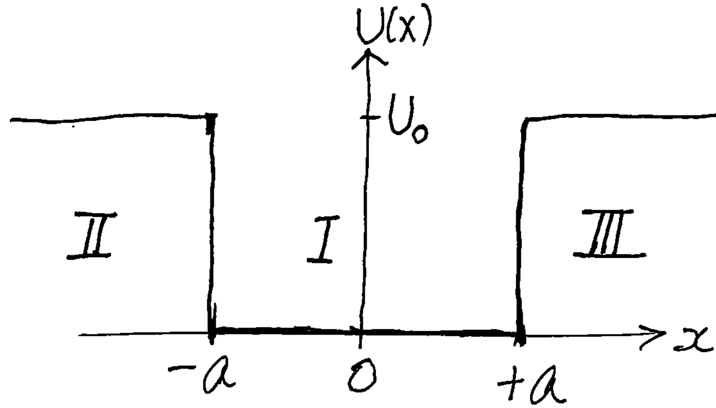
VI. 1D Finite Square Well and Harmonic Oscillator

A. 1D Finite Square Well

$$U(x) = \begin{cases} 0, & -a \le x \le a \\ U_0, & |x| > a \end{cases}$$

- Study bound energy eigenstate(s)

Can finite well support bound states?



Strategy for "piece-wise constant" U(x)

- Write down solutions in different regions (Step 1)
- Apply B.C.'s at boundaries (Step 2)
- Focus on bound states (with $E < U_0$)

Known:
- $U(x)$ symmetric about $x=0$
- $\psi(x)$ symmetric or antisymmetric
- $\frac{d\psi}{dx}$ and ψ continuous everywhere
- $E < U_0$ bound states and $\psi \to 0$ as $x \to \pm\infty$

Region III $(x>+a)$: TISE $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + U_0\psi = E\psi$

$$\frac{d^2\psi}{dx^2} - \underbrace{\frac{2m}{\hbar^2}(U_0-E)}_{>0}\psi = 0 \qquad (x>+a)$$

to be solved

Def: $K^2 = \frac{2m}{\hbar^2}(U_0-E)$

$$\frac{d^2\psi}{dx^2} - K^2\psi = 0$$

$$\therefore \quad \psi_{III}(x) = Fe^{-Kx} + Ge^{+Kx} \qquad (x>a)$$

Apply B.C.: $x\to+\infty$, $\psi(x)\to 0$ (this is physics), $G=0$

$$\psi_{III}(x) = Fe^{-Kx} \qquad (x>a) \quad (1) \quad (\because G=0)$$

Region II $(x<-a)$:
$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}(U_0 - E)\psi = 0 \quad (x<-a)$$

$$\Rightarrow \frac{d^2\psi}{dx^2} - K^2\psi = 0 \quad \text{(same as Region III)}$$

$$\therefore \psi_{II}(x) = De^{-Kx} + Ce^{Kx} \quad (x<-a)$$

Apply B.C.: $x \to -\infty$, $\psi(x) \to 0$ (bound state)

But De^{-Kx} term blows up as $x \to -\infty$, kill it by $D=0$.

$$\psi_{II}(x) = Ce^{Kx} \quad (x<-a) \quad (2)$$

<u>Region I</u> <u>$(-a < x < +a)$</u> : $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0$ ($\because U = 0$ in well)

$$\Rightarrow \frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{with } k^2 = \frac{2m}{\hbar^2}E$$ ← to solve for E

[cosine, sine, e^{ikx}, e^{-ikx} work]

$$\psi_I(x) = A\cos kx + B\sin kx \quad (-a < x < +a) \quad (3)$$

[this choice better reflects the expected symmetric/antisymmetric property]

- (1), (2), (3) give ψ in different regions
- A, B, C, F are coefficients to be determined
- B.C.'s at $x = \pm a$: ψ and $\frac{d\psi}{dx}$ are continuous (4 B.C.'s)

End of Step 1

Apply B.C.'s at $\underline{x=+a}$ to connect ψ_I to ψ_{III} properly (Ex.)

ψ continuous $\qquad A\cos ka + B\sin ka = F e^{-\kappa a} \qquad (4)$

$\frac{d\psi}{dx}$ continuous $\qquad -Ak\sin ka + Bk\cos ka = -\kappa F e^{-\kappa a} \qquad (5)$

Apply B.C.'s at $\underline{x=-a}$ to connect ψ_I to ψ_{II} properly (Ex.)

ψ continuous $\qquad A\cos ka - B\sin ka = C e^{-\kappa a} \qquad (6)$

$\frac{d\psi}{dx}$ continuous $\qquad Ak\sin ka + Bk\cos ka = \kappa C e^{-\kappa a} \qquad (7)$

Eqs. (4)–(7) are 4 equations for A, B, C, F (and E hidden in k and κ)

All physics has been used! The rest is math (or computing).

[End of Step 2]

Approach 1: General and think more like a computer

Inspect Eqs. (4)-(7), they can be expressed as

$$\begin{pmatrix} \cos ka & \sin ka & 0 & -e^{-\kappa a} \\ -k\sin ka & k\cos ka & 0 & \kappa e^{-\kappa a} \\ \cos ka & -\sin ka & -e^{-\kappa a} & 0 \\ k\sin ka & k\cos ka & -\kappa e^{-\kappa a} & 0 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ F \end{pmatrix} = 0 \qquad (8)$$

this zero is important for the math argument to follow

Of course, we don't want the solution $\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ as $\psi = 0$ everywhere and particle disappears! This is the trivial solution.

- For non-trivial solutions, the <u>determinant</u> must vanish (why?)

$$\begin{vmatrix} \cos ka & \sin ka & 0 & e^{-\kappa a} \\ -k\sin ka & k\cos ka & 0 & \kappa e^{-\kappa a} \\ \cos ka & -\sin ka & -e^{-\kappa a} & 0 \\ k\sin ka & k\cos ka & -\kappa e^{-\kappa a} & 0 \end{vmatrix} = 0 \quad (9)$$

<u>Recall:</u>

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

$$\kappa^2 = \frac{2m}{\hbar^2}(U_0 - E)$$

[Problem: m, a, U_0]

[For a (guess on) E, κ & k can be evaluated $\Rightarrow$ $|\vdots\vdots\vdots|$ elements are known]

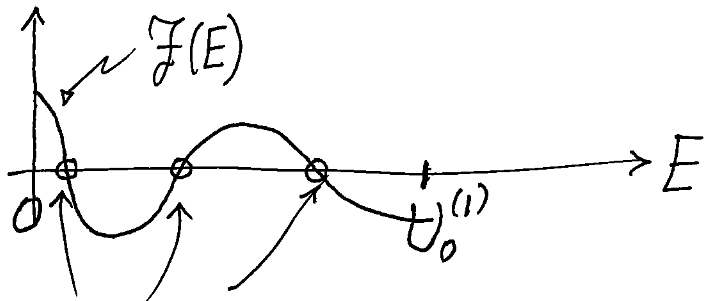
- Determinant is a number

$$\text{LHS} = \mathcal{F}(E) = \text{a number once a value of } E \text{ is input}$$
$$= \text{a function of } E$$

$\therefore$ Eq.(9) is $\underbrace{\mathcal{F}(E)}_{\text{or } \mathcal{F}(E;\, a,\, U_0)} = 0 \Rightarrow$ only some values of E with $E < U_0$ are allowed!

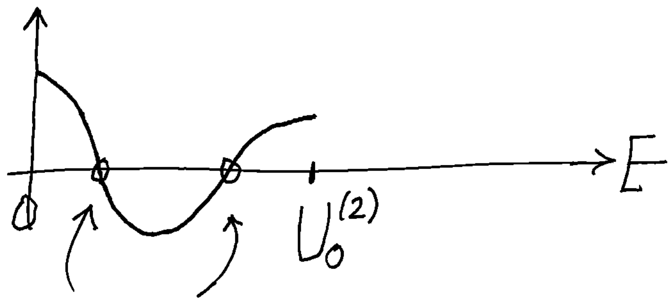
- Schematically, given m, a, $U_0^{(1)}$

  Expect to see only
  a finite number of bound states



These are the allowed energies for bound states

- Given m, a, $U_0^{(2)}$ ($< U_0^{(1)}$)



- How about narrower width?

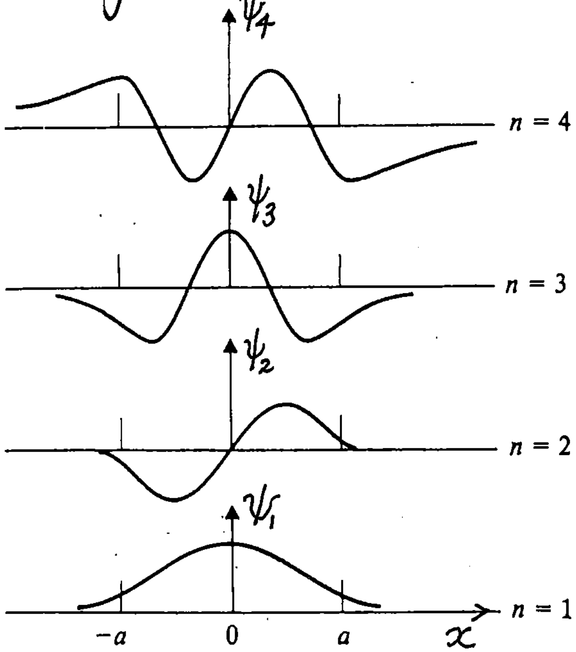
Allowed # bound states may vary with well depth

This turns the problem into a numerical problem of finding roots
[Go take computational physics course]

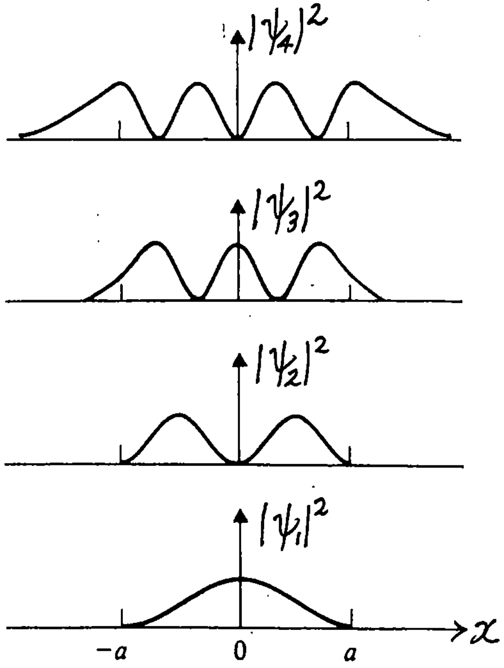
Key Features: Depending on U_0 and a

- Finite # bound states [sym., anti-sym., sym., anti-sym. ...]
- At least one symmetric bound state [Even U_0 is very shallow]

Energy Eigenfunctions of bound states

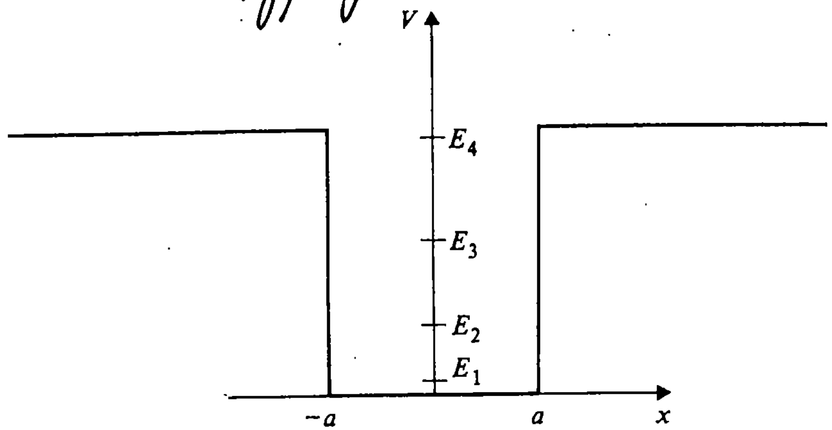


Probability Density

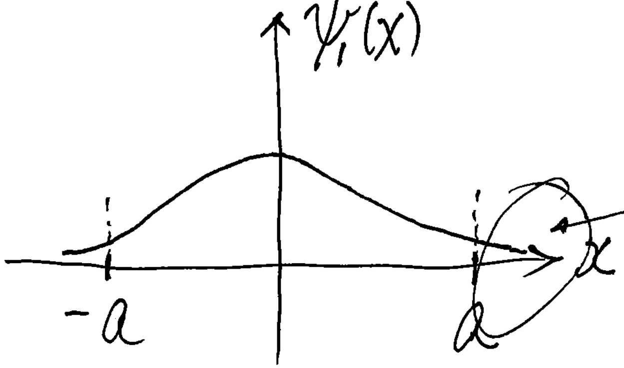


Example: $\boxed{\frac{2m}{\hbar^2} U_0 a^2 = 25}$

Energy of bound states



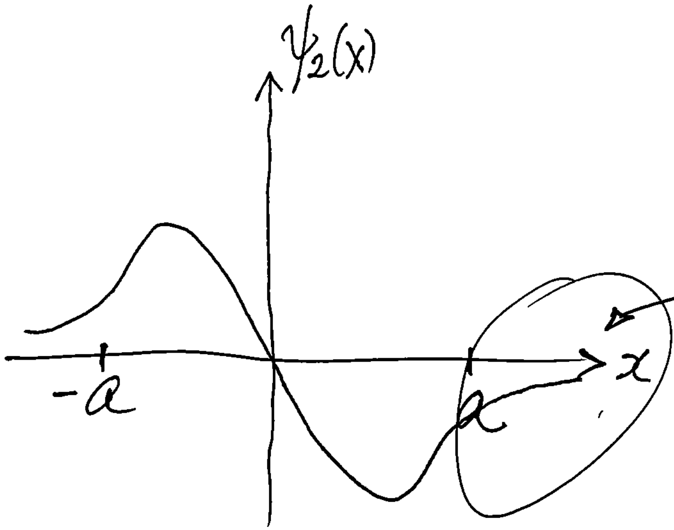
Finite number of bound states



$E_1 < U_0$

$\psi_1(x > +a) \neq 0 \quad \left(|\psi_1(x > |a|)|^2 \neq 0 \right)$

$\Rightarrow$ Possible to find particle in $|x| > a$ regions where $\underbrace{E_1 < U_0}_{\text{classically forbidden region}}$

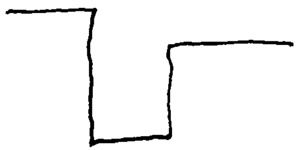
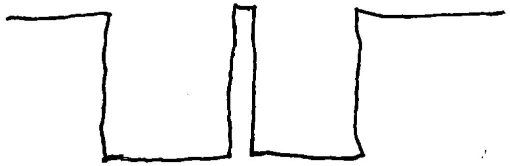
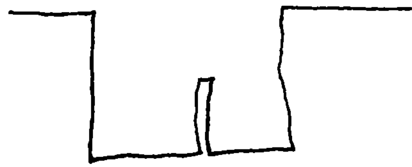


$\psi_2(x > |a|) \neq 0$ (if exist)

Tail is longer and bigger as eigenvalue increases

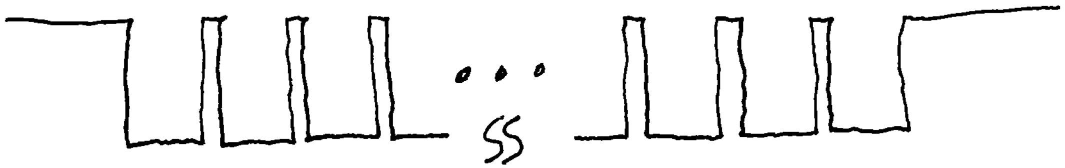
<u>Implication</u>: Tunneling if "tail" can be received before dropping too small

Extensions

- How about  ,   ?

  "molecules"

- How about

   ("1D solid") ?

- How about  ? Numerical solutions?

This page is repeated here for discussion on Approach 2 (see next page)

Set of Equations after Matching B.C.'s

Apply B.C.'s at $\underline{x = +a}$ to connect ψ_I to ψ_{III} properly (Ex.)

ψ continuous $$A\cos ka + B\sin ka = F e^{-\kappa a} \quad (4)$$

$\frac{d\psi}{dx}$ continuous $$-Ak\sin ka + Bk\cos ka = -\kappa F e^{-\kappa a} \quad (5)$$

Apply B.C.'s at $\underline{x = -a}$ to connect ψ_I to ψ_{II} properly (Ex.)

ψ continuous $$A\cos ka - B\sin ka = C e^{-\kappa a} \quad (6)$$

$\frac{d\psi}{dx}$ continuous $$Ak\sin ka + Bk\cos ka = \kappa C e^{-\kappa a} \quad (7)$$

Eqs. (4)–(7) are 4 equations for A, B, C, F (and E hidden in k and κ)

All physics has been used! The rest is math (or computing).

Approach 2: Stick to Paper and Pen (as far as possible)

Back to Eqs.(4)-(7).

Eq.(4) + Eq.(6): $\quad 2A\cos ka = (C+F)\,e^{-\kappa a} \qquad (4')$

Eq.(7) − Eq.(5): $\quad 2kA\sin ka = \kappa(C+F)\,e^{-\kappa a} \qquad (5')$

Eq.(4) − Eq.(6): $\quad 2B\sin ka = (F-C)\,e^{-\kappa a} \qquad (6')$

Eq.(5) + Eq.(7): $\quad 2kB\cos ka = -\kappa(F-C)\,e^{-\kappa a} \qquad (7')$

Note: We are isolating the "A" ($A\cos kx$ in ψ_I) and "B" ($B\sin kx$ in ψ) terms. "$A\cos kx$" is symmetric about $x=0$ and "$B\sin kx$" is antisymmetric about $x=0$.

$\dfrac{(5')}{(4')}$: $\quad k \tan ka = K \quad$ unless $\underbrace{A=0 \text{ and } C=-F}_{\text{then } (4') \,\&\, (5') \text{ are: } ``0" = ``0"}$ $\qquad (10)$

[Meaning: If $A=0$ & $C=-F$, nevermind about $k \tan ka = K$]

$\dfrac{(7')}{(6')}$: $\quad k \cot ka = -K \quad$ unless $B=0$ and $C=F$ $\qquad (11)$

[Meaning: If $B=0$ and $C=F$, nevermind about $k \cot ka = -K$]

- Conditions (10), (11) must be satisfied simultaneously (came from Eqs. (4)-(7)).

Two sets of solutions to TISE

Either
$$\begin{cases} k \tan ka = K \\ B = 0 \text{ and } C = F \end{cases} \quad (12)$$

OR

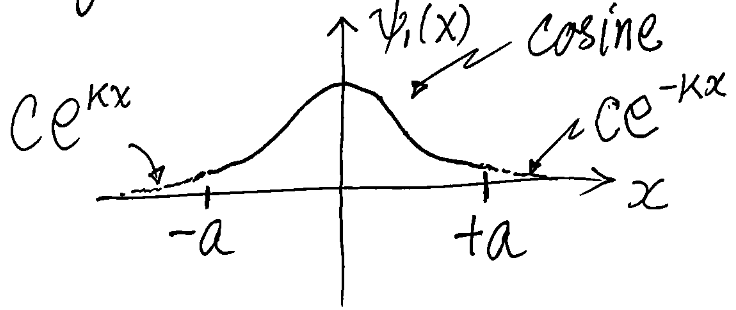
$$\begin{cases} k \cot ka = -K \\ A = 0 \text{ and } C = -F \end{cases} \quad (13)$$

Symmetric (Even) about $x=0$

$$\psi_I = A \cos kx$$

$$\psi_{II} = \underbrace{Ce^{Kx}}_{x<-a}, \quad \psi_{III} = \underbrace{Ce^{-Kx}}_{x>+a}$$

e.g. Ground state

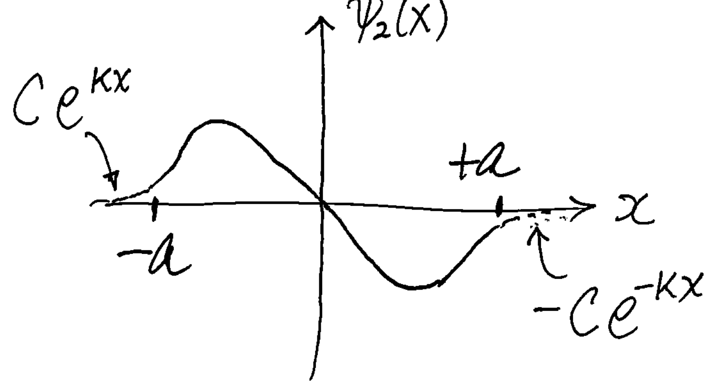


Antisymmetric (Odd) about $x=0$

$$\psi_I = B \sin kx$$

$$\psi_{II} = Ce^{Kx} \ (x<-a), \quad \psi_{III} = -Ce^{-Kx} \ (x>a)$$

e.g. 1st excited state



Solve $\underbrace{ka\tan(ka) = \kappa a}$ for symmetric solutions (12')

to solve for allowed energies E

Solve $\overbrace{ka\cot(ka) = -\kappa a}$ for antisymmetric solutions (13')

Can do the two searches separately

- Practically, still need a computer to solve for E that satisfies

$$ka\tan(ka) - \kappa a = 0 \quad \text{and} \quad ka\cot(ka) + \kappa a = 0$$

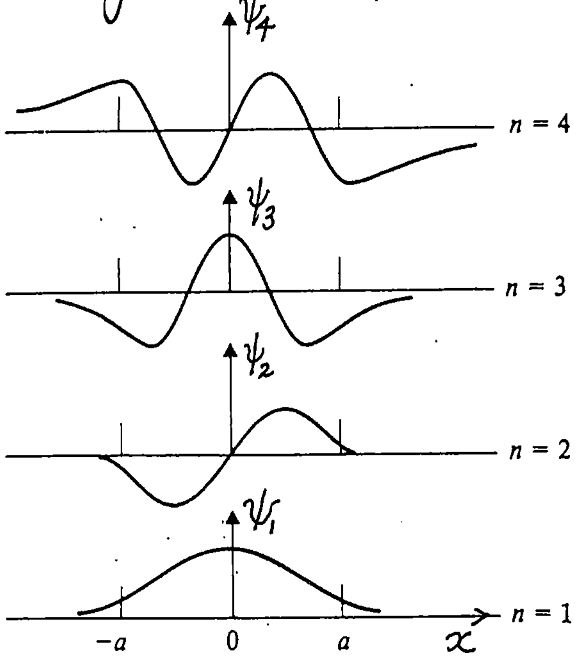
The fact is: 1D Finite Well Problem cannot be solved analytically

[∴ take computational physics courses!]

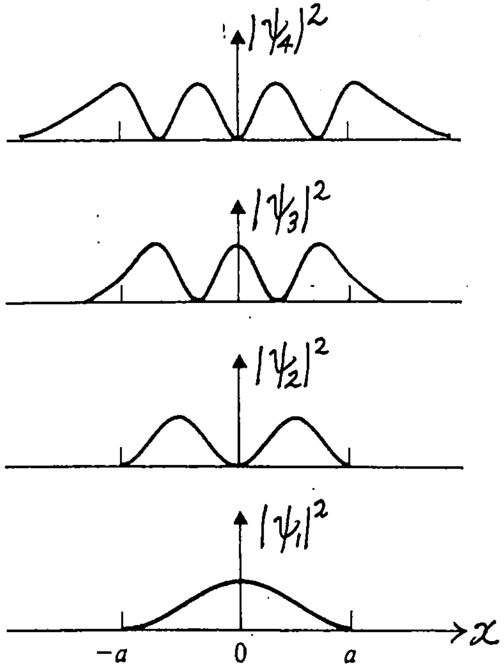
Key Features: Depending on U_0 and a

- Finite # bound states [sym., anti-sym., sym., anti-sym. . . .]
- At least one symmetric bound state [Even U_0 is very shallow]

Energy Eigenfunctions of bound states

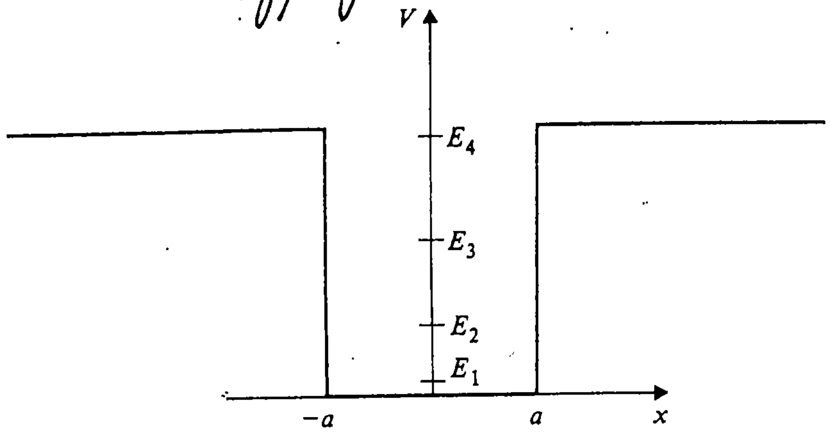


Probability Density



Example: $\frac{2m}{\hbar^2} U_0 a^2 = 25$

Energy of bound states

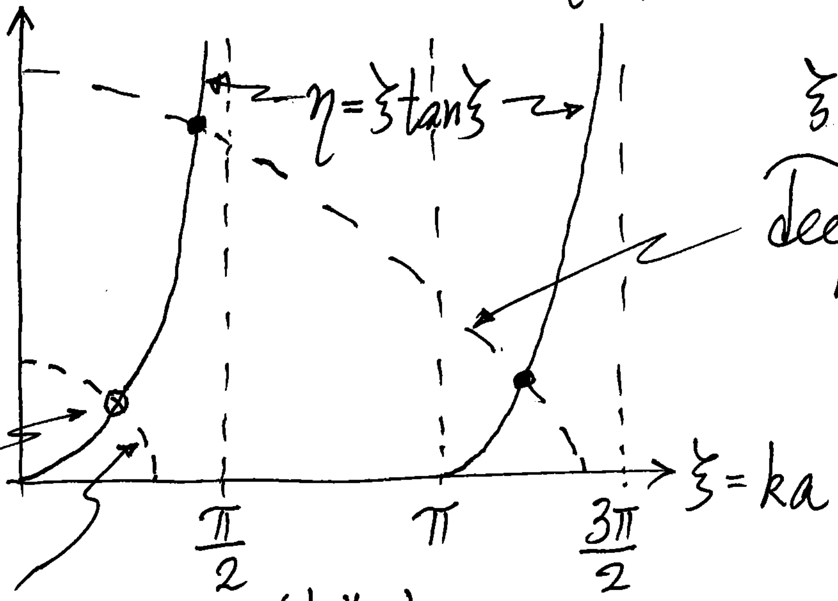


Finite number of bound states

Get a sense graphically $\quad \overbrace{(ka)}^{\xi}\tan\overbrace{(ka)}^{\xi} = \overbrace{\kappa a}^{\eta} \quad$ (Symmetric solutions)

$\therefore \quad \xi \tan \xi = \eta \quad , \quad \xi^2 + \eta^2 = (k^2 + \kappa^2)a^2 = \underbrace{\frac{2m}{\hbar^2} U_0 a^2}_{\text{constant for a problem}} = (\text{radius})^2$

- Draw 2 lines on $(\xi - \eta)$ plane



$\underbrace{\xi^2 + \eta^2}= \frac{2m}{\hbar^2} U_0^{(\text{deep})} \cdot a^2$

deeper well supports more bound states [2 symmetric ones] here

Intersection point
$\Downarrow$
ka
$\Downarrow$
E

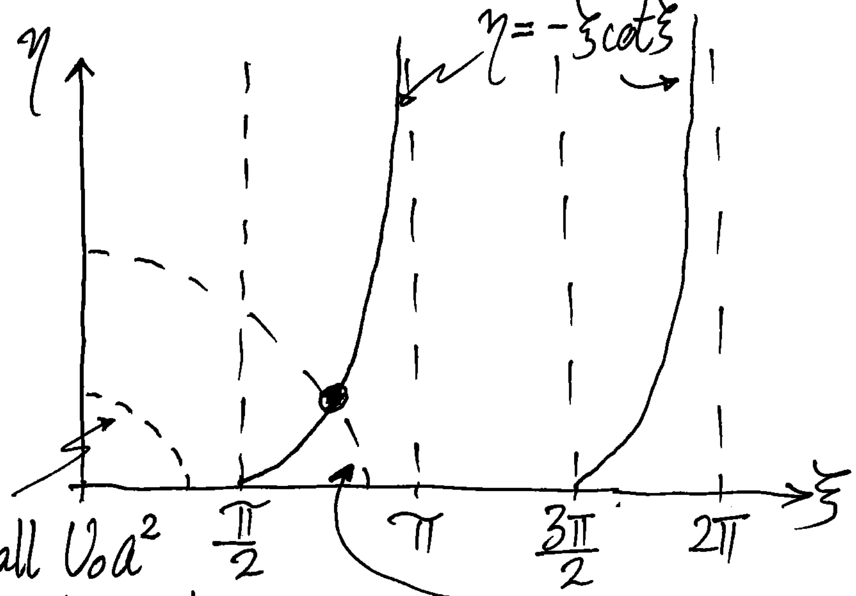
$\xi^2 + \eta^2 = \frac{2m}{\hbar^2} U_0^{(\text{shallow})} \cdot a^2$

<u>Note:</u> $(U_0 a^2)$ is the combination that matters!

<u>At least one symmetric</u> bound state no matter how shallow the well is.

Antisymmetric solutions $\quad ka \cot ka = -Ka$

$$\xi \cot \xi = -\eta \qquad \xi^2 + \eta^2 = \frac{2m}{\hbar^2} U_0 a^2$$



Small $U_0 a^2$

⇒ No intersection

⇒ No antisymmetric (odd) eigenstates

[only one symmetric state]

With picture on last page

⇒ sym, anti-sym, sym, anti-sym, ...

(even, odd, even, odd, ...)

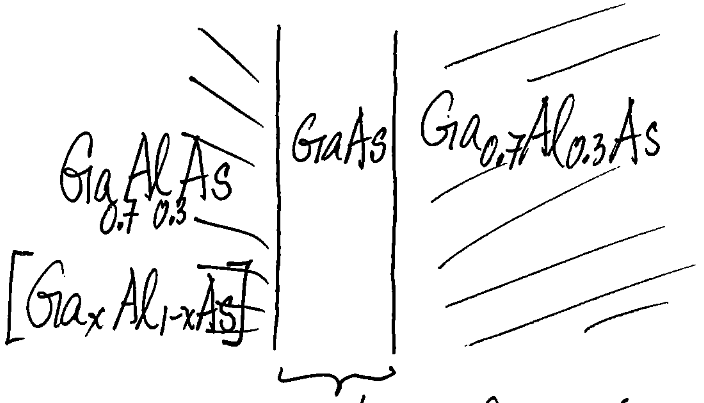
and

bound states governed by $(U_0 a^2)$

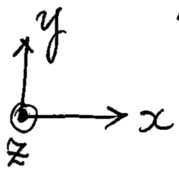
{Only sufficiently deep well could have anti-symmetric bound state(s)

Is 1D Finite Well Problem real?

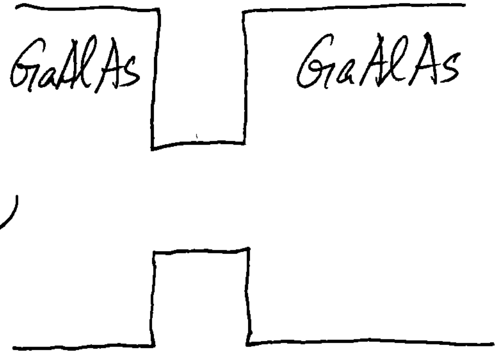
Yes! Semiconductor Sandwiches



W ~10 atomic layers (tens of Å)



Electrons see in x-direction

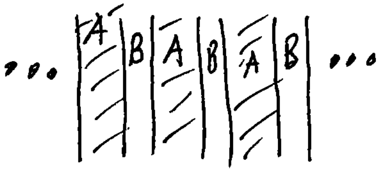


$U(x)$

Electrons free to move in y-z plane

MBE (Molecular beam epitaxy) can grow to atomic layer precision (分子束近延生長)

Quantum Well in Semiconductor heterostructures



superlattice (超晶格) [a man-made solid with tunable period]

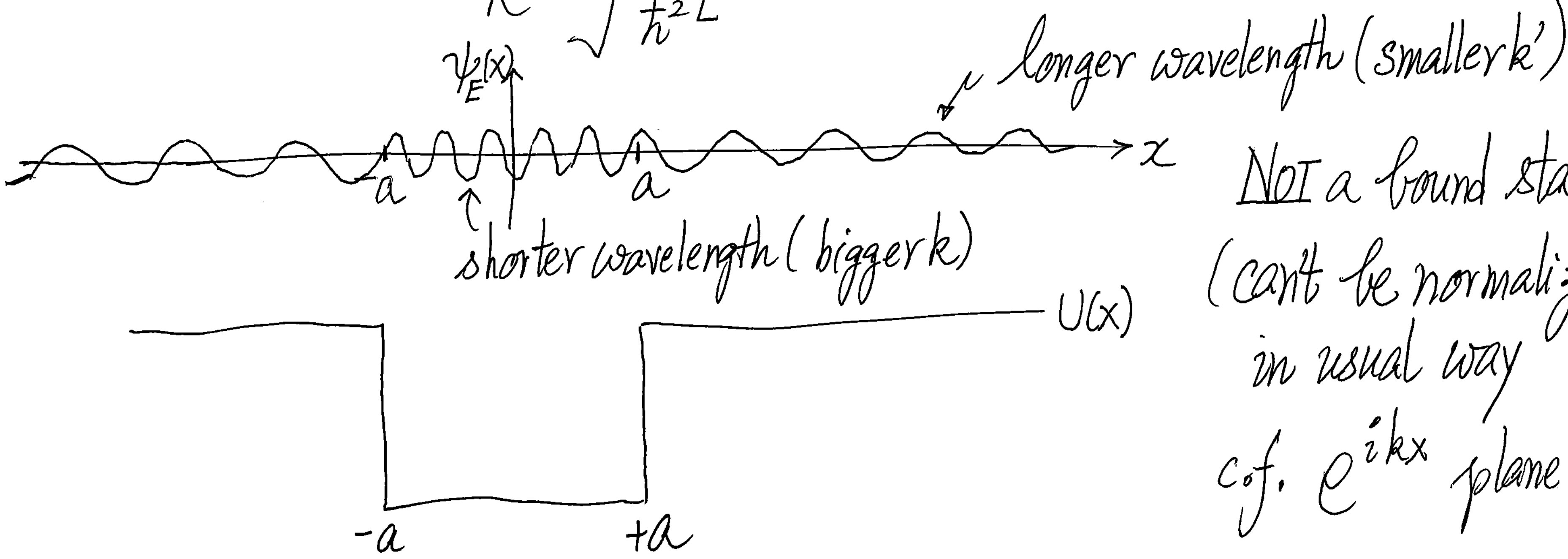
- How about <u>unbound states</u> ($E > U_0$)?

$$\frac{d^2\psi}{dx^2} + \underbrace{\frac{2m}{\hbar^2}(E - U(x))}_{>0 \text{ all } x}\psi = 0$$

There is solution for <u>any</u> $E > U_0$ ($\because$ no boundary)

$x < |a|$: $k' = \sqrt{\frac{2m}{\hbar^2}(E - U_0)} < k$

$-a < x < a$: $k = \sqrt{\frac{2m}{\hbar^2}E}$



<u>NOT</u> a bound state (can't be normalized in usual way)

c.f. e^{ikx} plane wave

Summary

- Finite Well Problems need numerical solutions
- Support a finite number of bound states determined by $\frac{2m}{\hbar^2} U_0 a^2$
- Has at least one bound state (symmetric) no matter how shallow (narrow) the well is
- $|\psi|^2$ has non-zero tail into classical forbidden region
- Developed into an area of semiconductor heterostructures[†]

† J. Singh, "Physics of Semiconductors and their heterostructures"

† D. Ferry, "Quantum Mechanics: An introduction for device physicists and electrical engineers"