

PART II

Phys 3010

Theorem: If the potential $V(x)$ is an even function of x , $V(-x) = V(x)$, then the stationary quantum states in this potential have definite parity:

$$\psi(-x) = P\psi(x), \quad P = \pm 1.$$

Proof:

$$H(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

$$H(-x) = -\frac{\hbar^2}{2m} \frac{d^2}{d(-x)^2} + V(-x) = H(x)$$

(1) $\boxed{\epsilon \psi(x) = H(x) \psi(x)}$ $\psi(x)$ is a stationary state with energy ϵ .

consider state $\varphi(x) = \psi(-x)$

$$H(x) \varphi(x) = H(-x) \varphi(x) = \boxed{H(-x) \psi(-x) = \epsilon \psi(-x)}$$

Hence

(2) $\boxed{\epsilon \varphi(x) = H(x) \varphi(x)}$

Thus, $\varphi(x)$ satisfies the same eq. as $\psi(x)$.

Hence $\varphi(x) = P\psi(x)$ where P is a number.

Consider now $\varphi(-x)$ (double reflection)

$$\varphi(-x) = \psi(-(-x)) = \underline{\underline{\psi(x)}}$$

on the other hand

$$\varphi(-x) = P\psi(-x) = P\varphi(x) = \underline{\underline{P^2\psi(x)}}$$

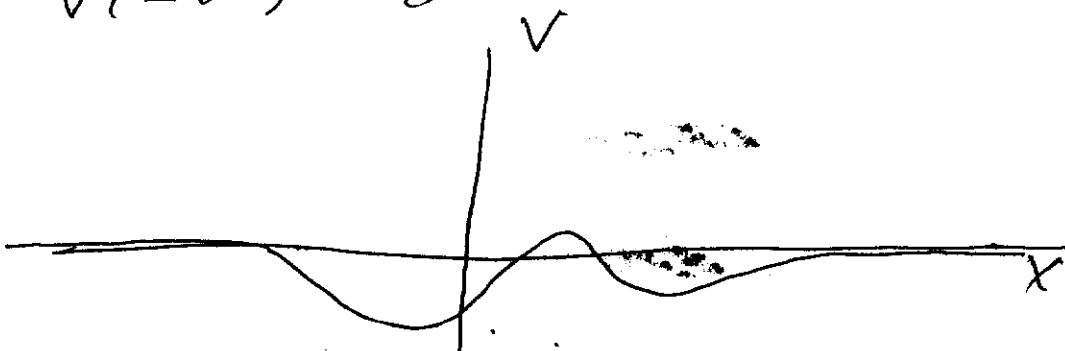
$$\boxed{\psi(x) = P^2\psi(x)} \Rightarrow P^2 = 1 \Rightarrow P = \pm 1.$$

End of proof.

Bound states and scattering (unbound) states

Consider a potential $V(x)$ such that

$$V(\pm\infty) = 0$$



Stationary states are given by
Schrödinger eq.

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

Consider very large value of x (positive or negative), then $V(x) = 0$ and the eq. reads

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

There are two possibilities:

(I) $E > 0$

(II) $E < 0$

(I) Consider $E > 0$. In this case $\psi = A e^{ikx} = a \cos kx + b \sin kx$

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

$$\frac{d\psi}{dx} = ik A e^{ikx}, \quad \frac{d^2\psi}{dx^2} = (ik)^2 A e^{ikx} = -k^2 A e^{ikx}$$

$$S.E.: \quad E A e^{ikx} = \frac{\hbar^2 k^2}{2m} A e^{ikx} \Rightarrow \boxed{E = \frac{\hbar^2 k^2}{2m} > 0}$$

This is an unbound state because there is a finite probability to find particle at arbitrary large distance.

At a given energy the wave number k can be positive (particle moving from left to right) or negative (particle moving from right to left).

$$k = \pm \sqrt{\frac{2mE}{\hbar^2}}$$

Thus, any unbound state is double degenerate

Bound.

(II) $E < 0$, then $\psi(x) = A e^{-kx}$

$$\psi' = -kA e^{-kx}, \quad \psi'' = (-k)^2 A e^{-kx} = k^2 A e^{-kx}$$

$$E\psi = E A e^{-kx} = -\frac{\hbar^2}{2m} \psi'' = -\frac{\hbar^2 k^2}{2m} A e^{-kx}$$

$$E = -\frac{\hbar^2 k^2}{2m}, \quad E = -|E|$$

$$k = \pm \sqrt{\frac{2m|E|}{\hbar^2}}$$

Consider $x > 0$. There are two solutions (27)

$$\psi = A e^{-\sqrt{\frac{2m|E|}{\hbar^2}} x}$$

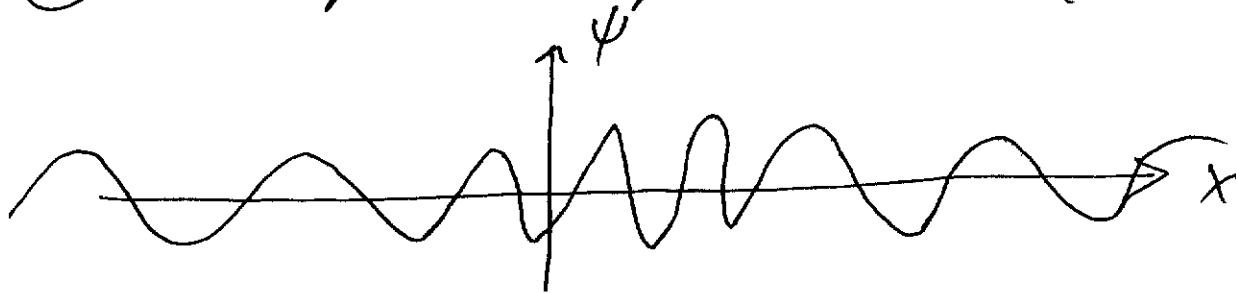
$$\psi = A e^{+\sqrt{\frac{2m|E|}{\hbar^2}} x}$$

However, there is also the normalization condition, $\int_{-\infty}^{+\infty} |\psi|^2 dx = 1$. Therefore

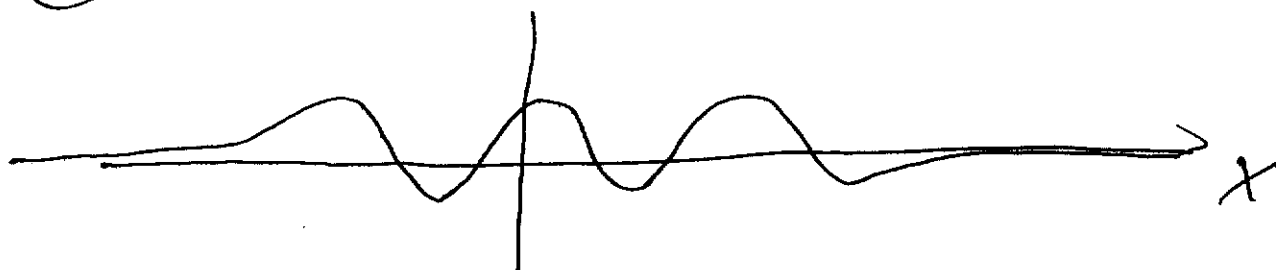
ψ must approach zero at $x \rightarrow \infty$.
Hence only the solution $\psi = A e^{-\sqrt{\frac{2m|E|}{\hbar^2}} x}$
is physical.

Similarly at $x < 0$, only $\psi = A e^{+\sqrt{\frac{2m|E|}{\hbar^2}} x}$ is physical.

① Wave function of the unbound (scattering) state

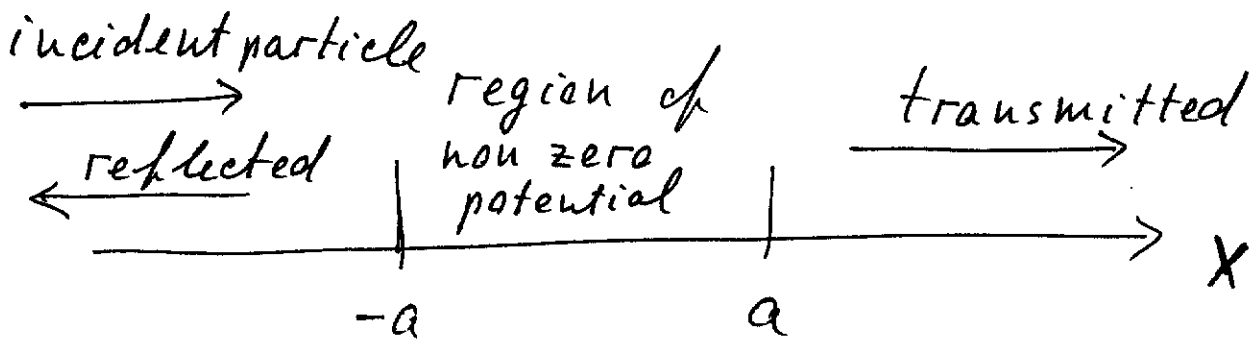


② Wave function of the bound state



Scattering

Reflection and transmission coefficients.
Scattering on the potential well.



stationary scattering state:

$$x < -a, \psi(x) = e^{ikx} + R e^{-ikx}$$

↑ incident wave ↑ reflected wave

$$x > +a, \psi(x) = T e^{ikx} \text{ - transmitted wave}$$

The probability flux at $x > +a$

$$j_{\text{transm}} = -\frac{i\hbar}{2m} \left[\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x} \psi \right] =$$

$$= -\frac{i\hbar}{2m} |T|^2 [ik + ik] = \underline{\underline{\frac{\hbar k}{m} |T|^2}}$$

Probability flux at $x < -a$.

$$\begin{aligned}
j &= -\frac{i\hbar}{2m} \left\{ (e^{-ikx} + R e^{ikx}) (i k e^{ikx} - i k R e^{-ikx}) - c.c. \right\} = \\
&= -\frac{i\hbar}{2m} \left\{ \underline{i k + i k R} e^{2ikx} - \underline{i k R} e^{-2ikx} - i k |R|^2 - \right. \\
&\quad \left. - \left[-i k - \underline{i k R} e^{-2ikx} + \underline{i k R} e^{2ikx} + i k |R|^2 \right] \right\} = \\
&= -\frac{i\hbar}{2m} 2ik (1 - |R|^2) = \underline{\underline{\frac{k}{m} (1 - |R|^2)}}
\end{aligned}$$

incident flux : $j_{inc} = \frac{k}{m}$

reflected flux : $j_{refl.} = -\frac{k}{m} |R|^2$

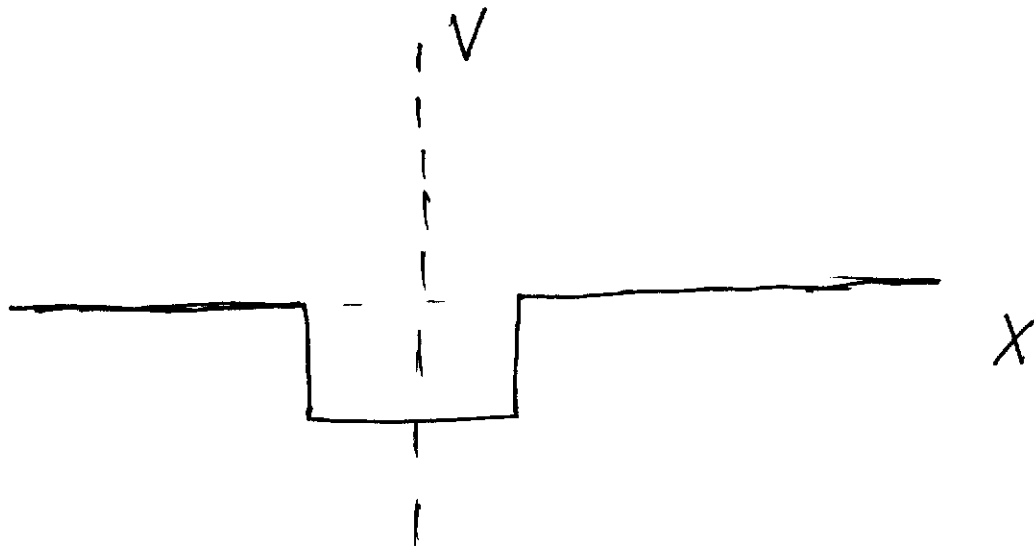
The flux is conserved:

$$j_{inc} + j_{refl.} = j_{transm} \Rightarrow \boxed{1 - |R|^2 = |T|^2}$$

$$\left\{ \begin{aligned}
\text{probability of transmission} &= \frac{j_{transm}}{j_{inc}} = |T|^2 \\
\text{probability of reflection} &= \frac{j_{refl.}}{j_{inc}} = |R|^2
\end{aligned} \right.$$

Scattering on the potential well.

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

$\epsilon > 0 \Leftrightarrow$ scattering

outside the well $\psi = A e^{ikx} + B e^{-ikx}$

$$\epsilon \psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \Rightarrow \epsilon (A e^{ikx} + B e^{-ikx}) = -\frac{\hbar^2}{2m} ((ik)^2 A e^{ikx} + (ik)^2 B e^{-ikx}).$$

S. eq. is satisfied at arbitrary A and B.

$$\boxed{\epsilon = \frac{\hbar^2 k^2}{2m}}$$

For scattering problem

$$\psi = \begin{cases} e^{ikx} + R e^{-ikx}, & x < -a \\ T e^{ikx}, & x > a \end{cases}$$

Within the well

(31)

$$-a < x < a$$

$$E\psi = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V_0\psi, \quad \psi = A e^{iqx} + B e^{-iqx}$$

$$\boxed{E = \frac{\hbar^2 q^2}{2m} + V_0} \Rightarrow \boxed{q = \sqrt{\frac{2m(V_0 + E)}{\hbar^2}}}$$

Matching conditions

The potential is finite ($|V| < \infty$), hence, due to S. eq. $\frac{d^2\psi}{dx^2}$ is also finite.

Therefore $\frac{\partial\psi}{\partial x}$ is continuous.

The wave function ψ is always (even if the potential is infinite) continuous.

Matching conditions at $x=a$

$$\text{limit } \delta \rightarrow 0 \begin{cases} \psi(a-\delta) = \psi(a+\delta) \\ \psi'(a-\delta) = \psi'(a+\delta) \end{cases}$$

(32)

$$\textcircled{\text{I}} \begin{cases} A e^{iqa} + B e^{-iqa} = T e^{ika} \\ iq[A e^{iqa} - B e^{-iqa}] = ikT e^{ika} \end{cases}$$

Matching conditions at $x = -a$

$$\text{limit } \delta \rightarrow 0 \begin{cases} \psi(-a-\delta) = \psi(-a+\delta) \\ \psi'(-a-\delta) = \psi'(-a+\delta) \end{cases}$$

$$\textcircled{\text{II}} \begin{cases} e^{-ika} + R e^{ika} = A e^{-iqa} + B e^{iqa} \\ ik[e^{-ika} - R e^{ika}] = iq[A e^{-iqa} - B e^{iqa}] \end{cases}$$

Solving 4 eqs. $\textcircled{\text{I}}$ $\textcircled{\text{II}}$ one can find

4 unknown variables A, B, R, T .

This completely solves the scattering problem.

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Transmission resonances.

Subbarrier tunneling

Let us solve eqs. (I) (II) on page 32.

Divide I.2 by I.1:
$$q \frac{Ae^{iqa} - Be^{-iqa}}{Ae^{iqa} + Be^{-iqa}} = K \quad (3)$$

Divide II.2 by II.1:
$$q \frac{Ae^{-iqa} - Be^{iqa}}{Ae^{-iqa} + Be^{iqa}} = K \frac{e^{-ika} - Re^{ika}}{e^{-ika} + Re^{ika}} \quad (4)$$

Let us introduce
$$\alpha = \frac{B}{A} e^{-2iqa}$$

Then from (3) we get

$$\frac{1-\alpha}{1+\alpha} = \frac{K}{q} \Rightarrow 1-\alpha = \frac{K}{q}(1+\alpha) \Rightarrow \alpha = \frac{q-K}{q+K}$$

From (4) one gets:

$$\frac{q}{k} \frac{1 - \alpha e^{4iqa}}{1 + \alpha e^{4iqa}} = \frac{1 - R e^{2ika}}{1 + R e^{2ika}}$$

\parallel
 Z

$$(1 + R e^{2ika}) \frac{q}{k} Z = 1 - R e^{2ika} \Rightarrow$$

$$R e^{2ika} \left[1 + Z \frac{q}{k} \right] = 1 - Z \frac{q}{k} \Rightarrow$$

$$R e^{2ika} = \frac{k - Zq}{k + Zq}$$

$$Z = \frac{1 - \frac{q-k}{q+k} e^{4iqa}}{1 + \frac{q-k}{q+k} e^{4iqa}} = \frac{(q+k) - (q-k) e^{4iqa}}{(q+k) + (q-k) e^{4iqa}}$$

$$R e^{2ika} = \frac{k-q \frac{(q+k) - (q-k)e^{4iqa}}{(q+k) + (q-k)e^{4iqa}}}{k+q \frac{(q+k) - (q-k)e^{4iqa}}{(q+k) + (q-k)e^{4iqa}}} =$$

$$= \frac{k[(q+k) + (q-k)e^{4iqa}] - q[(q+k) - (q-k)e^{4iqa}]}{k[(q+k) + (q-k)e^{4iqa}] + q[(q+k) - (q-k)e^{4iqa}]}$$

$$= \frac{(kq + k^2 - q^2 - kq) + (kq - k^2 + q^2 - kq)e^{4iqa}}{(kq + k^2 + q^2 + kq) + (kq - k^2 - q^2 + kq)e^{4iqa}}$$

$$= \frac{(k^2 - q^2) - (k^2 - q^2)e^{4iqa}}{(k+q)^2 + (k-q)^2 e^{4iqa}} = (q^2 - k^2) \frac{e^{2iqa} - e^{-2iqa}}{(k+q)^2 e^{-2iqa} - (k-q)^2 e^{2iqa}}$$

2i sin 2qa

$$R = 2i e^{-2ika} \frac{(q^2 - k^2) \sin 2qa}{(k+q)^2 e^{-2iqa} - (k-q)^2 e^{2iqa}}$$

Transmission resonances

Let $2qa = \pi n$, $n = 1, 2, 3 \dots$

hence $\sin 2qa = 0$, hence $R = 0$,

hence $|T| = 1$. Remember: $1 - |R|^2 = |T|^2$

No reflection, full transmission.

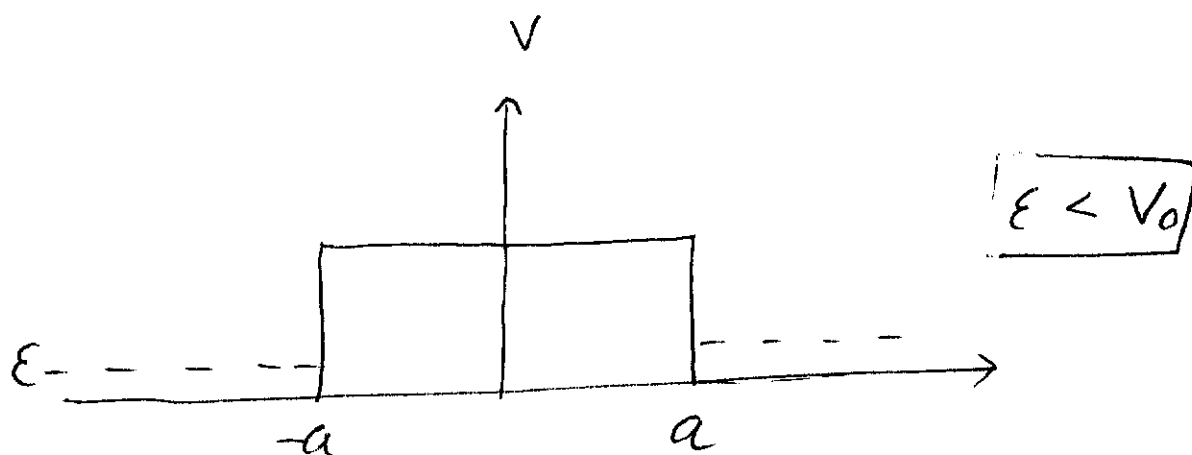
$$q = \frac{\pi n}{2a} = \sqrt{\frac{2m(V_0 + E)}{\hbar^2}} \leftarrow \text{see page 31}$$

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

E must be positive (scattering). It means that at given V_0 the integer n must be large enough.

At these values of energy the well is fully transparent. This is the transmission resonance.

Subbarrier tunneling



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

$$\psi = \begin{cases} e^{ikx} + R e^{-ikx}, & x < -a \\ A e^{-qx} + B e^{qx}, & -a < x < a \\ T e^{ikx}, & x > a \end{cases}$$

$$E\psi = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V_0\psi, \quad \text{at } -a < x < a:$$

$$E(A e^{-qx} + B e^{qx}) = -\frac{\hbar^2}{2m} q^2 (A e^{-qx} + B e^{qx}) + V_0 (A e^{-qx} + B e^{qx})$$

$$E = -\frac{\hbar^2 q^2}{2m} + V_0 \Rightarrow$$

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

Matching conditions

(38)

$$\textcircled{\text{I}} x=a: \begin{cases} Ae^{-qa} + Be^{qa} = Te^{ika} \\ -qAe^{-qa} + qBe^{qa} = ikTe^{ika} \end{cases}$$

$$\textcircled{\text{II}} x=-a: \begin{cases} Ae^{qa} + Be^{-qa} = e^{-ika} + Re^{ika} \\ -qAe^{qa} + qBe^{-qa} = ike^{-ika} - Rike^{ika} \end{cases}$$

There are 4 eqs. and 4 unknown variables A, B, R, T . So the eqs. can be resolved in general case. To avoid long algebra let us consider the case of thick barrier, $qa \gg 1$, or more precisely $e^{2qa} \gg 1$.

In this case the transmission is very small, hence $|R| \approx 1$, or we can write $R = -e^{-2ika + i\varphi}$, where φ is an unknown phase.

We will see that $A \sim e^{-qa}$ and $B \sim e^{-3qa}$. It means that B-terms can be neglected in (II) . Hence we get from (II)

$$\begin{cases} A e^{qa} = e^{-ika} (1 - e^{i\varphi}) \\ -q A e^{qa} = ik e^{-ika} (1 + e^{i\varphi}) \end{cases}$$

Divide second by first eq.:

$$ik \frac{1 + e^{i\varphi}}{1 - e^{i\varphi}} = -q \quad ; \quad ik \frac{e^{-i\frac{\varphi}{2}} + e^{i\frac{\varphi}{2}}}{e^{-i\frac{\varphi}{2}} - e^{i\frac{\varphi}{2}}} = -q$$

$$ik \frac{2 \cos \frac{\varphi}{2}}{-2i \sin \frac{\varphi}{2}} = -q \Rightarrow \boxed{\tan \frac{\varphi}{2} = \frac{k}{q}}$$

$$A = e^{-qa - ika} (1 - e^{i\varphi}) = e^{-qa - ika} e^{\frac{i\varphi}{2}} (e^{-i\frac{\varphi}{2}} - e^{i\frac{\varphi}{2}})$$

$$= -2i e^{-qa - ika} e^{\frac{i\varphi}{2}} \sin \frac{\varphi}{2} = -2i e^{-qa - ika} \times$$

$$\times \sin \frac{\varphi}{2} \left(\cos \frac{\varphi}{2} + i \sin \frac{\varphi}{2} \right)$$

$$\cos \frac{\varphi}{2} = \frac{1}{\sqrt{1 + \tan^2 \frac{\varphi}{2}}} = \frac{q}{\sqrt{k^2 + q^2}}, \quad \sin \frac{\varphi}{2} = \frac{k}{\sqrt{k^2 + q^2}}$$

$$A = -2i e^{-qa-ika} \frac{k(q+ik)}{k^2+q^2} = 2 e^{-qa-ika} \frac{k(k-iq)}{k^2+q^2} \quad (40)$$

$$A = \frac{2k}{k+iq} e^{-qa-ika}$$

Now, let us substitute A in (I):

$$\begin{cases} \frac{2k}{k+iq} e^{-2qa-ika} + B e^{qa} = T e^{ika} \\ -\frac{2k}{k+iq} e^{-2qa-ika} + B e^{qa} = \frac{ik}{q} T e^{ika} \end{cases}$$

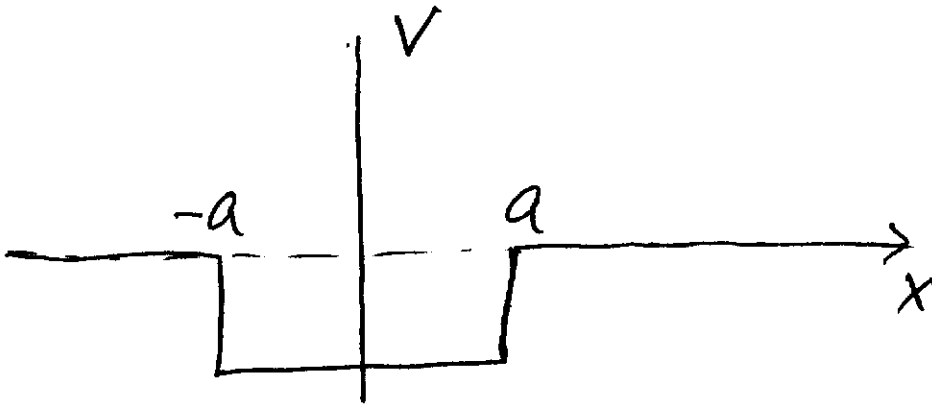
Subtract second from first eq.

$$\frac{4k}{k+iq} e^{-2qa-ika} = T e^{ika} \left(1 - \frac{ik}{q}\right) = T e^{ika} \frac{(-i)(k+iq)}{q}$$

$$T = \frac{4ikq}{(k+iq)^2} e^{-2qa-2ika}$$

$$\left. \begin{array}{l} \text{subbarrier tunneling} \\ \text{probability} \end{array} \right\} = |T|^2 = \left(\frac{4kq}{k^2+q^2}\right)^2 e^{-4qa}$$

Bound states in the potential well



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

$E = -|E|$ negative (bound)

$$\left. \begin{array}{l} x < -a, \quad \psi = c_1 e^{kx} \\ x > a, \quad \psi = c_2 e^{-kx} \end{array} \right\} \text{ see pp 26-27}$$

$$-a < x < a$$

$$\boxed{E\psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} - V_0 \psi}$$

$$\psi = A \cos qx + B \sin qx$$

$$\psi'' = -q^2 (A \cos qx + B \sin qx)$$

Substitute into S. eq.

$$E(A \cos qx + B \sin qx) = \frac{\hbar^2 q^2}{2m} (A \cos qx + B \sin qx) - V_0 (A \cos qx + B \sin qx)$$

Hence $\boxed{E = \frac{\hbar^2 q^2}{2m} - V_0} \Rightarrow \boxed{q = \sqrt{\frac{2m(V_0 - |E|)}{\hbar^2}}}$

$$E = -\frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 q^2}{2m} - V_0 \Rightarrow$$

$$\Rightarrow \boxed{k = \sqrt{\frac{2mV_0}{\hbar^2} - q^2}}$$

q is real, hence $V_0 - |E|$ is always positive.
It means that the energy level is always above bottom of the potential.

Let us use the parity theorem (page 23) and consider separately even and odd solutions.

(43)

(I) Positive parity solution, $P=+1$

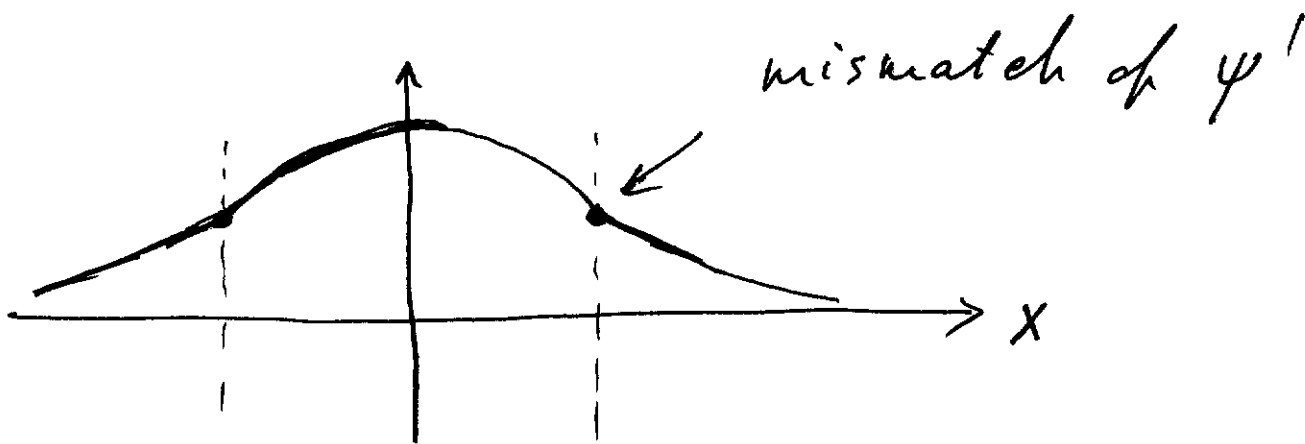
$$\psi = \begin{cases} c e^{-kx}, & x > a \\ A \cos qx, & -a < x < a \\ c e^{kx}, & x < -a \end{cases}$$

(II) Negative parity solution, $P=-1$

$$\psi = \begin{cases} D e^{-kx}, & x > a \\ B \sin qx, & -a < x < a \\ -D e^{kx}, & x < -a \end{cases}$$

(I) consider $P=+1$ solution.

plot of ψ at arbitrary q and κ .



mismatch in ψ' means $\psi''(x=\pm a) = \infty$
hence Schroedinger eq. is not satisfied
at $x = \pm a$.

Matching conditions at $x = a$

$$\begin{cases} A \cos qa = C e^{-\kappa a} \\ -q A \sin qa = -\kappa C e^{-\kappa a} \end{cases}$$

Similar conditions at $x = -a$ are fulfilled automatically because of symmetry of the solution.

Devide second eq. by first one

$$-q \tan qa = -k \Rightarrow \boxed{\tan qa = \frac{k}{q}}$$

Let us introduce new variable

$$y = qa$$

$$\boxed{\tan y = \frac{kq}{y}}$$

$$\text{or } \boxed{\tan y = \frac{\sqrt{\lambda - y^2}}{y}}$$

$$ka = \sqrt{\frac{2mV_0 a^2}{\hbar^2} - q^2 a^2} = \sqrt{\lambda - y^2}$$

↑
see page 42

denote $\boxed{\frac{2mV_0 a^2}{\hbar^2} = \lambda}$

λ is a dimensionless parameter

$\lambda \ll 1 \iff$ shallow potential

$\lambda \gg 1 \iff$ deep potential

consider electron ($m = 9.1 \cdot 10^{-31} \text{ kg}$) in potential of depth $V_0 = 10 \text{ eV} = 10 \cdot 1.6 \cdot 10^{-19} \text{ J} = 1.6 \cdot 10^{-18} \text{ J}$.

Two cases:

(A) length of the potential $2a = 10 \text{ \AA} = 10^{-9} \text{ m}$

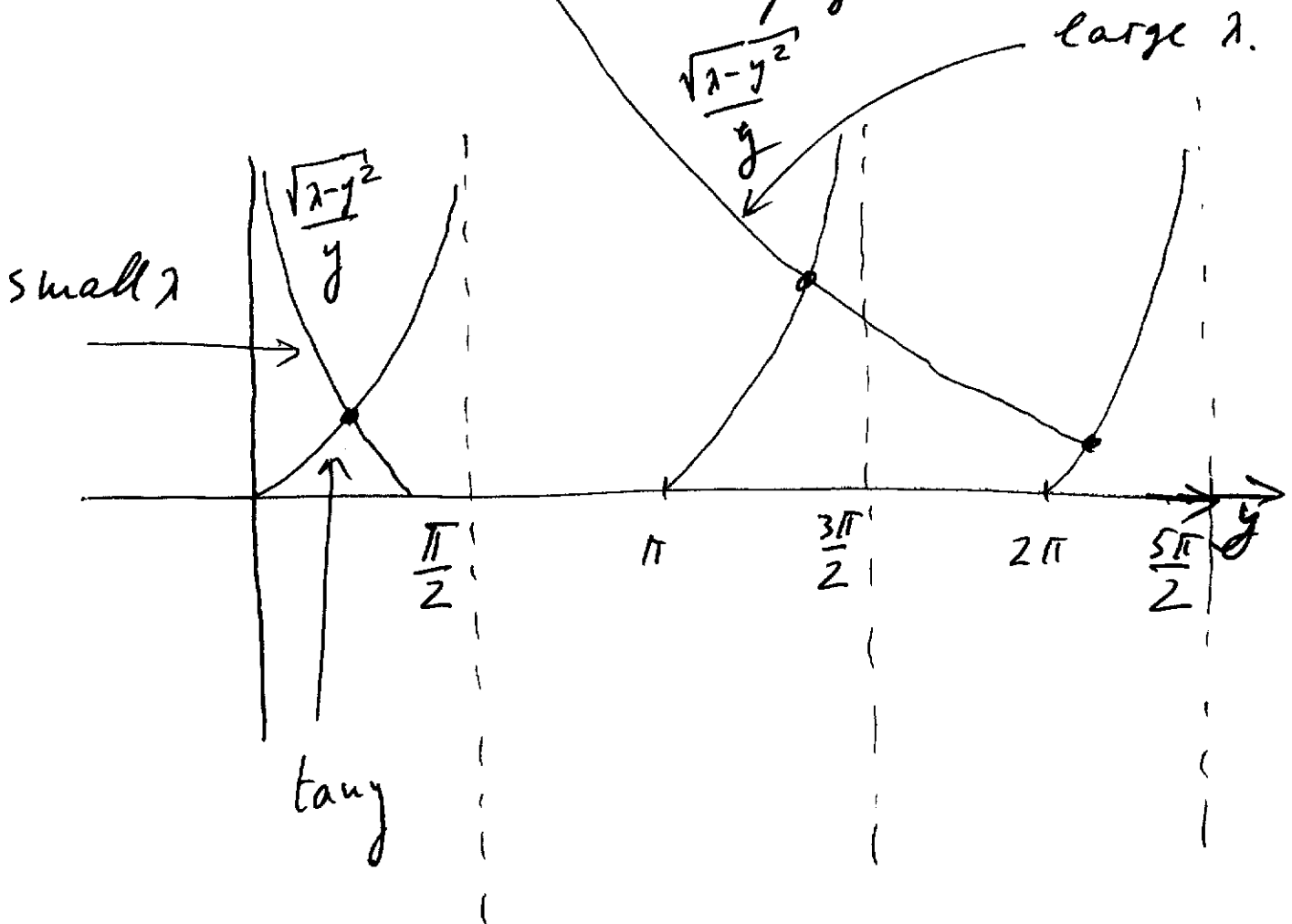
(B) length of the potential $2a = 0.1 \text{ \AA} = 10^{-11} \text{ m}$

(A)
$$\lambda = \frac{2 \cdot 9.1 \cdot 10^{-31} \cdot 1.6 \cdot 10^{-18} \cdot (0.5 \cdot 10^{-9})^2}{(1.054 \cdot 10^{-34})^2} \approx 70 \implies \text{very deep.}$$

(B)
$$\lambda = \frac{2 \cdot 9.1 \cdot 10^{-31} \cdot 1.6 \cdot 10^{-18} \cdot (0.5 \cdot 10^{-11})^2}{(1.054 \cdot 10^{-34})^2} = 0.007 \implies \text{very shallow}$$

$$\tan y = \frac{\sqrt{\lambda - y^2}}{y}$$

eq. for energy levels,
see page 45



at $\lambda \ll 1$ there is only one bound state

at $\lambda \gg 1$ there are many bound states

$\lambda \ll 1$ then $y^2 \approx \lambda$, actually y^2 is slightly smaller than λ

$$\sqrt{\lambda - y^2} = \kappa a \ll y \ll 1$$

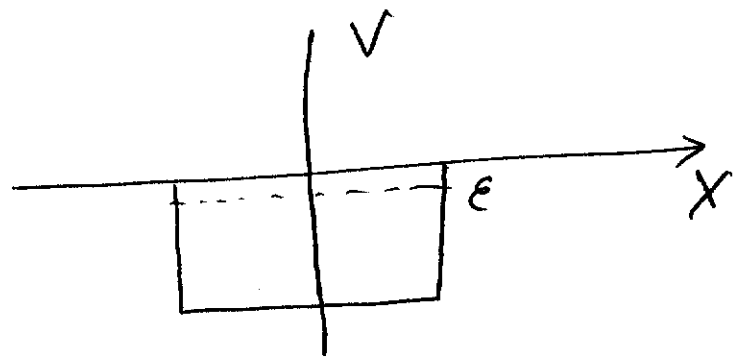
$$\tan y \approx y \approx \frac{\kappa a}{y} \Rightarrow \kappa a \approx y^2 \approx \lambda$$

$$\boxed{\kappa \approx \frac{\lambda}{a}}$$

$$E = -\frac{\hbar^2 \kappa^2}{2m} = -\frac{\hbar^2 \lambda^2}{2m a^2} = -\frac{\hbar^2 4m^2 V_0^2 a^4}{2m a^2 \hbar^4} =$$

$$= -\frac{2m a^2 V_0^2}{\hbar^2} = -\underbrace{\left(\frac{2m V_0 a^2}{\hbar^2}\right)}_{\lambda} V_0 = -\lambda V_0 \ll V_0$$

shallow level.



There is binding in arbitrary weak attractive potential.

↑
This statement is true only in 1D quantum mechanics.

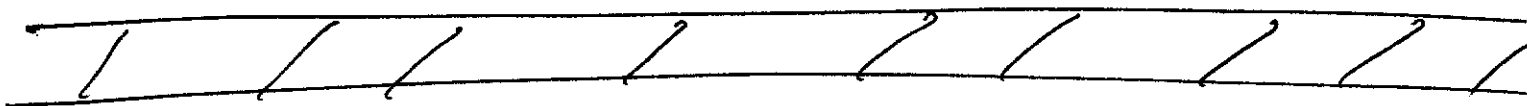
$$\lambda \gg 1$$

(43)

$$\tan y = \frac{\sqrt{\lambda^2 - y^2}}{y} \rightarrow \infty \Rightarrow y = (n + \frac{1}{2}) \pi$$
$$n = 0, 1, 2 \dots$$

$$q = \frac{7}{a} = \frac{\pi}{a} (n + \frac{1}{2})$$

The infinite potential well solution,
see page 20.



II Negative parity solution.

ψ is given in page 43.

Matching conditions at $x = a$

$$\begin{cases} B \sin qa = D e^{-ka} \\ qB \cos qa = -kD e^{-ka} \end{cases}$$

Divide eqs. \Rightarrow $\boxed{\cot qa = -\frac{k}{q}}$

Further solution is similar to the even ($n=1$) case. For details see text book