle moves between two classical turning points (may penetrate into classically forbidden region though) and $\int_{-\infty}^{\infty} |\psi|^2 \, dx < \infty$.

⋆ **Unbound States**

If $E > 0$, then classically, the kinetic energy of the particle is positive for any x and there is no classically-forbidden region.

Eigenvalues and Eigenfunctions of the Momentum Operator

Momentum Operator

Recall the form of the momentum operator

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}.$$

Find eigenvalues and eigenfunctions

$$\hat{p}_x \phi(x) = p_x \phi_x \quad \Longrightarrow \quad \begin{array}{c} -i\hbar \dfrac{\mathrm{d}\phi(x)}{\mathrm{d}x} = p_x \phi(x) \\ \Downarrow \\ \dfrac{\mathrm{d}\phi(x)}{\phi(x)} = \dfrac{i}{\hbar} p_x \mathrm{d}x \\ \Downarrow \\ \boxed{\phi(x) = Ce^{\frac{i}{\hbar} p_x x} = \phi_{p_x}(x)} \end{array}$$

Hence ϕ_{p_x} is the eigenfunction corresponding to eigenvalue p_x, which can be *any* real number.

Remarks

Summary

- $\star$ eigenvalues: $-\infty < p_x < \infty$
- $\star$ eigenfunctions: $\phi_{p_x}(x) = Ce^{\frac{i}{\hbar}p_x x}$

Comment

Note that ϕ_{p_x} is not square-integrable. This is a characteristic feature of unbound-state wave functions. We "normalize" eigenfunctions of $\hat{p}_x$ in the following way $\phi_{p_x}(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}p_x x}$. Then

$$\langle \phi_{p_x}, \phi_{p_{x'}} \rangle = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{\frac{i}{\hbar}(p_x' - p_x)x}\, \mathrm{d}x = \delta(p_x' - p_x).$$

Recall. The δ symbol here denotes the Dirac delta

$$\delta(u) = \begin{cases} 0, & \text{for } u \neq 0 \\ \infty, & \text{for } u = 0 \end{cases} \qquad \text{and} \qquad \int_{-\infty}^{\infty} \delta(u)\, \mathrm{d}u = 1$$

Free Quantum Particle

Schrödinger Equation for Free Quantum Particle

For a free quantum particle

$$V(x) \equiv 0 \qquad \text{and} \qquad E > 0,$$

and the stationary Schrödinger equation assumes the form

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi \qquad \Longleftrightarrow \qquad \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2mE}{\hbar^2}\psi = 0.$$

The general solution of the stationary Schrödinger equation for a free particle is therefore found as

$$\psi(x) = C_1 e^{ikx} + C_2 e^{-ikx},$$

with $k = \sqrt{\frac{2mE}{\hbar^2}}$. Equivalently, in terms of the momentum $(p_x = \hbar k)$,

$$\boxed{\psi(x) = C_1 e^{\frac{i}{\hbar}p_x x} + C_2 e^{-\frac{i}{\hbar}p_x x} = \psi_{p_x}(x)}$$

$$\boxed{E = \frac{\hbar^2 k^2}{2m} = \frac{p_x^2}{2m} = E_{p_x}}$$

Interpretation

Note that the wave function $\psi_{p_x}(x)$, which is the general solution to Schrödinger equation for free particle, is a linear combination of two eigenfunctions of $\hat{p}_x$

$$\psi_{p_x}(x) = C_1 e^{\frac{i}{\hbar} p_x x} + C_2 e^{-\frac{i}{\hbar} p_x x}$$

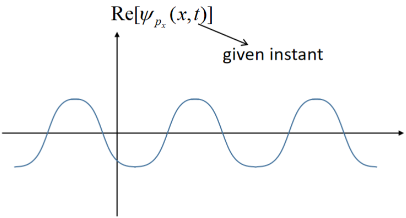
The term $C_1 e^{\frac{i}{\hbar} p_x x}$ represents the particle with momentum p_x, whereas the term $C_2 e^{-\frac{i}{\hbar} p_x x}$ represents the particle with the opposite momentum $-p_x$. But both particles have the same energy $E = \frac{p_x^2}{2m} = E_{p_x}$.

Note. Multiplying both sides of the expression for ψ_{p_x} by $e^{-\frac{i}{\hbar} E_{p_x} t}$, the full (time-dependent) solution is given by
$\Psi_{p_x}(x,t) = C_1 e^{\frac{i}{\hbar}(p_x x - E_{p_x} t)} + C_2 e^{-\frac{i}{\hbar}(-p_x x - E_{p_x} t)}$

Free Quantum Particle. Discussion

Problem: *The solution to Schrödinger equation for a free particle is not normalized!*

However, this is consistent with Heisenberg uncertainty principle: **definite momentum** $\Delta_{p_x} = 0$ implies **complete delocalization in space** $\Delta_x = \infty$.



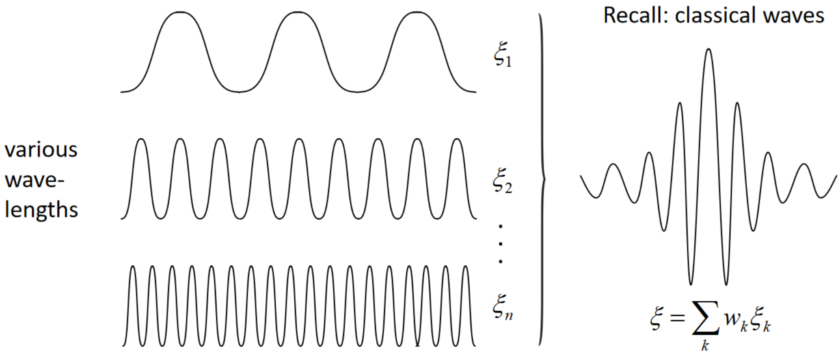
completely delocalized
(know nothing about the position)

How to Describe a (Partially) Localized Particle in QM?

Describing Partially Localized Particle

Question. Since $\Delta_{p_x}\,\Delta_x > \frac{\hbar}{2}$ prevents us from knowing simultaneously the position of a particle and its momentum with an arbitrarily small uncertainty, how to describe a (partially) localized particle in quantum mechanics?

Idea: Construct a wave-packet (superposition of free-particle wave functions)



Wave Packets

Here, de Broglie waves are superposed

$$\Psi(x,t) = \int_{-\infty}^{\infty} w(p_x) e^{\frac{i}{\hbar}(p_x x - Et)} \, \mathrm{d}p_x$$

where $w(p_x)$ is the weight (momentum distribution) and $e^{\frac{i}{\hbar}(p_x x - Et)}$ describes a particle with momentum p_x and energy $E = \frac{p_x^2}{2m}$.

free particle wave function (plane wave)
definite momentum
complete delocalization in space

$$\xrightarrow[\text{with different momenta}]{\text{superpostion of plane waves}}$$

wave packet
distribution of momentum
particles becomes more localized in space

It is a trade-off between <u>known position</u> and <u>known momentum</u>.

Gaussian Wave Packet

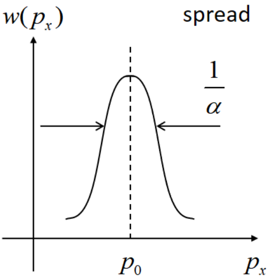
Example. Gaussian wave packet

$$w(p_x) = \sqrt{\frac{\alpha}{\sqrt{\pi}}} \exp[-\frac{1}{2}\alpha^2(p_x - p_0)^2].$$

For this weight function, the explicit form of $\Psi(x,t)$ can be found (tedious calculation!) and

$$|\Psi(x,t)|^2 = \frac{1}{\beta_t\sqrt{\pi}} \exp\left\{-\frac{(x - p_0 mt)^2}{\beta_t^2}\right\}$$

where $\beta_t = \alpha\hbar\sqrt{1 + \frac{t^2}{t_0^2}}$

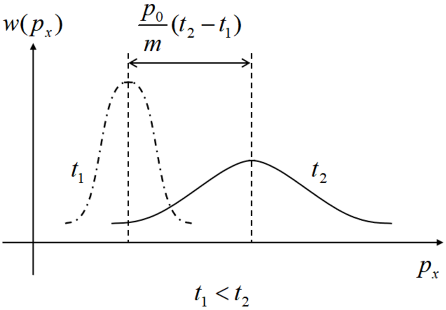


Gaussian

Features of Gaussian Wave Packet

$$|\Psi(x,t)|^2 = \frac{1}{\beta_t\sqrt{\pi}} \exp\left\{-\frac{(x - p_0 mt)^2}{\beta_t^2}\right\}, \quad \text{where} \quad \beta_t = \alpha\hbar\sqrt{1 + \frac{t^2}{t_0^2}}$$

- Describes a localized particle travelling with speed $\frac{p_0}{m}$.
- The shape of $|\Psi(x,t)|^2$ depends on time: it spreads with time (and well-located packets spread faster).

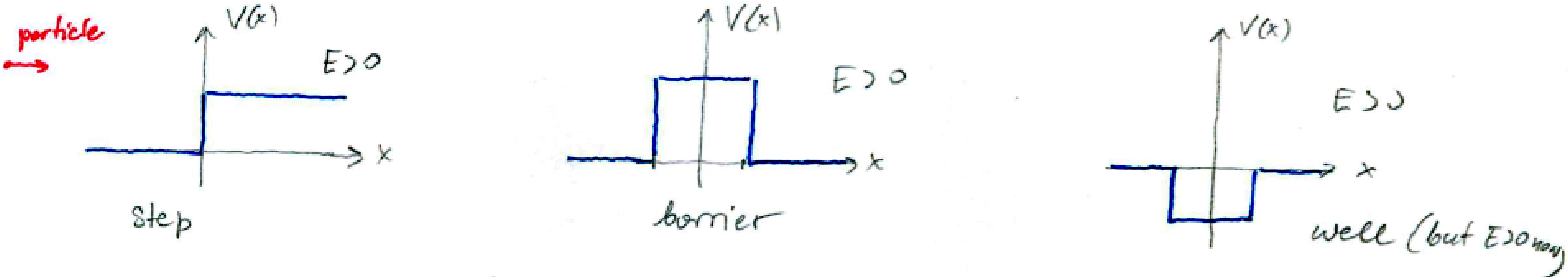


- Gaussian wave packet saturates the Heisenberg uncertainty principle at $t = 0$, that is $\Delta_x^{(\Psi)} \Delta_{p_x}^{(\Psi)} = \frac{\hbar}{2}$.

Scattering and Tunneling in 1D

1D Scattering. Introduction

Consider a particle moving from -∞ in one of the following 1D potential fields



General question: What happens to the particle that starts from x=-∞, and is incident on a potential step/barrier/well?

General answer: It may either bounce back or continue traveling in the positive *x*-axis direction.

What are the probabilities of these two outcomes?

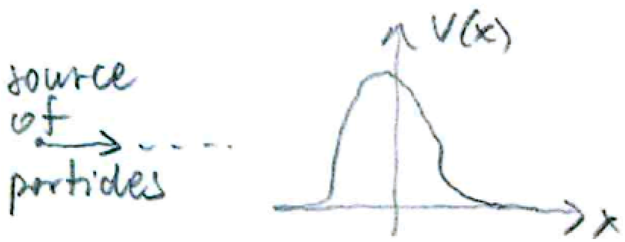
1D Scattering. Normalization

In general, in all these situations, the wave function of the particle is of the form

$$\Psi(x,t) = \underbrace{C_1 e^{i(kx-\omega t)}}_{\text{particle traveling to the right } (\rightarrow)} + \underbrace{C_2 e^{i(-kx-\omega t)}}_{\text{particle traveling to the left } (\leftarrow)} \qquad \text{where} \quad k = p/\hbar, \quad \omega = E/\hbar$$

Recall that such functions are not square-integrable.

How do we normalize wave functions in scattering problems?



$$|\Psi(x,t)|^2 dx = \rho \, dx = dN \quad \text{\# of particles in } (x, x+dx) \text{ at instant } t$$

$$\int_a^b |\Psi(x,t)|^2 dx = \text{\# of particles in } (a,b) \text{ at instant } t$$

Note. The wave-function is not dimensionless, it has units! $[\Psi] = \left[\frac{1}{\sqrt{m}}\right]$

1D Scattering. Normalization - Explanation

$$\Psi(x,t) = 10\left[\frac{1}{\sqrt{m}}\right] e^{i(kx-\omega t)}$$

↳ particle traveling (→) with momentum $\hbar k_0$

$$|\Psi(x,t)|^2 = 100\left[\frac{1}{m}\right]$$

contains 100 particles moving (→) with momentum $\hbar k_0$

1D Scattering. Probability Current Density

Fundamental quantity in scattering problems – **probability current density**

$$j_x(x,t) \stackrel{def}{=} \frac{\hbar}{2mi}\Big[\Psi^* \frac{\partial \Psi}{\partial x} - \underbrace{\Psi \frac{\partial \Psi^*}{\partial x}}_{\text{c.c.}}\Big]$$

c.c. – complex conjugate

Comments:

(1) for stationary states $\Psi(x,t) = e^{-i\omega t}\psi(x)$ and $j_x = j_x(x) = \frac{\hbar}{2mi}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right]$

(2)* this definition follows from a continuity eqn.: $\frac{\partial |\Psi|^2}{\partial t} + \frac{\partial j_x}{\partial x} = 0$ (see appendix*)

1D Scattering. Current Density - Examples

(1) particle traveling to the right with momentum $\hbar k$ and energy $\hbar\omega$

$$\Psi(x,t) = C\, e^{i(kx-\omega t)}$$

$$j_x(x,t) = j_x(x) = \frac{\hbar}{2mi}\left[C^* \cancel{e^{-ikx}}(ik)\, C\, e^{ikx} - C\cancel{e^{ikx}}(-ik)\, C^* e^{-ikx}\right]$$

$$= \underbrace{\frac{\hbar k}{m}}_{\text{velocity}} |C|^2 \quad \text{— compare with classical current density}$$

(1) particle described by the wave function

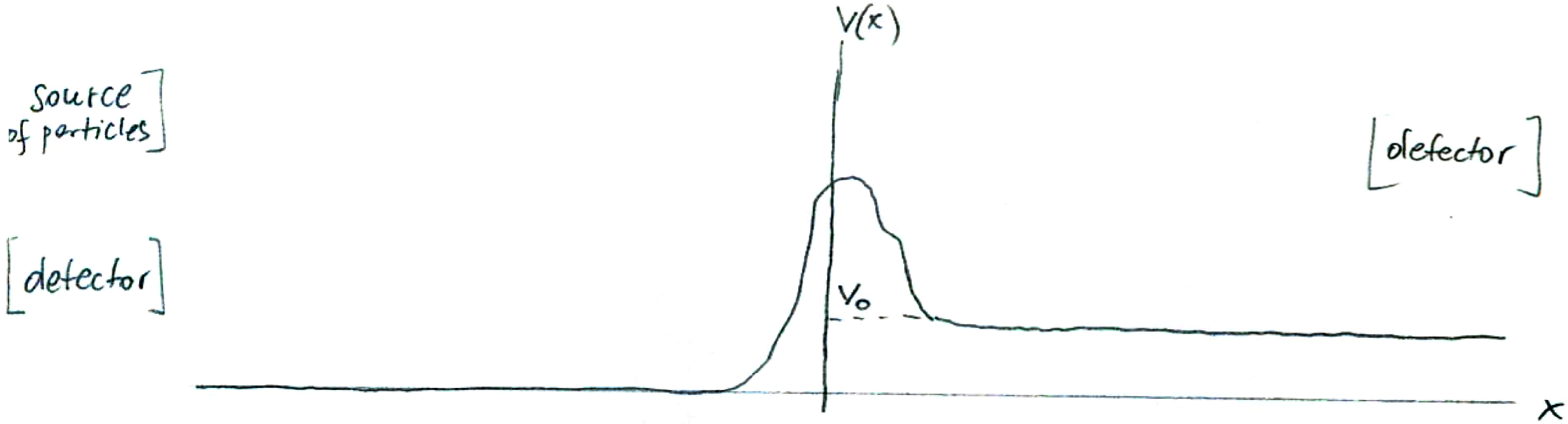
$$\Psi(x,t) = \underbrace{f(x)}_{\text{real function}}\, e^{-i\omega t}$$

(cf. particle in
a classically forbidden region)

Exercise: show that the current is zero.

Generic 1D Scattering Problem

Generic 1D Scattering Problem



Stationary Schrödinger equation (suppose that the particle's energy is $E > V_0$)

at $x \ll 0$ $\quad (V(x) = 0)$

$$-\frac{\hbar^2}{2m}\psi'' = E\psi$$

$$\psi'' + k_1^2\psi = 0\,, \qquad k_1^2 = \frac{2mE}{\hbar^2} > 0$$

$$E = \frac{\hbar^2 k_1^2}{2m} = \hbar\omega_1$$

at $x \gg 0$ $\quad (V(x) = V_0)$

$$-\frac{\hbar^2}{2m}\psi'' + V_0\psi = E\psi$$

$$\psi'' + k_2^2\psi = 0\,, \qquad k_2^2 = \frac{2m}{\hbar^2}(E - V_0) > 0$$

$$E = \frac{\hbar^2 k_2^2}{2m} + V_0 = \hbar\omega_2$$

Conservation of energy implies

$$\hbar\omega_1 = \hbar\omega_2 = \hbar\omega \qquad (\text{but } k_1 \neq k_2 \text{ in general})$$

Generic 1D Scattering Problem

Hence, the full solutions (stationary states)

at $x \ll 0$ $\quad (V(x)=0)$

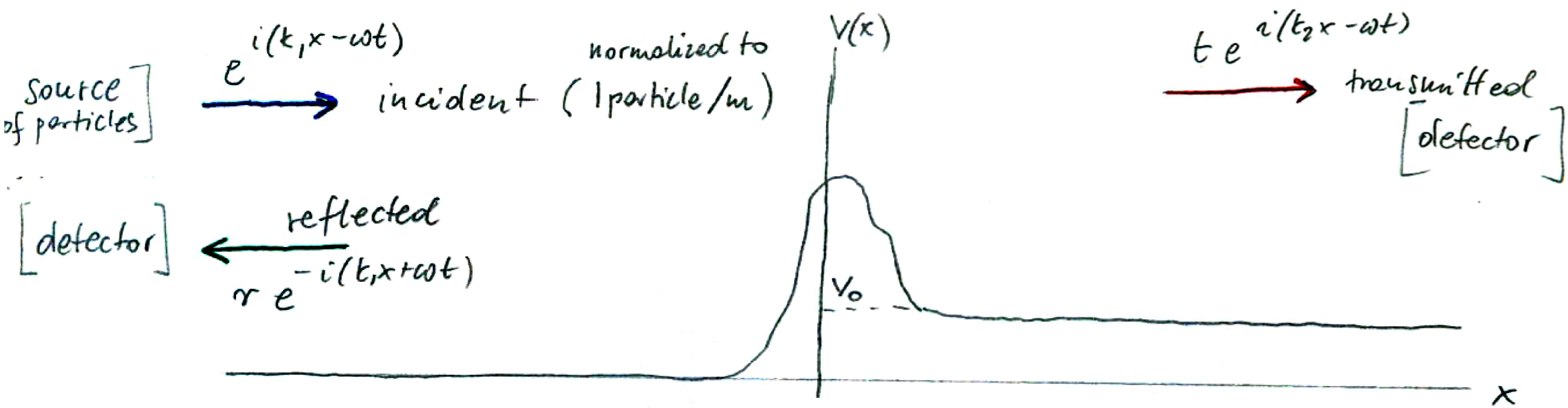
$$\Psi(x,t) = \underbrace{e^{i(k_1x-\omega t)}}_{\Psi_{inc}} + \underbrace{r\,e^{-i(k_1x+\omega t)}}_{\Psi_{ref}}$$

at $x \gg 0$ $\quad (V(x)=V_0)$

$$\Psi(x,t) = \underbrace{t\,e^{i(k_2x-\omega t)}}_{\Psi_{trans}}$$

Note: no particles travelling from $+\infty$ towards $-\infty$ (no term $\sim e^{-i(kx+\omega t)}$)

Comment. Again, everything we need follows from solving the stationary S.E.



Reflection and Transmission Coefficients

Recall that $$j_x = \frac{\hbar}{2mi}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right)$$

Having solved the S.E., we can calculate $j_{inc,x}$, $j_{ref,x}$, $j_{trans,x}$

Let us define

$$\boxed{R \overset{def}{=} \left| \frac{j_{ref,x}}{j_{inc,x}} \right| \quad \text{reflection coeff.}}$$

$$\boxed{T \overset{def}{=} \left| \frac{j_{trans,x}}{j_{inc,x}} \right| \quad \text{transmission coefficient}}$$

In particular, in the discussed generic problem

$$j_{inc,x} = \frac{\hbar k_1}{m}$$

$$j_{refl,x} = \frac{\hbar k_1}{m}|r|^2$$

$$j_{trans,x} = \frac{\hbar k_2}{m}|t|^2$$

$$R = |r|^2$$

$$T = |t|^2 \cdot \frac{k_2}{k_1}$$

r and t – to be found from continuity conditions

1D Scattering Problems: General Solving Strategy

(1) Solve the stationary Schrödinger equation in separate regions, implied by the form of the potential

(2) Require the wave function and its first derivative to be continuous at boundary points

(3) Find the probability current for incident, reflected, and transmitted particles

$$j_{inc}, \quad j_{refl}, \quad j_{trans}$$

(4) Calculate the reflection and transmission coefficients (i.e. reflection and transmission probabilities)

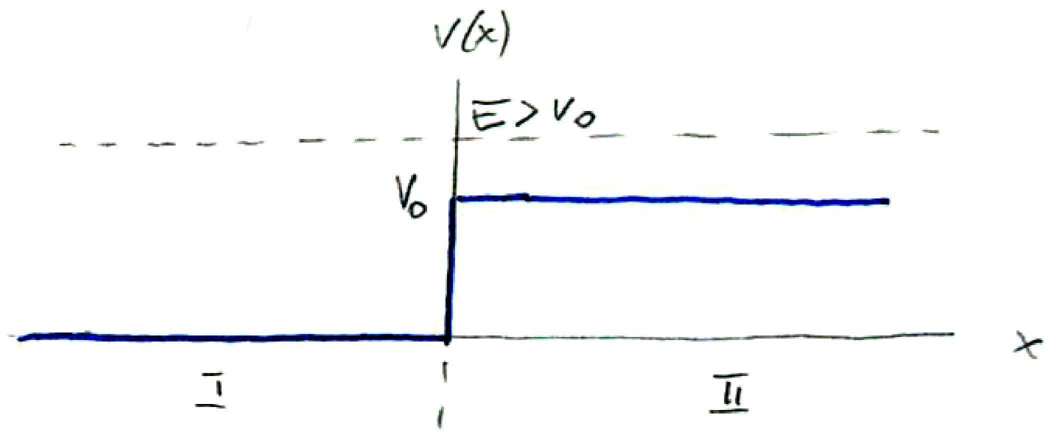
$$\boxed{R \stackrel{def}{=} \left| \frac{j_{ref,x}}{j_{inc,x}} \right| \quad \text{reflection coeff.}} \qquad \boxed{T \stackrel{def}{=} \left| \frac{j_{trans,x}}{j_{inc,x}} \right| \quad \text{transmission coefficient}}$$

Example 1: Potential Step

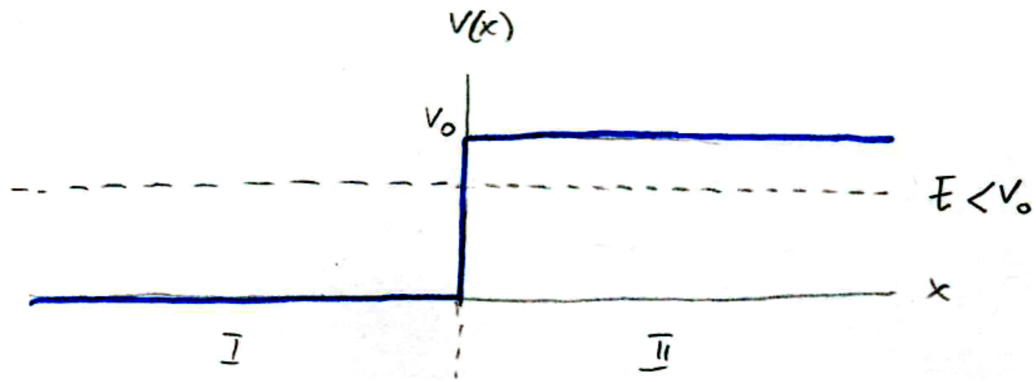
Potential Step

Depending on the energy of the incident particles, two cases need to be considered separately

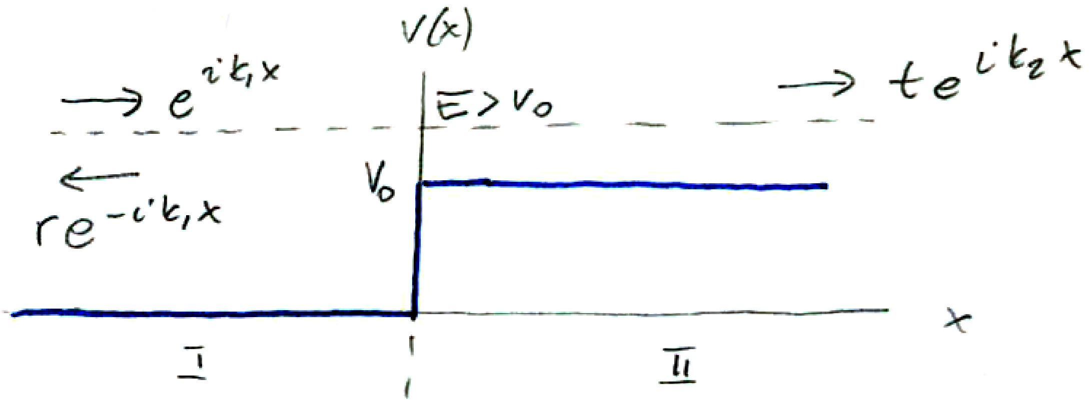
$E > V_0$



$E < V_0$



Potential Step. Case $E > V_0$



Solutions to the stationary S.E.

$$\psi_I(x) = e^{ik_1x} + re^{-ik_1x}$$

$$\psi_{II}(x) = te^{ik_2x}$$

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

Require the wave function and its derivative
to be continuous at $x = 0$

$$\begin{cases} \psi_I(0) = \psi_{II}(0) \\ \psi_I'(0) = \psi_{II}'(0) \end{cases} \Rightarrow \begin{cases} 1 + r = t \\ ik_1 - ik_1 r = ik_2 t \quad /: ik_1 \end{cases}$$

$$\begin{cases} 1 + r = t \\ 1 - r = \frac{k_2}{k_1} t \end{cases} \Rightarrow \quad t = \frac{2}{1 + \frac{k_2}{k_1}}, \quad r = \frac{1 - \frac{k_2}{k_1}}{1 + \frac{k_2}{k_1}}$$

Potential Step. Case $E > V_0$

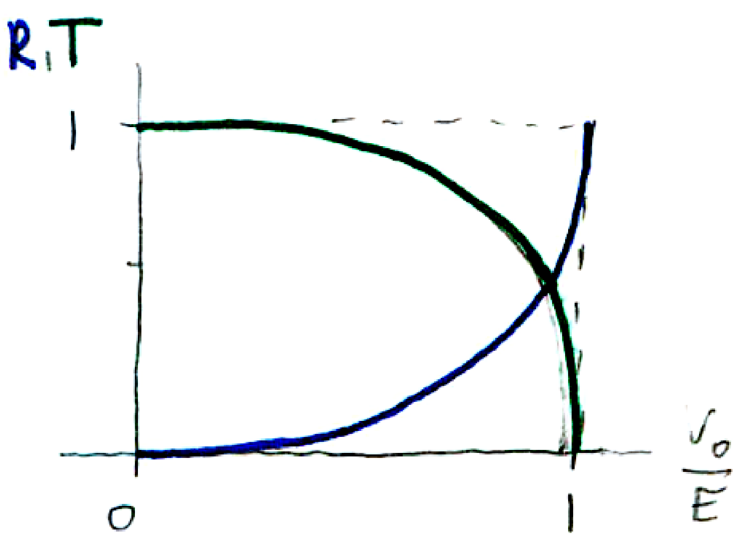
Hence the reflection and the transmission coefficient

$$R = |r|^2 = \left(\frac{1 - \frac{k_2}{k_1}}{1 + \frac{k_2}{k_1}} \right)^2 , \qquad T = \frac{k_2}{k_1} |t|^2 = \frac{4 \frac{k_2}{k_1}}{\left(1 + \frac{k_2}{k_1}\right)^2}$$

Or, recalling that $\left(\frac{k_2}{k_1}\right)^2 = 1 - \frac{V_0}{E} < 1$ we can rewrite both in terms of E and V_0

$$R = \left(\frac{1 - \sqrt{1 - \frac{V_0}{E}}}{1 + \sqrt{1 - \frac{V_0}{E}}} \right)^2 \qquad T = \frac{4 \sqrt{1 - \frac{V_0}{E}}}{\left(1 + \sqrt{1 - \frac{V_0}{E}}\right)^2}$$

Discussion



(*) $E \gg V_0 \Rightarrow \frac{V_0}{E} \to 0$ and $T \to 1$, $R \to 0$

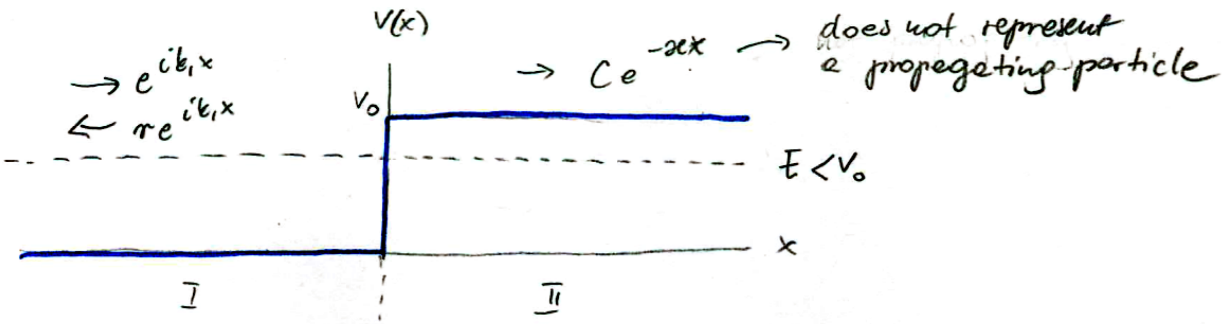
no reflection, total transmission

(*) $E = V_0 \Rightarrow \frac{V_0}{E} = 1$ and $T = 0$, $R = 1$

no transmission, total reflection

(*) $R + T = 1$

Potential Step. Case $E < V_0$



Solutions to the stationary S.E.

$$\psi_I(x) = e^{ik_1x} + r\,e^{-ik_1x}$$

$$\psi_{II}(x) = C\,e^{-\varkappa x}$$

$\hookrightarrow$ real !

$$k_1^2 = \frac{2mE^2}{\hbar^2} \qquad \varkappa^2 = \frac{2m}{\hbar^2}(V_0 - E) > 0$$

Continuity conditions

$$\begin{cases} \psi_I(0) = \psi_{II}(0) \\ \psi_I'(0) = \psi_{II}'(0) \end{cases} \Rightarrow \begin{cases} 1 + r = C \\ ik_1 - ik_1 r = -\varkappa C \end{cases} \Rightarrow \quad r = \frac{1 - i\frac{\varkappa}{k_1}}{1 + i\frac{\varkappa}{k_1}} \Rightarrow |r|^2 = 1$$

Hence $\boxed{R = 1}$ perfect reflection $\qquad \boxed{T = \left|\frac{j_{trans,x}}{j_{inc,x}}\right| = 0}$

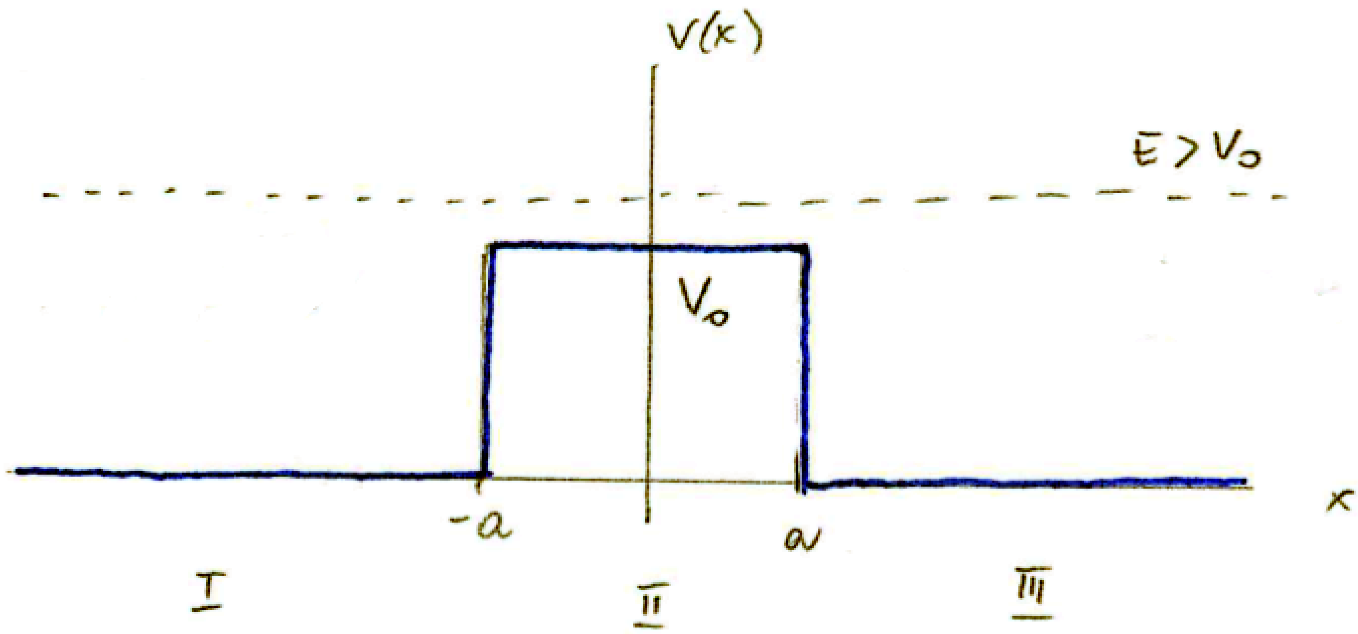
Note. $R + T = 1$
(see problem set)

Conclusion: All particles are reflected with probability 1.

Example 2: Potential Barrier

Rectangular barrier

$$V(x) = \begin{cases} V_0 & \text{for } |x| \leq a \\ 0 & \text{otherwise} \end{cases}$$



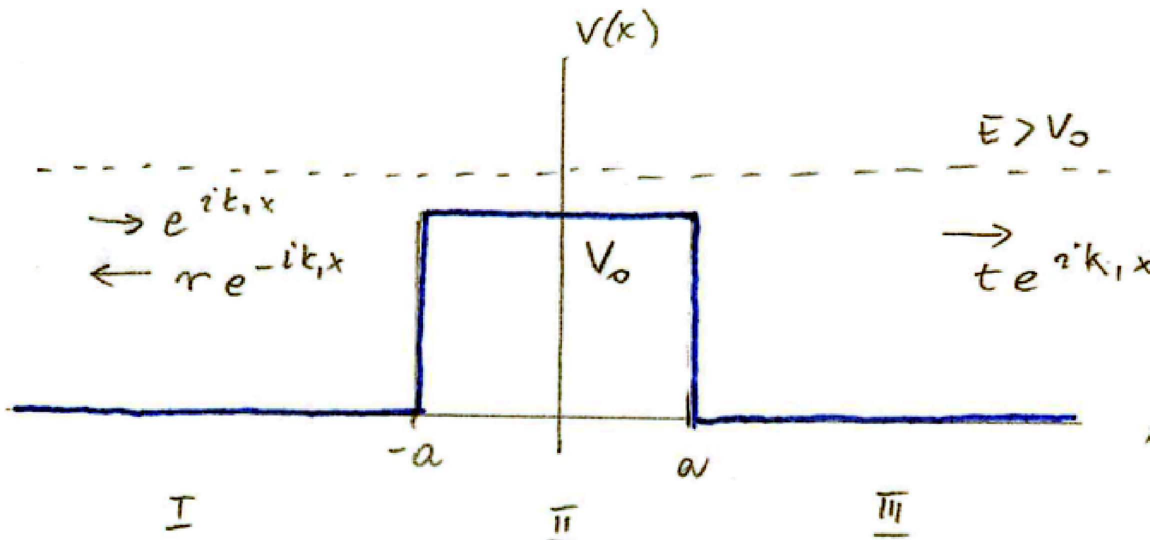
Rectangular barrier

$\boxed{1^\circ \; E > V_0}$ Solutions of stationary S.E. in $\underline{I}, \underline{II}, \underline{III}$

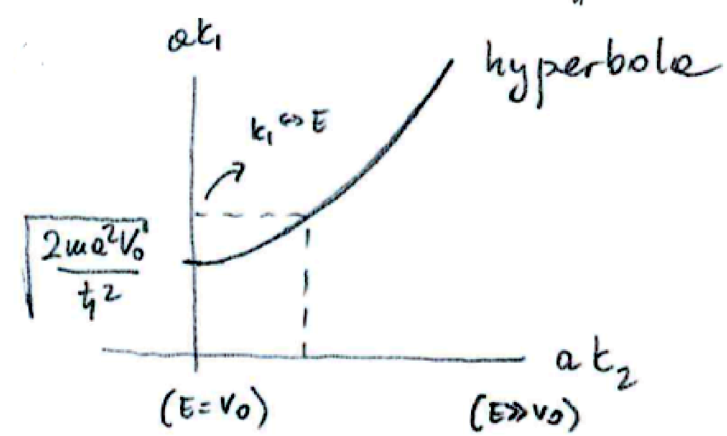
$$\psi_I(x) = e^{ik_1 x} + r e^{-ik_1 x} \quad ; \quad k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi_{II}(x) = A e^{ik_2 x} + B e^{-ik_2 x} \quad ; \quad k_2 = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$$

$$\psi_{III}(x) = t\, e^{ik_1 x}$$



Note: $(ak_1)^2 - (ak_2)^2 = \dfrac{2ma^2V_0}{\hbar^2}$



Continuous spectrum

Rectangular barrier

Continuity of ψ and ψ' at $x = \pm a$ allows to find (see recitation class)

$$T^{-1} = 1 + \frac{1}{4} \frac{V_0^2}{E(E-V_0)} \sin^2\left(2\sqrt{\frac{2ma^2}{\hbar^2}(E-V_0)}\right)$$

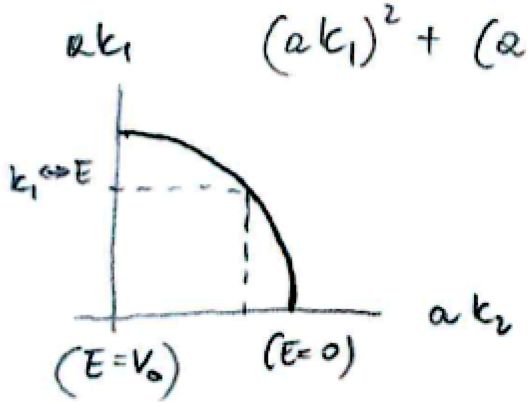
$$R = 1 - T$$

Rectangular barrier

$\boxed{2^\circ \quad E<V_0}$ Solutions of stationary S.E. in $\underline{\mathrm{I}}$, $\underline{\mathrm{II}}$, $\underline{\mathrm{III}}$

[Use same solutions, but replace k_2 with $i\varkappa$, where $\varkappa = \sqrt{\frac{2m}{\hbar^2}(V_0-E)}$]

$$(ak_1)^2 + (ak_2)^2 = \frac{2ma^2V_0}{\hbar^2}$$



Continuous spectrum

$$T^{-1} = 1 + \frac{1}{4}\frac{V_0^2}{E(V_0-E)}\sinh^2\left(2\sqrt{\frac{2ma^2}{\hbar^2}(V_0-E)}\right)$$

$$R = 1 - T$$

(recall $\sin(iz) = i\sinh z$)

Rectangular barrier. Discussion

→ for $0<E<V_0$, we have $T<1$ (but $T>0$) ⇒ tunneling

→ for $E \to V_0 \Rightarrow T \to \dfrac{1}{1+\frac{2ma^2V_0}{\hbar^2}} < 1$

→ for $E > V_0$, in general, transmission is not perfect

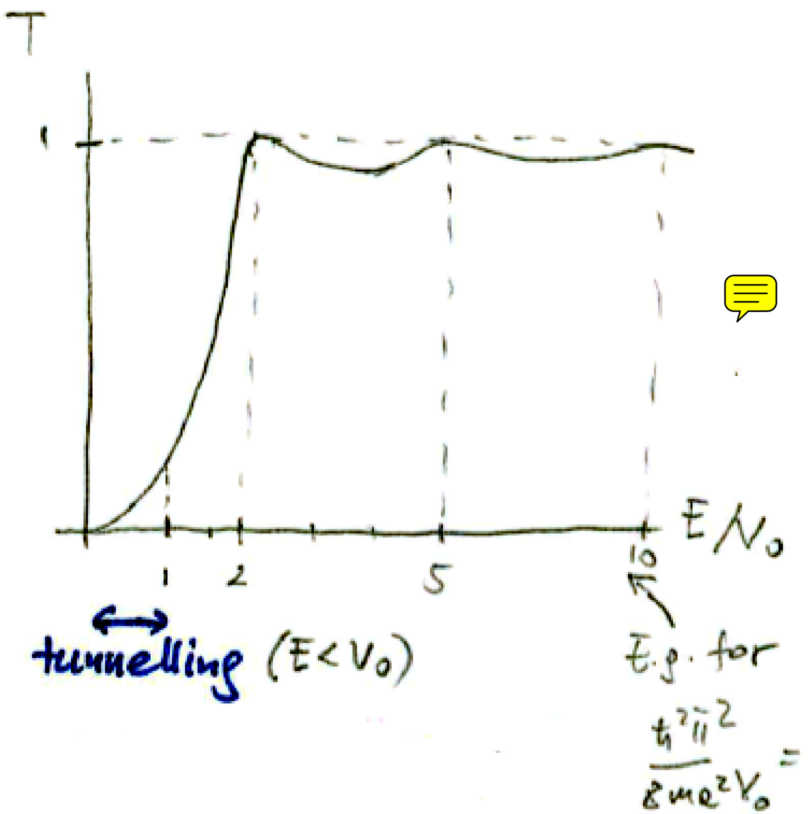
→ for $E>V_0$ perfect transmission

if $2\sqrt{\frac{2ma^2}{\hbar^2}(E-V_0)} = n\pi$, $(n=1,2,\dots)$

$$\Downarrow$$

$$E = V_0 + \underbrace{\frac{\hbar^2\pi^2}{8ma^2}n^2}$$

n-th energy level of infinite well with width $(2a)$

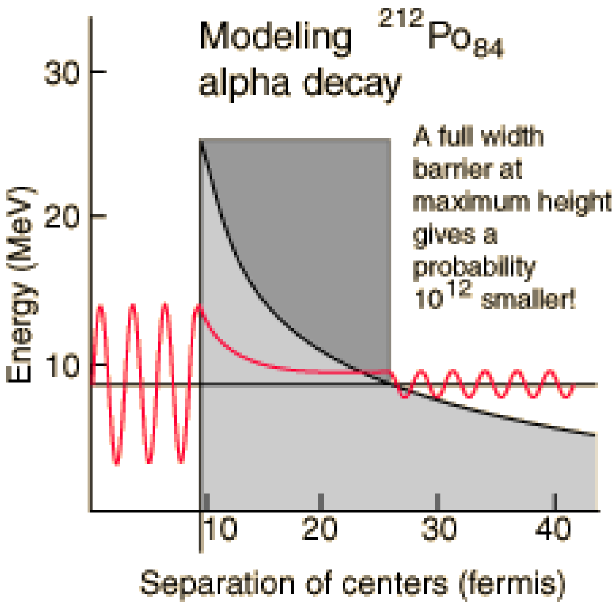


[Fig. 7.26/Liboff]

Applications

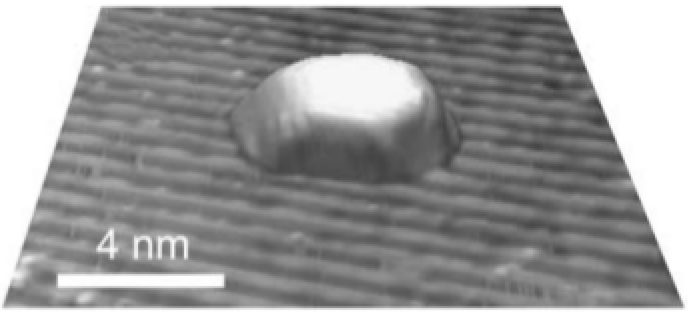
- NH_3 molecule

- alpha decay

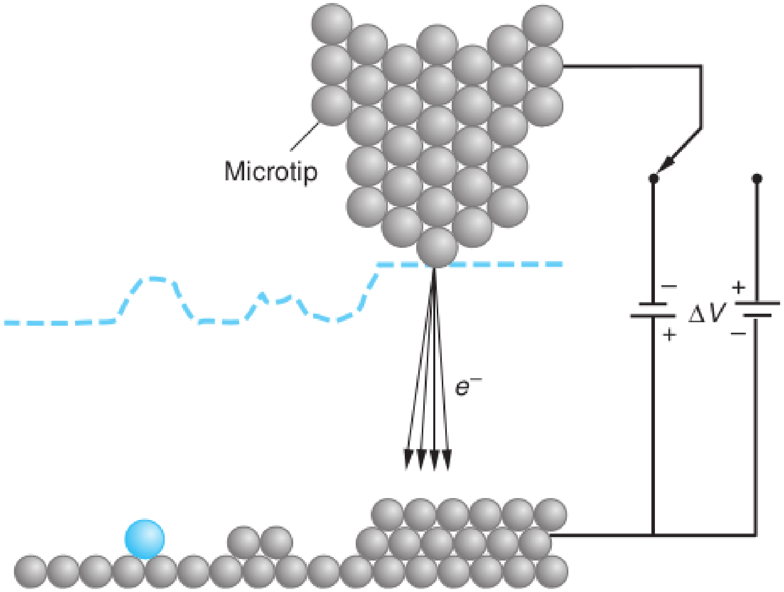


http://hyperphysics.phy-astr.gsu.edu/hbase/nuclear/alptun2.html#c1

- scanning tunneling microscopy



source: Tipler

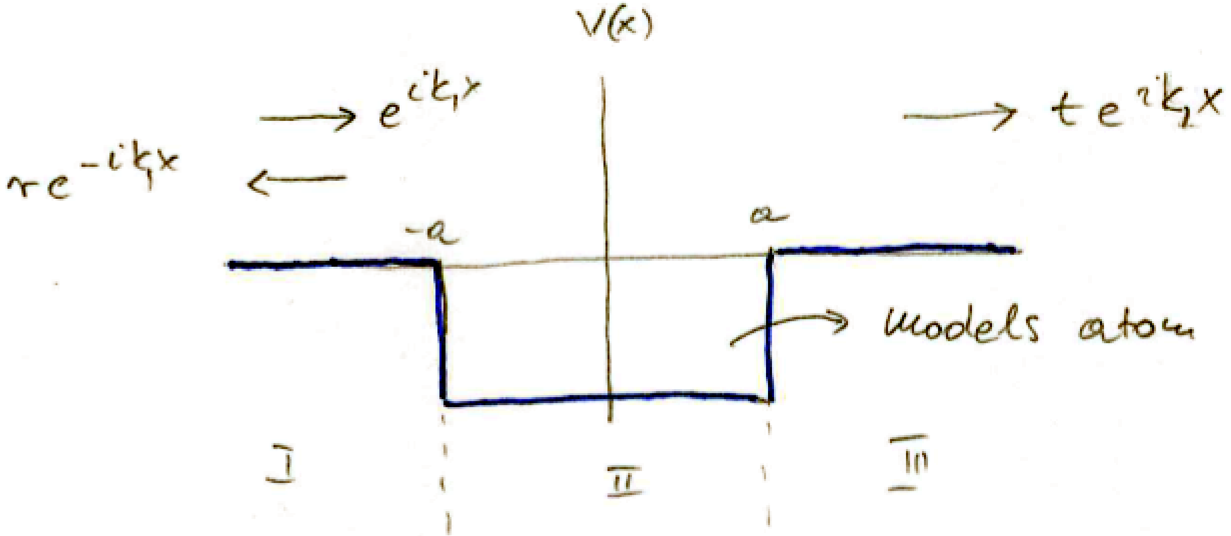


Example 3: Potential Well

(see problem set)

Scattering on a rectangular finite-depth well

Motivation: Ramsauer effect - rare gas atoms transparent to incident electrons



Solutions of stationary S.E.

$$\psi_I(x) = e^{ik_1x} + re^{-ik_1x} \qquad k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi_{II}(x) = Ae^{ik_2x} + Be^{-ik_2x} \qquad k_2 = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

$$\psi_{III}(x) = te^{ik_1x}$$

Scattering on a rectangular finite-depth well

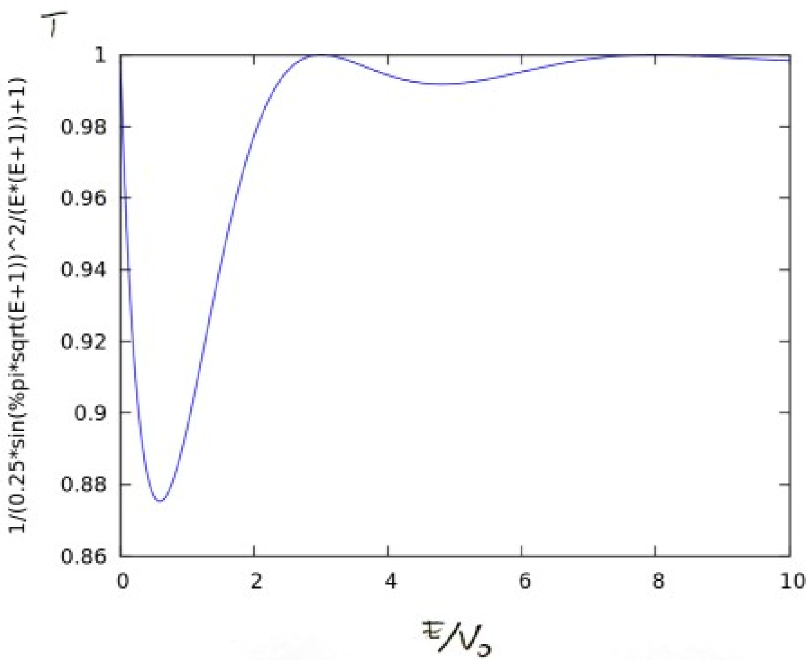
Again, the same procedure (see problem set)

$$\boxed{T^{-1} = 1 + \frac{1}{4}\frac{V_0^2}{E(E+V_0)}\sin^2\left(2\sqrt{\frac{2ma^2}{\hbar^2}(E+V_0)}\right) \qquad R = 1 - T}$$

Perfectly transparent if

$$2\sqrt{\frac{2ma^2}{\hbar^2}(E+V_0)} = n\pi, \qquad n = 1, 2, \ldots$$

$$= -V_0 + \frac{\hbar^2\pi^2}{8ma^2}n^2$$



For $\frac{\hbar^2\pi^2}{8ma^2V_0} = 1$