"Complementi di Fisica" Lectures 11, 12

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In these lectures

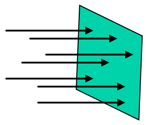
- Contents
  - Particles: probability density and flux; charge density and current density
  - Potential energy step: transmission and reflection coefficients
  - Potential well or barrier: limiting cases (Dirac δ)
- Reference textbooks
  - J.H.Davies, The physics of low-dimensional semiconductors, Cambridge University Press, 1998, p.9-13 ("1.4 Charge and current densities")
  - D.A. Neamen, Semiconductor Physics and Devices, McGraw-Hill, 3rd ed., 2003, p.38-42
  - D. Griffith, …

"Flux" of particles ?

Particle flux: **number of particles crossing a given surface per unit surface and per unit time**

Electrical current density: **(particle flux) × (charge/particle)**

Relationship with the wave function? Guess based on dimensions:



$$\left[|\Psi|^2 dx\,dy\,dz\right] = [\text{probability}] \quad \text{a - dimensional}$$

$$\Rightarrow \quad \left[|\Psi|^2\right] = \left[L^{-3}\right] = \left[\text{cm}^{-3}\right] = \left[|A|^2\right] \qquad \Psi = Ae^{ikx}$$

$$[F] = \left[\text{cm}^{-2}\text{s}^{-1}\right] \qquad \text{velocity}: [v] = \left[LT^{-1}\right] = \left[\text{cm s}^{-1}\right]$$

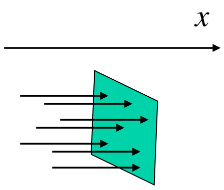
$$[F] = \left[|\text{A}|^2 v\right] = \left[\text{cm}^{-2}\ \text{s}^{-1}\right]$$

"Flux" of particles ?

Relationship with the wave function? Guess based on dimensions:

$$[F] = \left[|\text{A}|^2 v\right] = \left[\text{cm}^{-2}\ \text{s}^{-1}\right]$$

$$\boxed{F = v A^* A}$$



$$[F] = \left[\text{cm}^{-2}\text{s}^{-1}\right]$$

"flux of incident particles"
for a wave function with space part:

$$\psi = A\,e^{ikx}$$

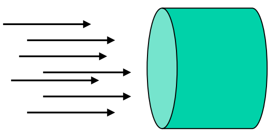
normalization (large but finite volume V):

$$\int_V |\psi|^2 dV = \int_V |A|^2 dV = \begin{cases} 1 & \text{one particle} \\ N & \text{N particles} \end{cases}$$

Fluxes and Currents

More refined treatment, based on the equation of continuity in electromagnetism:

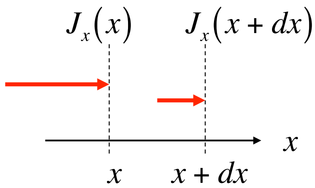
(flux of current through a closed surface) = - d/dt (charge inside)



$$\oint_S \vec{J} \bullet \vec{n}\, dS = -\frac{\partial}{\partial t}\oint_V \rho\, dV$$

$$\vec{\nabla} \bullet \vec{J} = -\frac{\partial \rho}{\partial t}$$

$$\frac{\partial J_x}{\partial x} + \ldots = -\frac{\partial \rho}{\partial t}$$



In the simplest 1-d case the "current density vector" reduces to a "current" J:

Summary of Classical Physics

Maxwell's equations

I. $\nabla \cdot E = \frac{\rho}{\epsilon_0}$ (Flux of E through a closed surface) = (Charge inside)/ϵ_0

II. $\nabla \times E = -\frac{\partial B}{\partial t}$ (Line integral of E around a loop) = $-\frac{d}{dt}$ (Flux of B through the loop)

III. $\nabla \cdot B = 0$ (Flux of B through a closed surface) = 0

IV. $c^2 \nabla \times B = \frac{j}{\epsilon_0} + \frac{\partial E}{\partial t}$ c^2(Integral of B around a loop) = (Current through the loop)/ϵ_0 $+ \frac{\partial}{\partial t}$(Flux of E through the loop)

Conservation of charge

$\nabla \cdot j = -\frac{\partial \rho}{\partial t}$ (Flux of current through a closed surface) = $-\frac{\partial}{\partial t}$ (Charge inside)

Force law

$F = q(E + v \times B)$

Law of motion

$\frac{d}{dt}(p) = F$, where $p = \frac{mv}{\sqrt{1 - v^2/c^2}}$ (Newton's law, with Einstein's modification)

Gravitation

$F = -G\frac{m_1 m_2}{r^2} e_r$

From: The Feynman Lectures on Physics, vol.II

Continuity and Schrödinger

The wave function is a solution of the Schrödinger equation (1-d for simplicity):

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

From the QM postulates on the wave function, the charge density must be identified with:

$$\rho \equiv q\left|\Psi(x,t)\right|^2$$

Since there is a charge density, there should be also a current J (in general, 3-d: current density vector), satisfying the continuity equation (1-d)

$$\frac{\partial \rho}{\partial t} = -\frac{\partial J_x}{\partial x} \qquad \text{where: } J_x(x,t) \equiv ???$$

Continuity and Schrödinger

From the Schrödinger equation to a continuity equation (1-d):

$$i\hbar\Psi^* \frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\Psi^*\frac{\partial^2}{\partial x^2}\Psi + U\Psi^*\Psi \qquad \Psi^* \times \text{(S.eq.)}$$

$$-i\hbar\Psi \frac{\partial}{\partial t}\Psi^* = -\frac{\hbar^2}{2m}\Psi\frac{\partial^2}{\partial x^2}\Psi^* + U\Psi\Psi^* \qquad \Psi \times \text{(S.eq.)}^*\text{, } U \text{ real}$$

$$\frac{\partial}{\partial t}\Psi^*\Psi = -\frac{\hbar}{2im}\left(\Psi^*\frac{\partial^2}{\partial x^2}\Psi - \Psi\frac{\partial^2}{\partial x^2}\Psi^*\right)$$

Subtracting, regrouping: time evolution of $|\Psi|^2$

$$\frac{\partial}{\partial t}\left[q\Psi^*\Psi\right] = -\frac{\partial}{\partial x}\left[\boxed{\frac{q\hbar}{2im}\left(\Psi^*\frac{\partial}{\partial x}\Psi - \Psi\frac{\partial}{\partial x}\Psi^*\right)}\right]$$

$\Rightarrow$ continuity equation (1-d)

Charge density $\rho(x,t)$ Current $J_x(x,t)$

Probability (charge) current density

A few specific examples (easy to verify):

1. Stationary wave functions: $\rho = \text{constant} \qquad J_x = 0$
2. Plane waves $\Psi(x,t) = Ae^{i(kx-\omega t)}$

$$\rho = q|A|^2 = q|\Psi|^2 \qquad J_x = \frac{q\hbar k}{m}|A|^2 = q|A|^2 v$$

3. Superposition of plane waves travelling in opposite directions $\Psi(x,t) = \left(A_+e^{ikx} + A_-e^{-ikx}\right)e^{i\omega t}$

$$J_x = \frac{q\hbar k}{m}\left(|A_+|^2 - |A_-|^2\right)$$

4. Decaying waves (real exponential for the space part)

$$\Psi(x,t) = \left(B_+e^{Kx} + B_-e^{-Kx}\right)e^{i\omega t} \qquad K \text{ real}$$

$$J_x = \frac{q\hbar K}{im}\left(B_+^*B_- - B_-^*B_+\right) = \frac{2q\hbar K}{m}\Im\left(B_+B_-\right)$$

“Step” potential energy barrier

Analysis method

- *Separable* solutions: time-independent Schrödinger equation
  - The energy eigenvalue must be *the same* everywhere; it may correspond to
    - a "bound" particle state
    - a "free" particle state
  - *the energy eigenvalue E* determines the type of solution in each region (interval)
  - *Continuity of the wave function and its derivative*, at the boundaries between different intervals, determine the coefficients of the different terms
- transmission and reflection coefficients for a given finite *barrier* or *well* can be defined for "free" particle states

Solution types

- If in some region the potential $U(x) = U_0$ is constant: possible separable stationary solutions:
  - If $E > U_0$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U_0\psi = E\psi \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} + k^2\psi = 0, \quad k^2 = \frac{2m(E-U_0)}{\hbar^2} > 0$$

$$\Rightarrow \quad \psi(x) = Ae^{ikx} + Be^{-ikx}, \quad A \text{ and } B \text{ arbitrary complex constants, or}$$

$$\psi(x) = C\sin kx + D\cos kx \quad (\text{equivalent}); \quad k \text{ is real!}$$

  - If $E < U_0$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U_0\psi = E\psi \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} + q^2\psi = 0, \quad q^2 = \frac{2m(E-U_0)}{\hbar^2} < 0$$

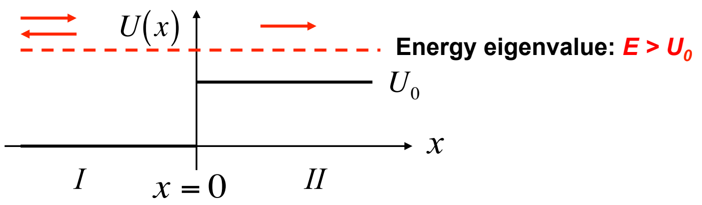
$$\Rightarrow \quad q = \sqrt{(-1)\frac{2m(U_0-E)}{\hbar^2}} = i\alpha, \quad \alpha^2 = \frac{2m(U_0-E)}{\hbar^2} > 0$$

$$\Rightarrow \quad \psi(x) = Ae^{\alpha x} + Be^{-\alpha x}, \quad A \text{ and } B \text{ arbitrary complex constants}$$

$$\text{in this case: } q \text{ imaginary}, \quad \alpha \text{ real;}$$

$$\text{equivalent notation: } \frac{d^2\psi}{dx^2} - \alpha^2\psi = 0, \quad \alpha^2 = \frac{2m(U_0-E)}{\hbar^2} > 0$$

Step potential energy, $E > U_0$



$$I: \quad \psi_I(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x} \qquad k_1 = \sqrt{2mE/\hbar^2} \quad \text{real}$$

$$II: \quad \psi_{II}(x) = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x} \qquad k_2 = \sqrt{2m(E-U_0)/\hbar^2} \quad \text{real}$$

Coefficients: boundary conditions, particles coming from the left

$$I: \quad A_1 = 1 \quad (\text{arbitrary}) \qquad B_1 \quad (\text{"reflected"})$$

$$II: \quad A_2 \quad (\text{"transmitted"}) \qquad B_2 = 0$$

Step potential energy, $E > U_0$

Wave function and its derivative: continuity at $x = 0$

$$\psi_I(0) = \psi_{II}(0) \quad \Rightarrow \quad 1 + B_1 = A_2$$

$$\left.\frac{d\psi_I}{dx}\right|_{x=0} = \left.\frac{d\psi_{II}}{dx}\right|_{x=0} \quad \Rightarrow \quad ik_1 - ik_1 B_1 = ik_2 A_2$$

The coefficients B_1, A_2 can be determined in terms of k_1, k_2 and therefore are uniquely determined by the energy eigenvalue E

$$B_1 = \frac{k_1 - k_2}{k_1 + k_2} = B_1(E) \qquad A_2 = \frac{2k_1}{k_1 + k_2} = A_2(E)$$

These coefficients are expressing the relative "weights" of the reflected and transmitted waves: as we have seen, they can be used to find the corresponding "fluxes" or "currents"!

Reflection and transmission, *E > U_0*

Reflection coefficient: ratio of "reflected flux" to "incoming flux"
Reflection probability = fraction of particles "reflected back"

$$R = \frac{v_1 |B_1|^2}{v_1 |A_1|^2} = \frac{|B_1|^2}{|A_1|^2} = \ldots = R(E)$$

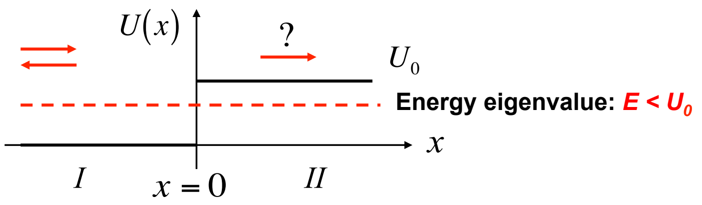
Transmission coefficient: ratio of "transmitted flux" to "incoming flux"
Transmission probability = fraction of particles "transmitted on"

$$T = \frac{v_2 |A_2|^2}{v_1 |A_1|^2} = \ldots = T(E)$$

Exercise:
compute *R(E), T(E)*
for an electron
with *E = 20 eV, U_0 = 10 eV*

Unlike the classical case,
not all particles with *E > U_0* "climb" over the step!

Step potential energy, *E < U_0*



$$I: \quad \psi_I(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x} \qquad k_1 = \sqrt{2mE/\hbar^2} \quad \text{real}$$

$$II: \quad \psi_{II}(x) = A_2 e^{\alpha_2 x} + B_2 e^{-\alpha_2 x} \qquad \alpha_2 = \sqrt{2m(U_0 - E)/\hbar^2}$$

$$(q_2 = i\alpha_2 \ \ \text{imaginary}, \ \ \alpha_2 \ \text{real})$$

Coefficients: boundary conditions, particles coming from the left

$$I: \quad A_1 = 1 \quad \text{(arbitrary)} \qquad B_1 \quad \text{("reflected")}$$

$$II: \quad A_2 = 0 \quad \text{(divergent!!!)} \qquad B_2 \quad \text{("transmitted"??)}$$

Step potential energy, *E* < U_0

Wave function and its derivative: continuity at *x = 0*

$$\psi_I(0) = \psi_{II}(0) \qquad \Rightarrow \quad 1 + B_1 = B_2 \qquad \text{setting } A_1 = 1$$

$$\left.\frac{d\psi_I}{dx}\right|_{x=0} = \left.\frac{d\psi_{II}}{dx}\right|_{x=0} \qquad \Rightarrow \quad ik_1 - ik_1 B_1 = -\alpha_2 B_2$$

Exercise:
compute *R(E), T(E)* defined as before

Solving for the coefficients B_1, B_2 as before:

$$B_1 = -\frac{\alpha_2 + ik_1}{\alpha_2 - ik_1} \qquad |B_1|^2 = 1$$

The *"reflection" R* seems to be total: same weight as the incoming wave, with a phase shift

$$B_2 = -\frac{2ik_1}{\alpha_2 - ik_1} \qquad |B_2|^2 = 4\frac{k_1^{\,2}}{\alpha_2^{\,2} + k_1^{\,2}}$$

"Transmission" T is not zero: the wave function "leaks" at *x > 0* !?!

Step potential energy, *E* < U_0

Non-zero probability for the particle to be found at *x > 0*
(classically impossible!);
The corresponding probability density P(x) is:

$$P(x) = |\psi_{II}(x)|^2 = |B_2|^2 e^{-2\alpha_2 x} \qquad \alpha_2 = \sqrt{2m(U_0 - E)/\hbar^2}$$

Exercise 1:
Evaluate the typical "penetration depth" *L = 1/(2α)*
For an electron with *E = 8 eV* and a step U_0 *= 10 eV*

Exercise 2:
Evaluate the probability (with the above data) that an electron is found at a distance > L from the position of the step:

$$p(x \geq L) = \int_L^{+\infty} P(x)\,dx = \dots$$

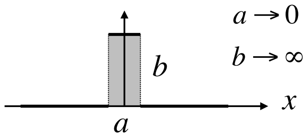
However, the net flux for *x > 0* is zero
(can be checked by computing the current density)
and eventually the particle must turn back !

Limiting cases: Dirac δ

Dirac δ "function": potential energy well
Bound particle solution
Free (scattering) solution
Reflection and transmission coefficients
Similar results for potential barrier

Dirac δ "function"

- "Generalized function" concept
  - You can think of it as a "limit" case in a family of functions (for instance gaussians)
    - Integral = unity
    - Decreasing width, increasing max. value



$$a \to 0 \qquad ab = 1$$
$$b \to \infty$$

$$\delta(x) = \begin{cases} 0 & x \neq 0 \\ \infty & x = 0 \end{cases}$$

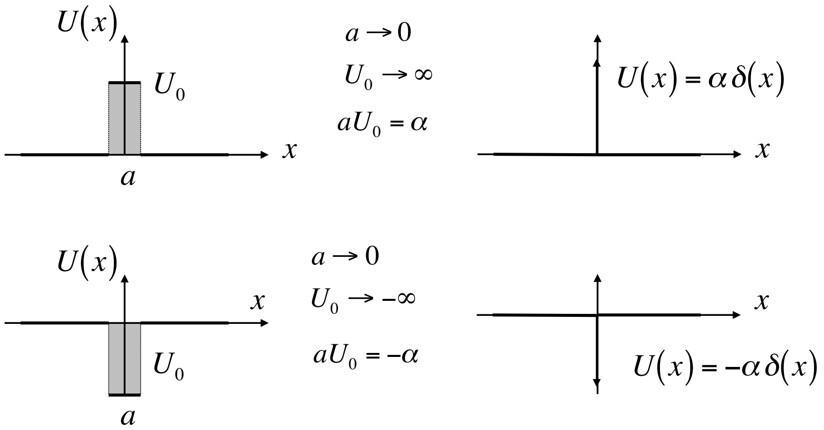
$$\int_{-\infty}^{+\infty} \delta(x)\, dx = 1$$

  - Extending the definition of integrals, one can show that:

$$f(x)\delta(x-a) = f(a)\delta(x-a)$$
$$\int_{-\infty}^{+\infty} f(x)\delta(x-a)\, dx = f(a)$$

Dirac δ potential

- **Represent wells or barriers in a simplified way:**

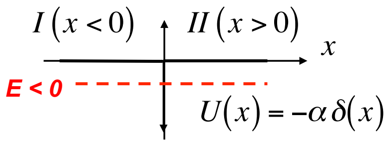


The product of U_0 (barrier "height") and a (barrier "width") represents the "strenght" α of the interaction, determining transmission probability etc

δ-potential well: bound states (E < 0)

Time-independent S.eq.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\,\delta(x)\psi = E\psi$$



Separable solutions: look for wave functions ψ and energy eigenvalues E

$$I\,(x<0):\quad U(x) = 0 \quad\Rightarrow\quad \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

$$\psi_I(x) = \cancel{Ae^{-Kx}} + Be^{+Kx} \qquad K^2 = -\frac{2mE}{\hbar^2} > 0$$

$II\,(x<0)$:

Exclude divergent terms: *A* = *D* = *0*

$$\psi_I(x) = Ce^{-Kx} + \cancel{De^{+Kx}}$$

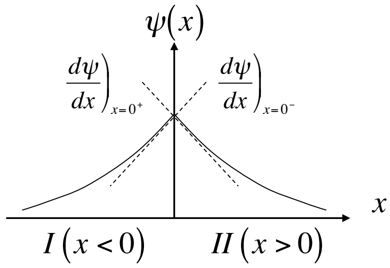
δ-potential well: bound states (E < 0)

To find allowed values for E
and B, C, K: continuity conditions.

(a) Wave function continuity.

$$\lim_{x\to 0^-}\psi_I(x) = \lim_{x\to 0^+}\psi_{II}(x) \Rightarrow B = C$$

$$\Rightarrow \psi(x) = Be^{-K|x|} = \begin{cases} Be^{Kx} & x \le 0 \\ Be^{-Kx} & x \ge 0 \end{cases}$$



(b) First derivative: discontinuous at $x = 0$, where the potential has a singularity.
The Schr.eq. constrains the difference of the limits of the first derivatives,
as it can be seen integrating on [- ε, + ε] and taking the limit for $\varepsilon \to 0$

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{+\varepsilon}\frac{d^2\psi}{dx^2}dx - \alpha\int_{-\varepsilon}^{+\varepsilon}\delta(x)\psi(x)\,dx = E\int_{-\varepsilon}^{+\varepsilon}\psi(x)\,dx$$

δ-potential well: bound states (E < 0)

Integrating we obtain:

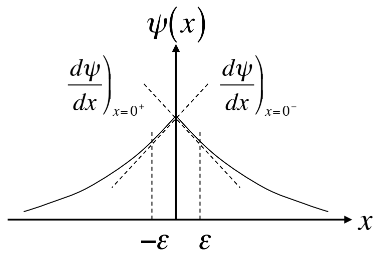
$$-\frac{\hbar^2}{2m}\left[\frac{d\psi}{dx}\right]_{-\varepsilon}^{+\varepsilon} - \alpha\psi(0) = E\underbrace{\int_{-\varepsilon}^{+\varepsilon}\psi(x)\,dx}_{\to\, 0}$$

In the limit $\varepsilon \to 0$

$$-\frac{\hbar^2}{2m}\left[\frac{d\psi}{dx}\right]_{-\varepsilon}^{+\varepsilon} - \alpha\psi(0) = E\int_{-\varepsilon}^{+\varepsilon}\psi(x)\,dx$$

$$\left.\frac{d\psi}{dx}\right)_{x=0^+} - \left.\frac{d\psi}{dx}\right)_{x=0^-} = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

$$-KB - KB = -\frac{2m\alpha}{\hbar^2}B$$



$$x<0: \quad \frac{d\psi}{dx} = KBe^{+Kx}$$

$$x>0: \quad \frac{d\psi}{dx} = -KBe^{-Kx}$$

(dis)continuity constrains therefore K and E to only one possible value:

$$K = \frac{m\alpha}{\hbar^2} \quad \Rightarrow \quad E = -\frac{\hbar^2K^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}$$

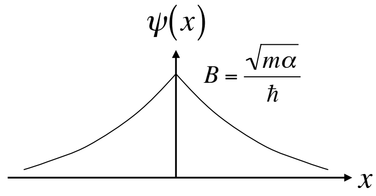
δ-potential well: bound states (E < 0)

The only missing parameter B is determined by the normalization condition:

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 \, dx = 1$$

$$2\int_{0}^{+\infty} |B|^2 e^{-2Kx} dx = \frac{|B|^2}{K} = 1$$

$$\Rightarrow \quad B = \sqrt{K} = \frac{\sqrt{m\alpha}}{\hbar}$$



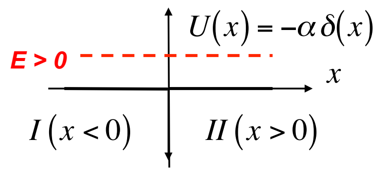
⇒ Only one bound solution:

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2} \qquad E = -\frac{m\alpha^2}{2\hbar^2}$$

δ-potential well: free states (E > 0)

Time-independent S.eq.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\,\delta(x)\psi = E\psi$$



Separable solutions: look for wave functions ψ and energy eigenvalues E

$I: \quad x<0 \qquad \psi_I(x) = Ae^{ikx} + Be^{-ikx} \qquad k = \frac{\sqrt{2mE}}{\hbar} > 0 \quad \text{real}$

$II: \quad x>0 \qquad \psi_{II}(x) = Fe^{ikx} + \cancel{G}e^{-ikx}$

$G = 0$ **Particles coming From the left**

(Dis)continuity at $x = 0$

$\psi_I(0) = \psi_{II}(0): \qquad A + B = F$

$$\left.\frac{d\psi_{II}}{dx}\right)_{0^+} - \left.\frac{d\psi_I}{dx}\right)_{0^-} = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

$$ik(F - A + B) = -\frac{2m\alpha}{\hbar^2}(A + B)$$

$\longrightarrow$

$$B = \frac{-\beta}{\beta + i}A \qquad \beta = \frac{m\alpha}{\hbar^2 k}$$

$$F = \frac{1}{1 - i\beta}A$$

Reflection and transmission

reflection coefficient

$$R \equiv \frac{\text{reflected flux}}{\text{incoming flux}} = \frac{v|B|^2}{v|A|^2} = \frac{\beta^2}{1+\beta^2} = \dots \qquad \beta \equiv \frac{m\alpha}{\hbar^2 k}$$

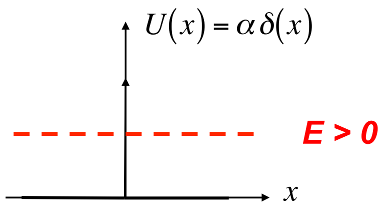
$$= \frac{1}{1+\hbar^4 k^2/(m^2\alpha^2)} = \frac{1}{1+2\hbar^2 E/(m\alpha^2)} = R(E)$$

transmission coefficient

$$T \equiv \frac{\text{transmitted flux}}{\text{incoming flux}} = \frac{v|F|^2}{v|A|^2} = \frac{1}{1+\beta^2} = \dots$$

$$= \frac{1}{1+m^2\alpha^2/(\hbar^4 k^2)} = \frac{1}{1+2m\alpha^2/(2\hbar^2 E)} = T(E) \qquad R+T=1$$

δ-potential barrier



identical solution method, but:

- **no bound solution**
- **only E > 0, "scattering" solutions**
- **the reflection and transmission coefficients R(E) and T(E) have the same expressions**

Lectures 13-15: summary

- **In these lectures we learned:**
  - How to represent the charge density (proportional to the probability density) and the current density, in terms of the wave function
  - To find the separable solutions of the Schrödinger equation, (the allowed energy eigenvalues and the corresponding eigenfunctions) for a potential energy varying in steps with intervals in which it can be considered constant
  - In particular, we treated in detail the simplest cases:
    - Single potential step
    - δ-function wells and barriers

  (Computing in particular t*ransmission* and *reflection coefficients*)

Lectures 14-16: exercises

1. Compute the current densities in the special cases listed at p.8
2. Compute the transmission and reflection coefficients *R(E), T(E)* for an electron with kinetic energy $E = 20\ eV$, crossing a potential energy step $U_0 = 10\ eV$
3. Evaluate the typical "penetration depth" $L = 1/(2\alpha)$ for an electron with $E = 8\ eV$ and a step $U_0 = 10\ eV$
4. Evaluate the probability (with the above data) that an electron is found at a distance > L from the position of the step
5. Compute the reflection and transmission coefficients for an electron with energy E = 10 eV crossing a barrier approximated with $U(x) = \alpha\, \delta(x)$, where $\alpha = 20$ eV Å

Back-up slides

Finite potential barrier

"bound" particle

"free" particle

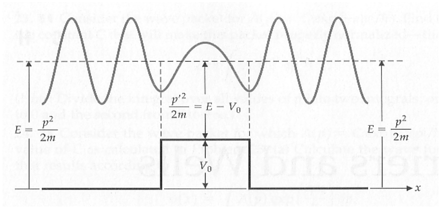
Reflection and transmission coefficients

Tunnel effect

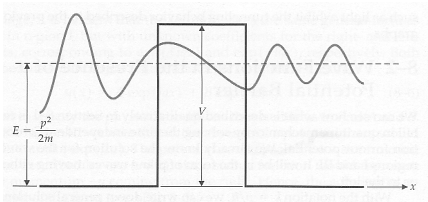
(NB: this section is given for reference only)

Finite potential barrier - introduction

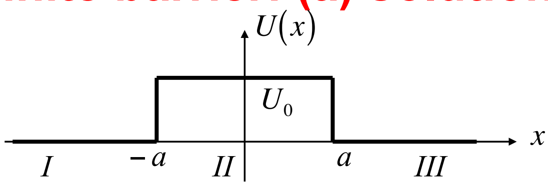
- ***E* > *U*$_0$: wavelength always real;**
  - **But: there is usually reflection in addition to transmission!**



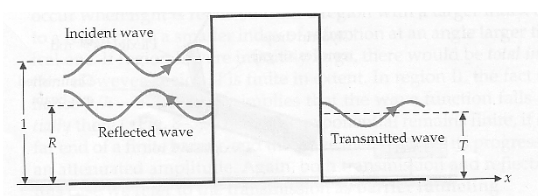
- ***E* < *U*$_0$: wavelength becomes imaginary (analog to classical: "evanescent waves");**
  - **the wave function falls off exponentially in the barrier**
  - **There is a "transmitted" wave with reduced amplitude**



Finite barrier: (a) solutions



Similar to finite well, but we use slightly different notations: to describe both "bound" and "free" solutions with the same equations, here *q* may be real or imaginary depending on the sign of *E*-*V*$_0$



$$I: \quad \psi_I = e^{ikx} + B_1 e^{-ikx} \qquad k = \sqrt{2mE/\hbar^2}$$

$$II: \quad \psi_{II} = A_2 e^{iqx} + B_2 e^{-iqx} \qquad q = \sqrt{(E - U_0)2m/\hbar^2}$$

$$III: \quad \psi_{III} = A_3 e^{ikx} \qquad k = \sqrt{2mE/\hbar^2}$$

Reflection and transmission

Continuity conditions:

$$x = -a: \quad e^{-ika} + B_1 e^{ika} = A_2 e^{-iqa} + B_2 e^{iqa}$$

$$ike^{-ika} + (-ik)B_1 e^{ika} = iqA_2 e^{-iqa} - iqB_2 e^{iqa}$$

$$x = a: \quad A_2 e^{iqa} + B_2 e^{-iqa} = A_3 e^{ika}$$

$$iqA_2 e^{iqa} - iqB_2 e^{-iqa} = ikA_3 e^{ika}$$

4 equations for 4 unknowns: A_2, B_2, B_1, A_3; we are interested mainly in reflection and transmission probabilities, represented by $|B_1|^2$ and $|A_3|^2$, where B_1 and A_3 are given by (see details in back-up slides):

$$B_1 = \frac{i(q^2 - k^2)\sin(2qa)}{2kq\cos(2qa) - i(k^2 + q^2)\sin(2qa)} e^{-2ika}$$

$$A_3 = \frac{2kq}{2kq\cos(2qa) - i(k^2 + q^2)\sin(2qa)} e^{-2ika}$$

"free" solution for $E > U_0$

- By inspection of the equations for R and T, their features for $E > U_0$:
  - B_1 and A_3 are complex numbers ("probability amplitudes")
  - B_1 is not zero, even for $E > U_0$
  - $B_1 \rightarrow 0$ for $U_0 \rightarrow 0$
  - $|B_1| \leq 1$
  - $|B_1|^2 + |A_3|^2 = R + T = 1$
  - $R=|B_1|^2$ and $T=|A_3|^2$ can be interpreted respectively as ***probabilities for reflection and transmission of the particle*** by the potential barrier (see coefficients defined previously for the step potential)
- A similar method is used in more complicated 3-d problems found in the physics of semiconductors !
  - For instance, scattering of an electron by an impurity or defect in a crystal lattice…
  - computation of "scattering amplitudes" and "probabilities" !

"tunneling" solution for *E* < U_0

- **When *E* < U_0:**
  - **Classically, the particle can only bounce back (perfect reflection)**
  - **Here: non-zero transmission probability**
  - **Convenient to show explicitely that q becomes purely imaginary**

$$q^2 = \frac{2m}{\hbar^2}(E - U_0) < 0 \quad \Rightarrow \quad \text{express it as} \quad q = i\eta \quad \text{purely imaginary}$$

$$\eta^2 = \frac{2m}{\hbar^2}(U_0 - E) > 0$$

$$\boxed{A_3 = \frac{4ik\eta\, e^{-2\eta a}}{2ik\eta\left(1 + e^{-4\eta a}\right) + \left(k^2 - \eta^2\right)\left(1 - e^{-4\eta a}\right)} e^{-2ika} \qquad e^{-4\eta a} << 1 \quad \Rightarrow \quad T = |A_3|^2 \approx \frac{16k^2\eta^2}{\left(k^2 + \eta^2\right)^2} e^{-4\eta a}}$$

$$\cos(2qa) \to \frac{e^{-2\eta a} + e^{2\eta a}}{2}$$

$$\sin(2qa) \to \frac{i\left(e^{2\eta a} - e^{-2\eta a}\right)}{2}$$

"tunneling" solution for *E* < U_0

Exponentially decreasing "tunneling" (transmission) probability, depending on the interaction strength, product of η (barrier "height") and *a* (barrier "width"):

$$\boxed{e^{-4\eta a} << 1 \quad \Rightarrow \quad T = |A_3|^2 \approx \frac{16k^2\eta^2}{\left(k^2 + \eta^2\right)^2} e^{-4\eta a}}$$

η = barrier "height"

***a* = barrier "width"**

Qualitatively similar behavior for arbitrary barrier shape, with more complicated coefficients in the exponential, obtained by integrating over many "thin square barriers"