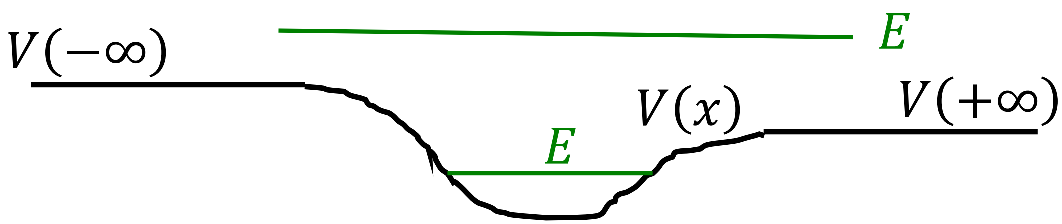
EE201/MSE207 Lecture 5

Bound and “scattering” (unbound) states

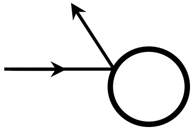


When a particle is limited in space (“bound”) and when not (“unbound”)?

In QM the answer is somewhat similar to the classical case:

If $\begin{cases} E < V(+\infty) \\ E < V(-\infty) \end{cases}$, then bound (localized, cannot go to infinity)

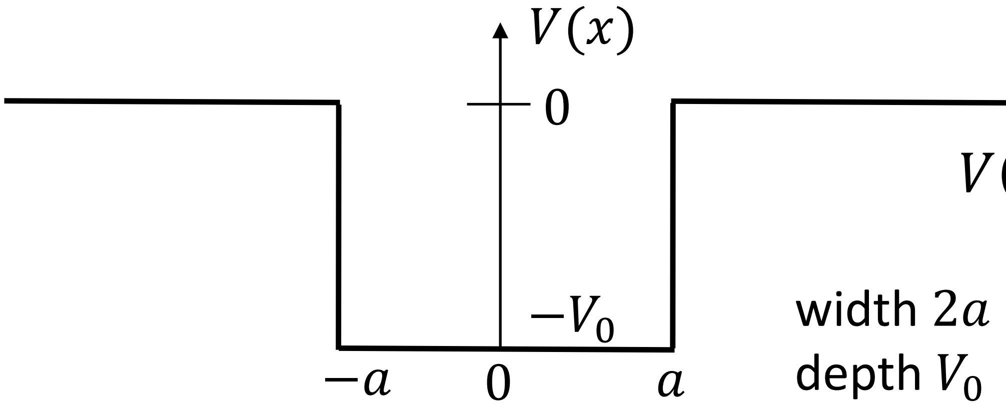
If $E > V(\infty)$ or $E > V(-\infty)$, then unbound (“scattering”);
can be at infinity, free particle there, $\psi \propto \exp(\pm ikx)$.
Why called “scattering”? Scattered particles (2D, 3D).



Important: Bound states $\Rightarrow$ discrete energy spectrum (as for infinite QW and oscillator)
Scattering states $\Rightarrow$ continuous energy spectrum (as for free particle)

We will analyze bound and scattering states in an important for applications example: finite square well

Finite square well



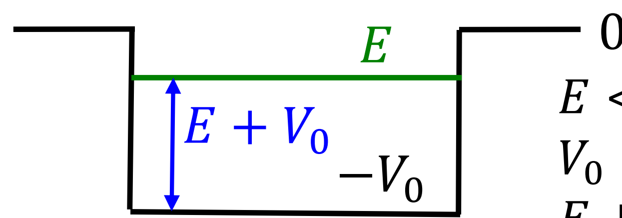
$$V(x) = \begin{cases} -V_0\,, & -a < x < a \\ 0\,, & |x| > a \end{cases}$$

width $2a$ (it was a for infinite well)

depth V_0

Today: Bound states, $E < 0$ ($E < E(\pm\infty) = 0$)

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



$E < 0$

$V_0 > 0$

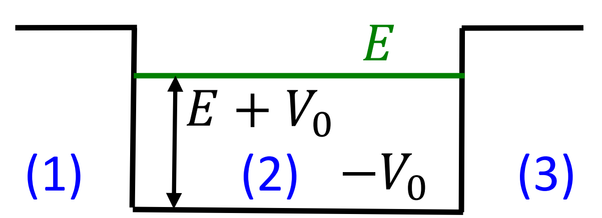
$E + V_0 > 0$

Three regions: (1) $x < -a$, (2) $-a < x < a$, (3) $x > a$

(1) (2) (3)

Solving TISE in 3 regions

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



$E < 0,\ V_0 > 0,$
$E + V_0 > 0$

(1) $x < -a \quad \Rightarrow \quad V = 0 \quad \Rightarrow \quad \dfrac{d^2\psi}{dx^2} = -\underbrace{\dfrac{2mE}{\hbar^2}}_{>0,\ =k^2}\psi$

$$\psi(x) = \cancel{A\,e^{-kx}} + B\,e^{kx}, \qquad k = \frac{\sqrt{-2mE}}{\hbar}$$

$A = 0$ because $\psi(-\infty) = 0$

(2) $-a < x < a \quad \Rightarrow \quad V = -V_0 \quad \Rightarrow \quad \dfrac{d^2\psi}{dx^2} = -\underbrace{\dfrac{2m(V_0 + E)}{\hbar^2}}_{<0,\ =-l^2}\psi$

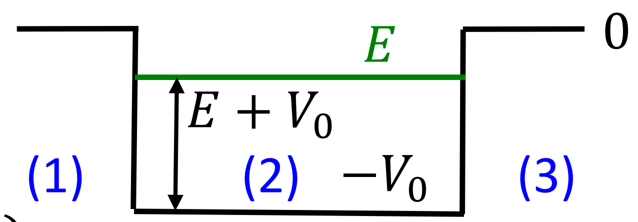
$$\psi(x) = C\sin(lx) + D\cos(lx) \qquad l = \frac{\sqrt{2m(V_0 + E)}}{\hbar}$$

(sin and cos are more convenient for bound states,
$e^{\pm ilx}$ more convenient for scattering states)

(3) $x > a \quad \Rightarrow \quad V = 0 \quad \Rightarrow \quad \psi(x) = F\,e^{-kx} + \cancel{G\,e^{kx}}$ (the same k)

$G = 0$ because $\psi(+\infty) = 0$

(1) $x < -a$ $\qquad \psi(x) = B\, e^{kx}, \quad k = \frac{\sqrt{-2mE}}{\hbar}$



(2) $-a < x < a$ $\qquad \psi(x) = C\sin(lx) + D\cos(lx)$

$$l = \sqrt{2m(V_0 + E)}/\hbar$$

(3) $x > a$ $\qquad \psi(x) = F\, e^{-kx}$

Boundary conditions:

1) $\psi(x)$ is continuous

2) $d\psi/dx$ is also continuous

2') actually, in semiconductors condition 2) is different:

$$\frac{1}{m_{eff}} \frac{d\psi}{dx} \text{ is continuous}$$

(this is not discussed in Griffiths' book)

Follows from continuity of probability current $\quad \frac{i\hbar}{2m}\left(\psi \frac{d\psi^*}{dx} - \psi^* \frac{d\psi}{dx}\right)$

We have 5 equations (4 boundary conditions and normalization) and 5 unknowns (B, C, D, F, and E). Possible to solve, but too many.

Simplification: trick of odd and even functions

$f(-x) = f(x)$ even

$f(-x) = -f(x)$ odd

Trick of odd and even functions for even potential, $V(-x) = V(x)$

In our case $V(x)$ is even

Theorem

If $V(-x) = V(x)$ and $\psi(x)$ is a solution of TISE with energy E, $\hat{H}\psi = E\psi$, then $\psi(-x)$ is also a solution with the same energy, $\hat{H}\psi(-x) = E\psi(-x)$.

(simple to prove, and also quite obvious)

Then $\psi(x) + \psi(-x)$ is also a solution, and $\psi(x) - \psi(-x)$ is also a solution

(because TISE is linear in ψ), (not necessarily normalized, but not a problem)

$\psi(x) + \psi(-x)$ is even $\qquad$ $\psi(x) - \psi(-x)$ is odd

(actually, if $\psi(x)$ is even or odd, then one of the combinations is zero)

Therefore, it is sufficient to find only even and odd solutions of TISE

Even solutions for finite square well

$$\psi(x) = \begin{cases} B\exp(kx), & x < -a \\ D\cos(lx), & |x| < a \quad \text{(no sin-term)} \\ B\exp(-kx), & x > a \quad \text{(the same factor } B\text{)} \end{cases}$$

only 3 unknowns: B, D, E

Boundary condition at $x = a$ (b.c. at $x = -a$ gives the same):

$$\begin{cases} B\exp(-ka) = D\cos(la) \\ -kB\exp(-ka) = -lD\sin(la) \end{cases}$$

Divide equations: $\boxed{k = l\tan(la)}$ This equation gives energy E since $k(E)$, $l(E)$

Rewrite:

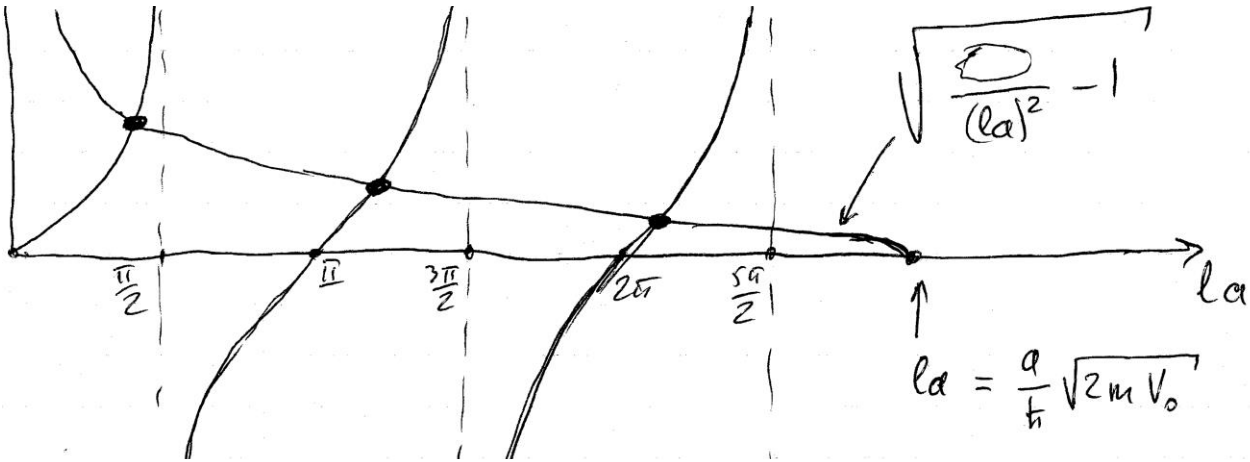
$$\tan(la) = \frac{k}{l} = \frac{\sqrt{-2mE}/\hbar}{\sqrt{2m(V_0+E)}/\hbar} = \sqrt{\frac{-E}{V_0+E}} = \sqrt{\frac{V_0}{V_0+E} - 1} = \sqrt{\frac{V_0 2m}{l^2\hbar^2} - 1}$$

$$\tan(la) = \sqrt{\frac{\frac{a^2 V_0 2m}{\hbar^2}}{(la)^2} - 1}$$

Even solutions for finite square well

$$\tan(la) = \sqrt{\frac{\frac{a^2 V_0 2m}{\hbar^2}}{(la)^2} - 1}$$

Solve graphically



$$l = \frac{\sqrt{2m(V_0 + E)}}{\hbar}$$

Finite number of solutions: $$N_{\text{even}} = \text{int}\left(\frac{\frac{a}{\hbar}\sqrt{2mV_0}}{\pi}\right) + 1$$

Limiting cases 1) $\frac{a^2 V_0 2m}{\hbar^2} \gg 1$ (wide, deep well)

Low levels: $la \approx (2n+1)\,\pi/2,$ $E_n + V_0 = \frac{l^2\hbar^2}{2m} \approx \frac{(2n+1)^2\pi^2\hbar^2}{2m(2a)^2}$

(similar to infinite well, but only odd states and $a \to 2a$)

2) $\frac{a^2 V_0 2m}{\hbar^2} \ll 1$ (shallow, narrow well) Only one level: $la \approx a\sqrt{2mV_0}/\hbar \ll 1,$ $|E| \ll V_0$

Even solutions for finite square well: normalization

(not important)

$$\psi(x) = \begin{cases} B\exp(kx)\,, & x < -a \\ D\cos(lx), & |x| < a \\ B\exp(-kx)\,, & x > a \end{cases}$$

Normalization

$$\int_{-\infty}^{\infty} |\psi(x)|^2\, dx = 1 \quad \Longrightarrow \quad \begin{cases} B = \dfrac{\exp(ka)\cos(la)}{\sqrt{a + 1/k}} \\ D = \dfrac{1}{\sqrt{a + 1/k}} \end{cases}$$

Odd solutions (similar)

$$\psi(x) = \begin{cases} B\exp(kx), & x < -a \\ C\sin(lx), & |x| < a \quad \text{(no cos-term)} \\ -B\exp(-kx), & x > a \quad (-B \text{ since odd}) \end{cases}$$

Boundary condition at $x = a$:

$$\begin{cases} -B\exp(-ka) = C\sin(la) \\ kB\exp(-ka) = Cl\cos(la) \end{cases}$$

Divide equations: $\boxed{k = -l\cot(la)}$

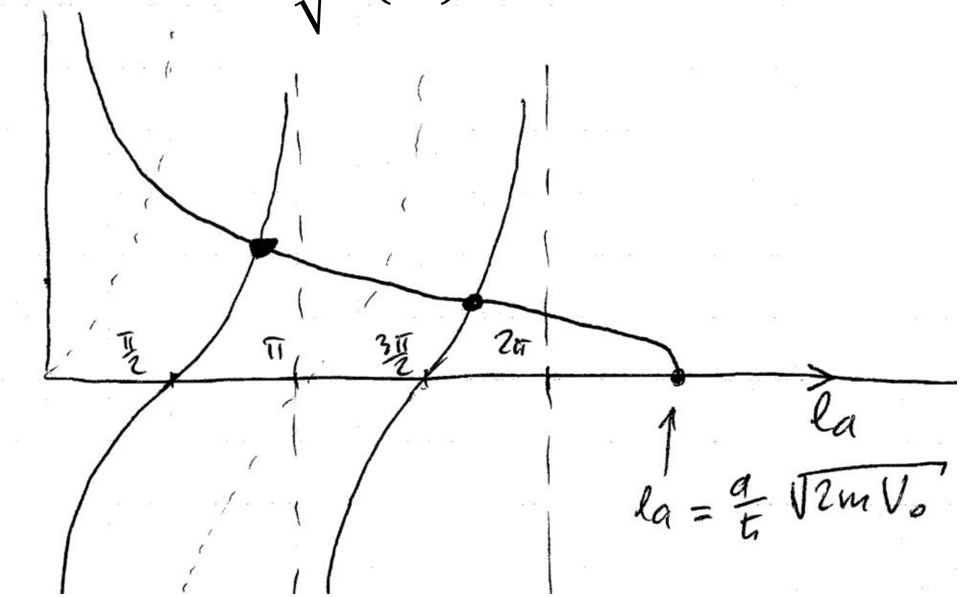
After some algebra: $$-\cot(la) = \sqrt{\frac{\frac{a^2V_0 2m}{\hbar^2}}{(la)^2} - 1}$$

Similar to the even case, the only difference: $\tan(la) \rightarrow -\cot(la)$

(just shifted by $\pi/2$)

Odd solutions for finite square well

$$-\cot(la) = \sqrt{\frac{\frac{a^2 V_0 2m}{\hbar^2}}{(la)^2} - 1}$$



Number of solutions:

$$N_{\text{odd}} = \text{int}\left(\frac{\frac{a}{\hbar}\sqrt{2mV_0}}{\pi} + \frac{1}{2}\right)$$

Total number of solutions:

$$N_{\text{even}} + N_{\text{odd}} = \text{int}\left(\frac{\frac{a}{\hbar}\sqrt{2mV_0}}{\pi/2}\right) + 1$$

Limiting cases 1) $\frac{a^2 V_0 2m}{\hbar^2} \gg 1$ (wide, deep well)

Low levels: $la \approx n\pi,\quad E_n + V_0 = \frac{l^2\hbar^2}{2m} \approx \frac{(2n)^2\pi^2\hbar^2}{2m(2a)^2}$

(these are remaining solutions for infinite well with $a \to 2a$)

2) Shallow, narrow well No odd solutions if $V_0 < \frac{\pi^2\hbar^2}{8ma^2}$

Digression: some integrals

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

(easy to derive by squaring and considering as a double-integral; also from normalization of a Gaussian: $\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi D}} e^{-x^2/2D} dx = 1.$

Take derivative in respect to parameter a

$$\int_{-\infty}^{\infty} (-x^2)\, e^{-ax^2} dx = -\frac{\sqrt{\pi}}{2a^{3/2}} \quad \Rightarrow \quad \boxed{\int_{-\infty}^{\infty} x^2\, e^{-ax^2} dx = \frac{\sqrt{\pi}}{2a^{3/2}}}$$

Take another derivative with respect to a, similarly:

$$\int_{-\infty}^{\infty} x^4\, e^{-ax^2} dx = \frac{3\sqrt{\pi}}{4a^{5/2}}$$

(and so on: x^6, x^8, etc.)

Can construct a similar series, starting with

$$\int_{0}^{\infty} x\, e^{-ax^2} dx = \frac{1}{2a}$$