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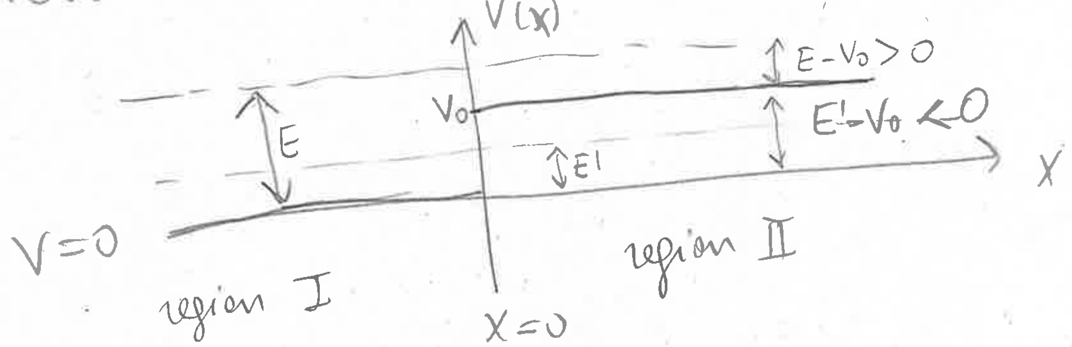
SS 2017 Ik-1, FAU

* Lecture 11 *

- The potential step -

Consider the potential in the figure:



The stationary Schr. eq. is:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + V(x)u(x) = E\,u(x), \qquad E > 0$$

$$\Leftrightarrow \quad \boxed{\frac{d^2u}{dx^2} = \frac{2m}{\hbar^2}\left[V(x) - E\right]u(x)}$$

u'' and u have the same (opposite) sign in the region where $V(x) - E > 0$ $\left(V(x) - E < 0\right)$.

Now

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & x > 0 \end{cases}$$

Define:

$$\boxed{K^2 \equiv \frac{2mE}{\hbar^2} > 0}$$

$$\boxed{q^2 \equiv \frac{2m}{\hbar^2}(E - V_0)} \Longrightarrow \begin{cases} q = \dfrac{\sqrt{2m(E - V_0)}}{\hbar} & \text{if } E > V_0 \\ q = i\dfrac{\sqrt{2m(V_0 - E)}}{\hbar} & \text{if } E < V_0 \end{cases}$$

In region I, $V=0$ and the Sch. eq is:

$$\frac{d^2u}{dx^2}+k^2u=0$$

whose solution is:

$$\boxed{u_I(x)=Ae^{ikx}+Be^{-ikx}}$$

region index

In region II, $V=V_0$ and

$$\frac{d^2u}{dx^2}+q^2u=0 \Rightarrow \boxed{u_{II}(x)=Ce^{iqx}+De^{-iqx}}$$

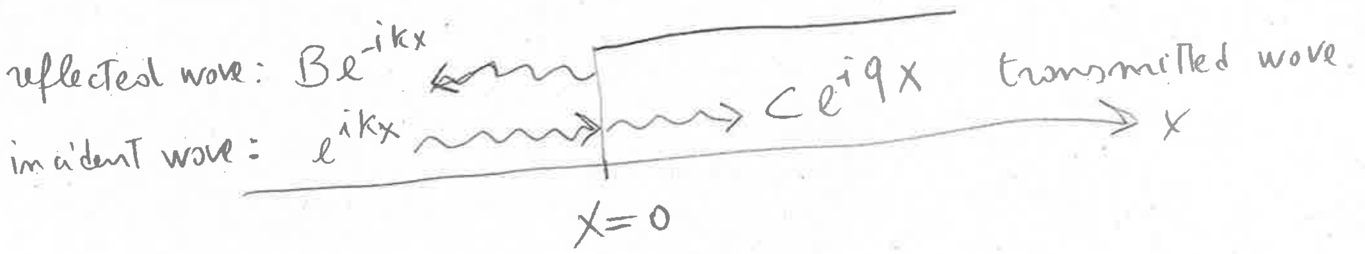
Suppose that in region I, for $x<0$, there is an impinging wave (from left) of unit amplitude, that is:

$$A=1$$

Moreover, since this is the only incident wave, in the region II ($x>0$) we can only have a wave moving towards rigth, that is

$$D=0$$

The PHYSICAL situation is depicted as follow:



We must join $u_I(x)$ and $u_{II}(x)$ imposing the continuity of the wave function:

$$\boxed{u_I(0) = u_{II}(0)} \qquad (1.13)$$

and the continuity of the first derivative.

$$\boxed{\left.\frac{du_I}{dx}\right|_{x=0} = \left.\frac{du_{II}}{dx}\right|_{x=0}} \qquad (2.13)$$

This second requirement follows from Sch. eq:

consider:
$$\frac{d^2}{dx^2}u(x) + \frac{2m}{\hbar^2}[E-V(x)] = 0$$

Integrate between $-\varepsilon<0$ and $\varepsilon>0$:

$$\int_{-\varepsilon}^{\varepsilon}\frac{d^2u(x)}{dx^2}dx = \frac{2m}{\hbar^2}\int_{-\varepsilon}^{\varepsilon}[V(x)-E]dx$$

$$\Leftrightarrow \left.\frac{du}{dx}\right|_{x=\varepsilon} - \left.\frac{du}{dx}\right|_{x=-\varepsilon} = \frac{2m}{\hbar^2}\int_{-\varepsilon}^{\varepsilon}V(x)\,dx - \frac{2mE}{\hbar^2}(2\varepsilon)$$

$$= \frac{2m}{\hbar^2}(V_0-2E)\varepsilon$$

Taking the limit $\varepsilon\to0$ we obtain (2.13).

Therefore:

$$u_I(0) = u_{II}(0) \Leftrightarrow 1 + B = C \qquad \equiv (\alpha)$$

$$u'_I(0) = u'_{II}(0) \Leftrightarrow ik(1-B) = iq\, C \qquad \equiv (\beta)$$

We take:

$$k(\alpha) + \beta \Leftrightarrow k(1+\cancel{B}) + k(1-\cancel{B}) = kC + qC$$

$$\Rightarrow \quad C(k+q) = 2k \quad \Rightarrow \quad \boxed{C = \frac{2k}{k+q}}$$

Then we take:

$$q(\alpha) - (\beta) \Leftrightarrow q(1+B) - k(1-B) = \cancel{qC} - \cancel{qC}$$

$$\Leftrightarrow (q-k) + B(q+k) = 0$$

$$\Rightarrow \quad \boxed{B = \frac{k-q}{k+q}}$$

So:

$$u(x) = \begin{cases} e^{ikx} + \dfrac{k-q}{k+q} e^{-ikx} & , \; x < 0 \\[2ex] \dfrac{2k}{k+q} e^{iqx} & , \; x \geq 0 \end{cases}$$

In summary:

$$\boxed{C = \frac{2}{1+q/k} \; ; \qquad B = \frac{1-q/k}{1+q/k}} \qquad (1.4)$$

What is the meaning of these expressions?

The probability current $\vec{j}$ in This case is equal to

$$\vec{J} = \vec{e}_x j \quad , |\vec{e}_x| = 1 \; ; \; \vec{e}_x = \text{unit vector directed along the x-axis}$$

where
$$j = \frac{\hbar}{2mi}\left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right)$$

In our case we have:

Incident wave : $\psi_{inc} = e^{ikx} \Rightarrow \frac{d\psi_{inc}}{dx} = ik\psi_{inc}$

Reflected wave : $\psi_{ref} = \frac{k-q}{k+q} e^{-ikx} \Rightarrow \frac{d\psi_{ref}}{dx} = -ik\psi_{ref}$

Transmitted wave : $\psi_{tran} = \frac{2k}{k+q} e^{iqx} \Rightarrow \frac{d\psi_{tran}}{dx} = iq\psi_{tran}$

For the moment, let us assume $q^2 > 0$. The case $q^2 < 0$ will be considered later.

We calculate:

$$j_{inc} = \frac{\hbar}{2mi}\left(ik|\psi_{inc}|^2 + ik|\psi_{inc}|^2\right) = \frac{\hbar}{2m\cancel{i}} 2\cancel{i}k = \frac{\hbar k}{m}$$

$$j_{ref} = \frac{\hbar}{2mi}\left|\frac{k-q}{k+q}\right|^2(-2ik) = -\frac{\hbar k}{m}\left|\frac{k-q}{k+q}\right|^2$$

$$j_{Tran} = \frac{\hbar}{2mi}\left[\frac{2k}{k+q^*} e^{-iq^*x} \, iq \frac{2k}{k+q} e^{iqx} + \right.$$
$$\left. - \frac{2k}{k+q} e^{iqx} (-iq^*) \frac{2k}{k+q^*} e^{-iq^*x}\right]$$

This is valid if either $q^2 > 0$ or $q^2 < 0$

$$j_{tran} = \frac{\hbar}{2mi}\left|\frac{2k}{k+q}\right|^2\left[\cancel{i}q\, e^{ix(q-q^*)} + \cancel{i}q^* e^{i(q-q^*)x}\right]$$

$$= \frac{\hbar}{m}\frac{q+q^*}{2}\left|\frac{2k}{k+q}\right|^2 \exp[ix(q-q^*)]$$

$$\boxed{j_{Tran} = \frac{\hbar}{m}\mathrm{Re}(q)\left|\frac{2k}{k+q}\right|^2 e^{ix\,\mathrm{Im}(q)}} \qquad (1.6)$$

For $q^2>0$, $\mathrm{Im}(q)=0$ and $\mathrm{Re}(q)=q \Rightarrow$

$$\Rightarrow j_{tran} = \frac{\hbar q}{m}\left|\frac{2k}{k+q}\right|^2 \; ; \text{For } q^2<0, \mathrm{Re}(q)=0 \Rightarrow j_{Trans}=0$$

We define the TRANSMISSION (T) and the REFLECTION (R) coefficients as: (in the formulas below we assume $q^2>0$)

$$T \equiv \left|\frac{j_{Tran}}{j_{inc}}\right| = \frac{\hbar q}{\cancel{m}}\left|\frac{2k}{k+q}\right|^2 \frac{1}{\frac{\cancel{\hbar} k}{\cancel{m}}} = \frac{q}{k}\left|\frac{2k}{k+q}\right|^2$$

$$R \equiv \left|\frac{j_{ref}}{j_{inc}}\right| = \frac{\hbar \cancel{k}}{m}\left|\frac{k-q}{k+q}\right|^2 \frac{1}{\frac{\hbar \cancel{k}}{\cancel{m}}} = \left|\frac{k-q}{k+q}\right|^2$$

or

$$\boxed{T = 4\frac{q/k}{(1+q/k)^2}\; ; \quad R = \frac{(1-q/k)^2}{(1+q/k)^2}} \qquad (2.6)$$

Note that

$$T+R = \frac{4\frac{q}{k}+1+\frac{q^2}{k^2}-\frac{2q}{k}}{(1+q/k)^2} = 1 \checkmark$$

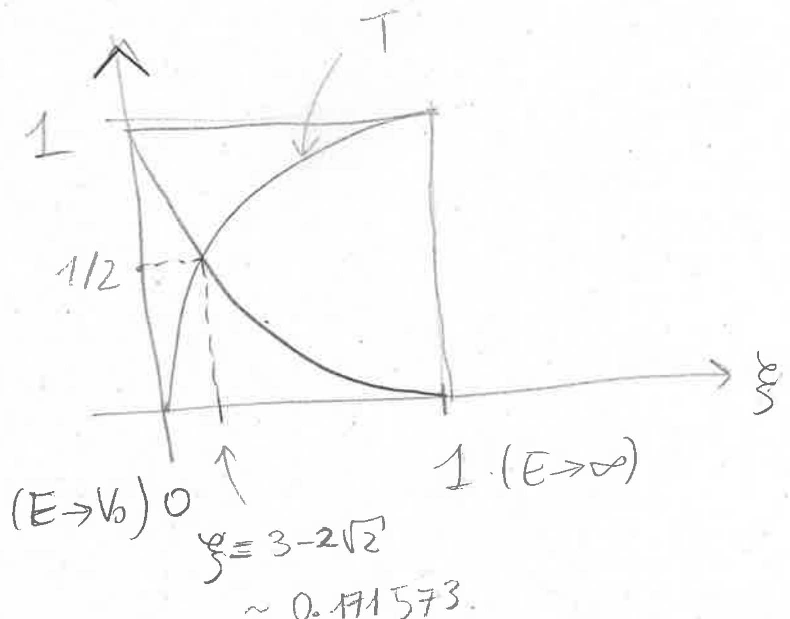
Since $\frac{q^2}{k^2} = \frac{\frac{2\cancel{m}}{\cancel{\hbar^2}}(E-V_0)}{\frac{2\cancel{m}E}{\cancel{\hbar^2}}} = 1 - \frac{V_0}{E} < 1$

$\Rightarrow \frac{q}{k} = \sqrt{1 - \frac{V_0}{E}} \equiv \xi$ at $E = V_0 \Rightarrow \frac{q}{k} = 0$

at $E = \infty \Rightarrow \frac{q}{k} = 1$

So, if ξ: $0 \leq \xi \leq 1$ with $\xi \equiv \frac{q}{k}$

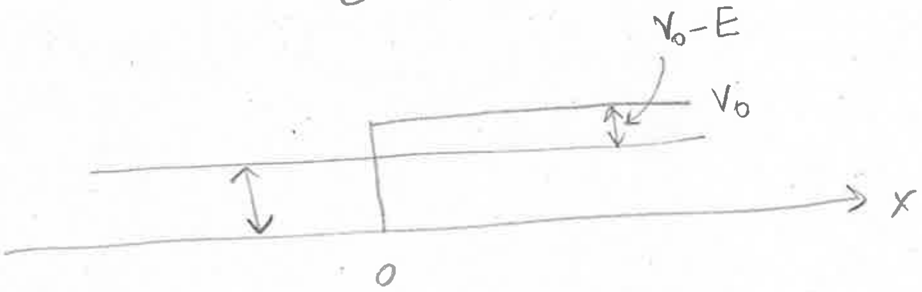
$$T = \left(\frac{2\sqrt{\xi}}{1+\xi}\right)^2 ; \quad R = \left(\frac{1-\xi}{1+\xi}\right)^2$$



Note: $R \neq 0$ $\forall$ $V_0 < E < \infty$, even if the energy is lower than V_0, the particle can be reflected.

Now, consider the case

$$E - V_0 < 0$$



Now

$$q^2 = -\frac{2m}{\hbar^2}(V_0 - E) \Rightarrow q = i|q|; \qquad |q| = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

and $\quad u_{II}(x) = C e^{iqx} = C e^{-|q|x}$ ← exponentially decaying wave (evanescent wave)

This wave is REAL, therefore $\vec{J} = 0 \Leftrightarrow$ there is no probability current flow associated to it.

Moreover, from (1.4) it follows that:

$$C = \frac{2}{1 + i|q|/k}; \qquad B = \frac{1 - i|q|/k}{1 + i|q|/k}$$

Defining again $\frac{|q|}{k} \equiv \xi$, then $\quad B = \frac{1 - i\xi}{1 + i\xi} \equiv \frac{Z^*}{Z}$

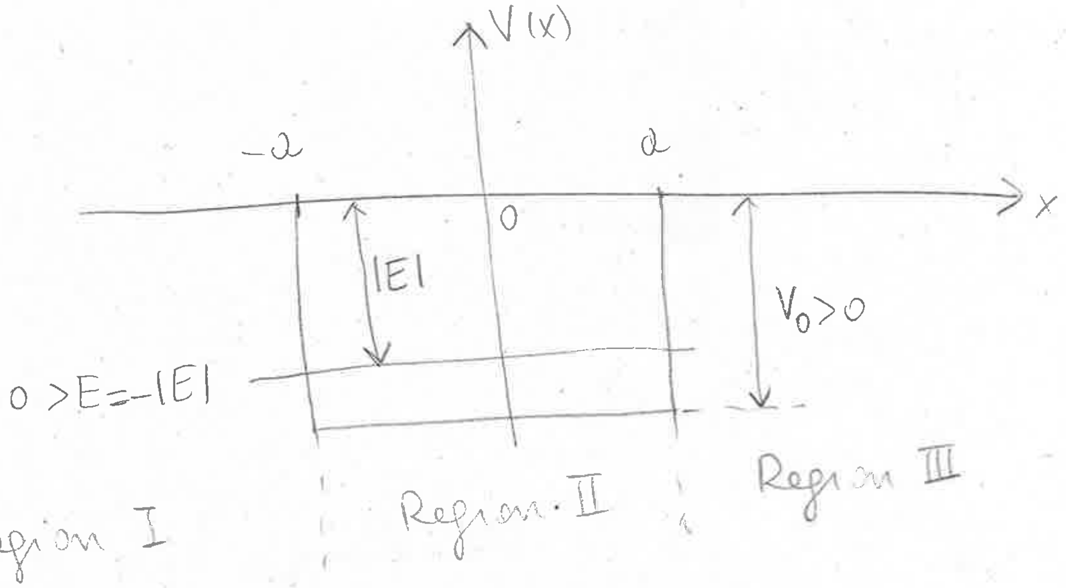
where $Z \equiv 1 + i\xi$. Therefore:

$$|B| = 1; \quad B = \exp\left[-2i \operatorname{ArcTan}\left(\frac{|q|}{k}\right)\right]$$

The Transmission and reflection coefficients are:

$$T = 0 \begin{pmatrix}\text{from 1.6} \\ \text{with } \mathrm{Re}\, q = 0\end{pmatrix}; \qquad R = |B|^2 = 1 \,!$$

– BOUND STATES IN THE POTENTIAL WELL –



Assume $\quad V_0-|E|\geq 0$

$$V(x)=\begin{cases}0, & x\leq -a \quad (\mathrm{I})\\ -V_0, & -a<x<a \quad (\mathrm{II})\\ 0, & x\geq a \quad (\mathrm{III})\end{cases}$$

The sch equation is, as usual:

$$-\frac{\hbar^2}{2m}u''(x)=\left(E-V(x)\right)u(x)$$

$$\Leftrightarrow \quad \boxed{u''(x)+\frac{2m}{\hbar^2}\left(E-V(x)\right)u(x)=0} \qquad (1.9)$$

where

$$\frac{2m}{\hbar^2}\left[E-V(x)\right]=\begin{cases}-\frac{2m}{\hbar^2}|E|\equiv -q^2, & x\leq -a\\ +\frac{2m}{\hbar^2}(V_0-|E|)\equiv +K^2, & |x|<a\\ -\frac{2m}{\hbar^2}|E|\equiv -q^2, & x\geq a\end{cases} \qquad (2.9)$$

Therefore, the three Sch. eqs. are:

$$u_I''(x) - q^2 u_I(x) = 0 \Rightarrow u_I(x) = A e^{qx} + \underline{B e^{-qx}}$$

$$u_{II}''(x) + K^2 u_{II}(x) = 0 \Rightarrow u_{II}(x) = C e^{ikx} + D e^{-ikx}$$

$$u_{III}''(x) - q^2 u_{III}(x) = 0 \Rightarrow u_{III}(x) = \underline{E e^{qx}} + F e^{-qx}$$

For $x \leq a$, the solution $B e^{-qx}$ is exponentially growing, therefore not acceptable. We put $B=0$

For $x \geq a$, $E e^{qx}$ is not acceptable $\Rightarrow E=0$

Continuity of functions and first derivatives require:

- At $x=-a$:

$$A e^{-qa} = C e^{-ika} + D e^{ika}$$

$$q A e^{-qa} = ik(C e^{-ika} - D e^{ika})$$

- At $x=a$:

$$C e^{ika} + D e^{-ika} = F e^{-qa}$$

$$ik(C e^{ika} - D e^{-ika}) = -q F e^{-qa}$$

This algebraic system can be written in matrix form as:

$$\underbrace{\begin{bmatrix} e^{-qa} & -e^{-ika} & -e^{ika} & 0 \\ qe^{-qa} & -ike^{-ika} & ike^{ika} & 0 \\ 0 & e^{ika} & e^{-ika} & -e^{-qa} \\ 0 & ike^{ika} & -ike^{-ika} & qe^{-qa} \end{bmatrix}}_{M} \begin{bmatrix} A \\ C \\ D \\ F \end{bmatrix} = 0 \qquad (1.11)$$

The solutions other than $A = C = D = F = 0$, exist only for that values of $|E|$ such that $\boxed{\det M = 0}$

A determinant does not change if a scalar multiple of one row (column) is added to another row (column). Therefore, we multiply the THIRD row of M by q and we sum it to the FOURTH row, obtaining:

$$\det \begin{bmatrix} \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & 0 \\ 0 & \cdot & \cdot & \cdot \\ 0 & (q+ik)e^{ika} & (q-ik)e^{-ika} & 0 \end{bmatrix} = \det M$$

Now, I exchange the last two rows. This changes the sign of det M:

$$\det M = -\left[\begin{array}{ccc|c} e^{-qa} & -e^{-ika} & -e^{ika} & 0 \\ q e^{-qa} & -ik e^{-ika} & ik e^{ika} & 0 \\ 0 & (q+ik)e^{ika} & (q-ik)e^{-ika} & 0 \\ \hline 0 & e^{ika} & e^{-ika} & -e^{-qa} \end{array}\right]$$

$\Leftrightarrow \det M = e^{-qa} \det M'$

where $M' = \left[\text{Principal } 3\times3 \text{ submatrix}\right]$

Now I multiply the firs row of M' by $-q$ and I sum it to the second one

$$\det M' = \det \left[\begin{array}{c|cc} e^{-qa} & -e^{-ika} & -e^{ika} \\ \hline 0 & (q-ik)e^{-ika} & (q+ik)e^{ika} \\ 0 & (q+ik)e^{ika} & (q-ik)e^{-ika} \end{array}\right]$$

Finally: $\det M = e^{-2qa} \underbrace{\det \begin{bmatrix} G^* & G \\ G & G^* \end{bmatrix}}_{=(G^*)^2 - G^2}$ where $G \equiv (q+ik)e^{ika}$

So, $\det M = 0 \Rightarrow G^2 = (G^*)^2$ or $G = \pm G^*$

$\Leftrightarrow \boxed{(q+ik)e^{ika} = \pm (q-ik)e^{-ika}}$

If we divide both sides by $\sqrt{q^2+k^2}$ we obtain:

$$\frac{q+ik}{\sqrt{q^2+k^2}}\, e^{ika} = \pm \frac{q-ik}{\sqrt{q^2+k^2}}\, e^{-ika} \iff z e^{ika} = \pm z^* e^{-ika}$$

But $|z| = 1 \Rightarrow z = e^{i\phi}$, where: $\begin{cases} q = \sqrt{q^2+k^2}\cos\phi \\ k = \sqrt{q^2+k^2}\sin\phi \end{cases}$

So we obtain:

$$e^{i(ka+\phi)} = \pm e^{-i(ka+\phi)}$$

The positive root gives:

$$ka + \phi = 0 \qquad (1,13)$$

The negative root:

$$ka + \phi = \frac{\pi}{2} \qquad (2,13)$$

Now, $(1,13) \iff \tan\phi = -\tan(ka) \iff \frac{k}{q} = -\tan(ka)$

$$\iff \boxed{k\cot(ka) = -q} \qquad (3,13a) \quad \left(\frac{G}{G^*} = 1\right)$$

While $(2,13) \iff \underbrace{\tan\phi}_{=\frac{k}{q}} = \tan\left(\frac{\pi}{2} - ka\right) = \cot ka$

$$\iff \boxed{k\tan(ka) = q} \qquad (3,13b) \quad \left(\frac{G}{G^*} = -1\right)$$

These equations can be solved numerically (or graphically). Defining:

$$ka \equiv \xi \,, \quad qa \equiv \eta$$

Then

$$(3.13a) \rightarrow \quad \xi \cot \xi = -\eta \qquad (2.14a)$$

$$(3.13b) \rightarrow \quad \xi \tan \xi = \eta \qquad (2.14b)$$

So, there are $\underline{\text{TWO}}$ classes of solutions. Let us see their form. After the several transformations, the system (1.11) becomes:

$$\begin{bmatrix} e^{-qa} & -e^{-ika} & -e^{ika} & 0 \\ 0 & G^* & G & 0 \\ 0 & G & G^* & 0 \\ 0 & e^{ika} & e^{-ika} & -e^{-qa} \end{bmatrix} \begin{bmatrix} A \\ C \\ D \\ F \end{bmatrix} = 0 \qquad (1.14)$$

This implies that:

$$\begin{cases} G^* C + G D = 0 \\ G C + G^* D = 0 \end{cases} \Leftrightarrow \begin{cases} G^* + G \dfrac{D}{C} = 0 \Rightarrow \boxed{\dfrac{D}{C} = -\dfrac{G^*}{G}} \\ G + G^* \dfrac{D}{C} = 0 \Rightarrow \dfrac{D}{C} = -\dfrac{G}{G^*} \end{cases}$$

From (3.13a) it follows

$$-D = C \qquad \text{"o"} \Leftrightarrow \text{ODD}$$

$$\text{"e"} \Leftrightarrow \text{EVEN}$$

and $\quad u^{o}_{II}(x) = 2iC\sin(kx)$

From (3.13b) it follows $D=C \Rightarrow u^{e}_{II}(x) = 2C\cos(kx)$

The other two equations in (1.14) give.

$$\begin{cases} Ae^{-qa} - Ce^{-ika} - De^{ika} = 0 \\ Ce^{ika} + De^{-ika} - Fe^{-qa} = 0 \end{cases}$$

- If $C=-D$ they become.

$$\left.\begin{aligned} &Ae^{-qa} + C(e^{ika} - e^{-ika}) = 0 \\ &C(e^{ika} - e^{-ika}) - Fe^{-qa} = 0 \end{aligned}\right\} \Rightarrow$$

$$\Rightarrow \begin{cases} A = -2Ci\sin(ka)e^{qa} \\ F = 2Ci\sin(ka)e^{qa} \end{cases}$$

- If $C=D$, instead:

$$\begin{cases} A = 2C\cos(ka)e^{qa} \\ F = 2C\cos(ka)e^{qa} \end{cases}$$

Gathering all these results, eventually we find:

$$\left.\begin{aligned} u_I(x) &= -2iC\sin(ka)\,e^{q(x+a)} \\ u_{II}(x) &= 2iC\sin(kx) \\ u_{III}(x) &= 2iC\sin(ka)\,e^{-q(x-a)} \end{aligned}\right\} \quad k\cot(ka) = -q$$

ODD solutions.

$$\left.\begin{aligned} u_I(x) &= 2C\cos(ka)\,e^{q(x+a)} \\ u_{II}(x) &= 2C\cos(kx) \\ u_{III}(x) &= 2C\cos(ka)\,e^{-q(x-a)} \end{aligned}\right\} \quad k\tan(ka) = q$$

EVEN SOLUTIONS.

The last parameter C is fixed by normalization:

$$\int_{-\infty}^{\infty} |u(x)|^2 dx = \int_{-\infty}^{-a} |u_I(x)|^2 dx + \int_{-a}^{a} |u_{II}(x)|^2 dx + \int_{a}^{\infty} |u_{III}(x)|^2 dx$$

$$= 1$$

Now, we look for the eigenvalues. From p14, we have:

$$\xi \equiv ka \quad ; \quad \eta \equiv qa$$

From (2.9) it follows that:

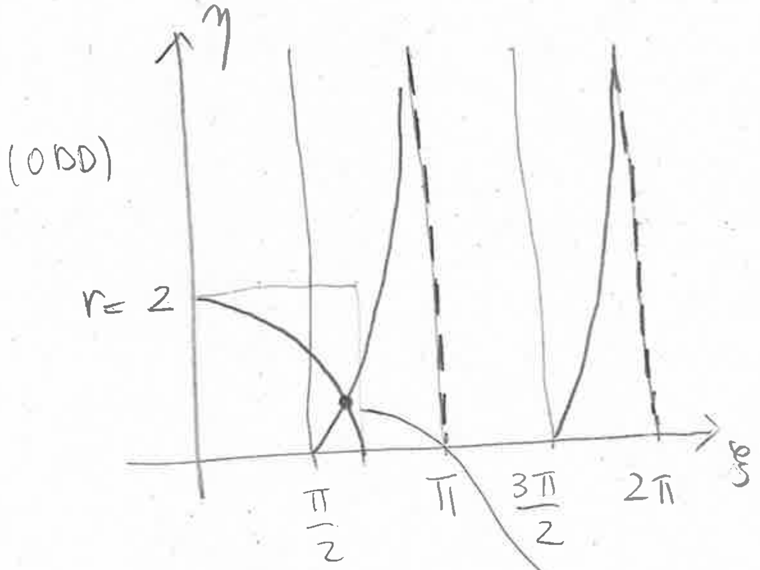
$$\xi^2 + \eta^2 = a^2(k^2+q^2) = \underbrace{\frac{2ma^2}{\hbar^2} V_0}_{\text{independent from } E!} - \cancel{\frac{2ma^2}{\hbar^2}|E|} + \cancel{\frac{2ma^2}{\hbar}|E|}$$

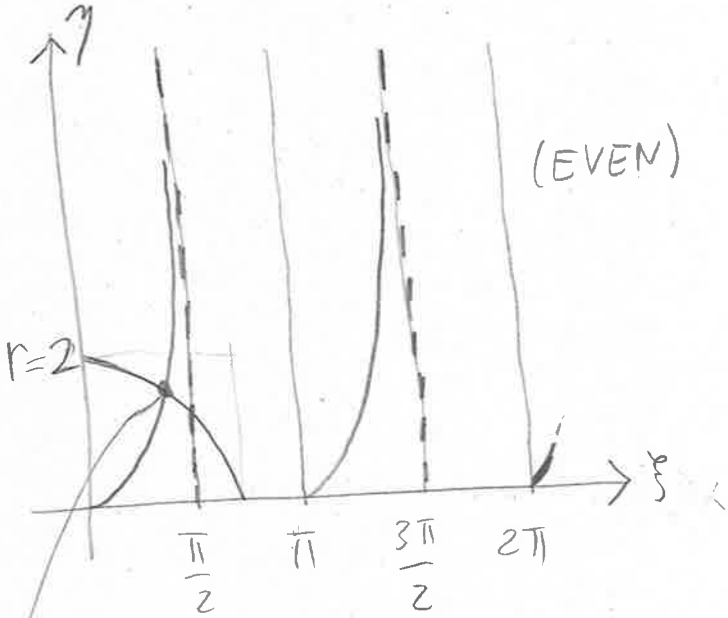
$$\equiv r^2$$

Combining this result with (2.14) we find.

$$\begin{cases} \xi \cot \xi = -\eta \\ \xi^2 + \eta^2 = r^2 \end{cases}$$ ODD eigenstates

$$\begin{cases} \xi \tan \xi = \eta \\ \xi^2 + \eta^2 = r^2 \end{cases}$$ EVEN eigenstates

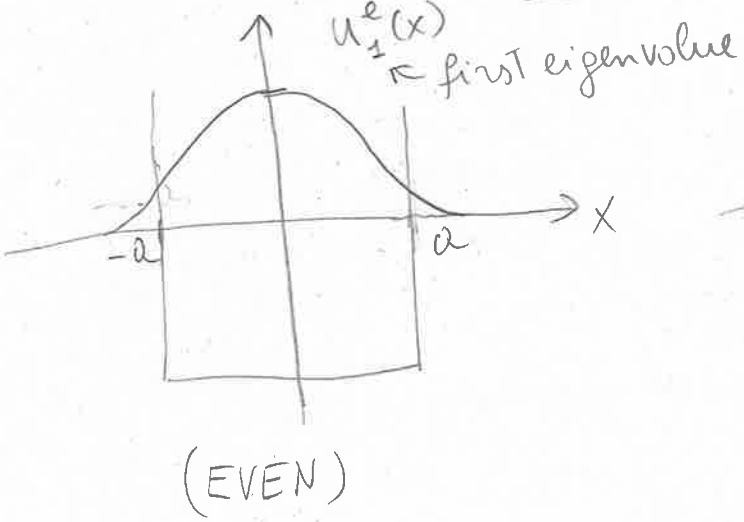


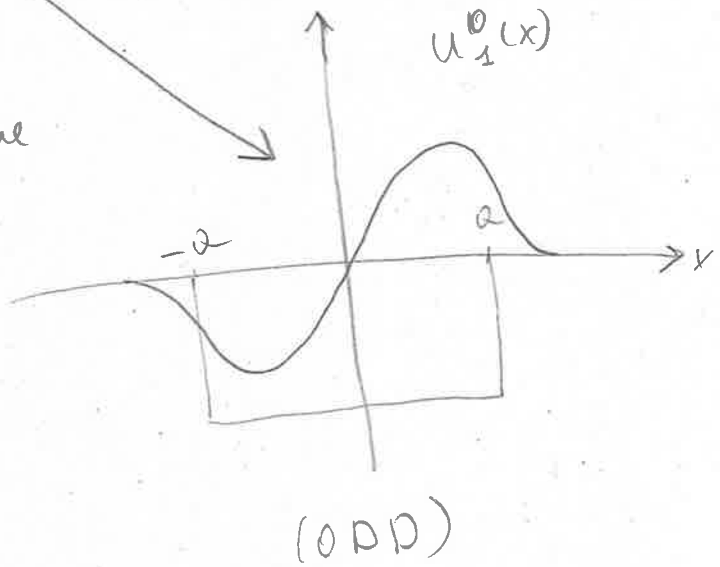


if $r = \sqrt{2mV_0}\,\frac{a}{\hbar} < \frac{\pi}{2}$

There are not solutions.

There is ALWAYS, at least, one solution





– HOMEWORK –

Solve the rectangular barrier problem, where

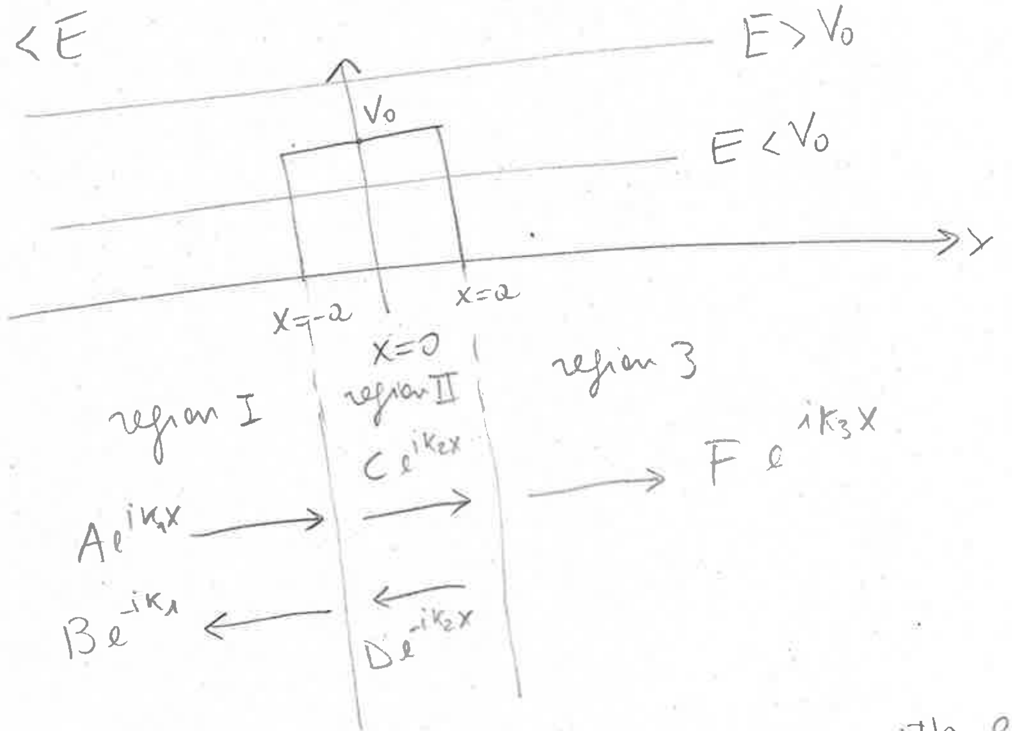
$$V(x) = \begin{cases} 0, & x < -a \\ V_0 > 0, & -a \le x \le a \\ 0, & a < x \end{cases}$$

Use the notation in the figure below to find;

Transmission and reflection coefficients for:

a) $0 < E < V_0$

b) $V_0 < E$



– Homework –

Consider the particle in a box, for $0 \le x \le a > 0$, with eigenvalues E_n and eigenfunctions $u_n(x)$ such that: $E_n = n^2 \frac{\hbar^2 \pi^2}{2ma^2}$; $u_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$

The particle is prepared in the state $\psi(x) = \frac{\sqrt{30}}{a^{5/2}} x(a-x)$. Calculate:

a) b_n, where $\psi(x) = \sum_{n=1}^{\infty} b_n u_n(x)$

b) $\langle \hat{H} \rangle_n = \sum_{n=1}^{\infty} |b_n|^2 E_n$

c) $\langle \hat{H} \rangle_n = \int_0^a u_n^*(x) \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} u_n(x) \right] u_n(x)$

d) $\langle \hat{H}^2 \rangle_n = \sum_{n=1}^{\infty} |b_n|^2 E_n^2$; e) $\langle \hat{H}^2 \rangle_n = \int_0^a u_n^*(x) \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right)^2 u_n(x)\, dx$

COMPARE ______ AND DISCUSS THE RESULTS.