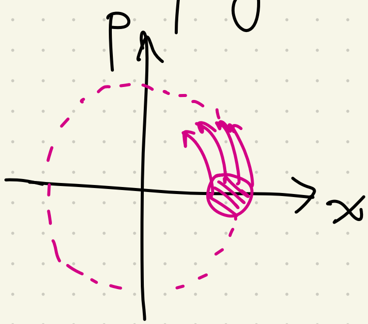
Remarks

① Thermal de Broglie wavelength $\dfrac{h}{\sqrt{2\pi m k_B T}}$ (A_I in C-T)

② Current associated to the probability density $|\psi(x,t)|^2$

③ A wave function of a free particle always spread because of the quadratic dependence of ω on k.

SHO is special because ω only depends on the mass and the spring constant. So different parts of the coherent state stay together.



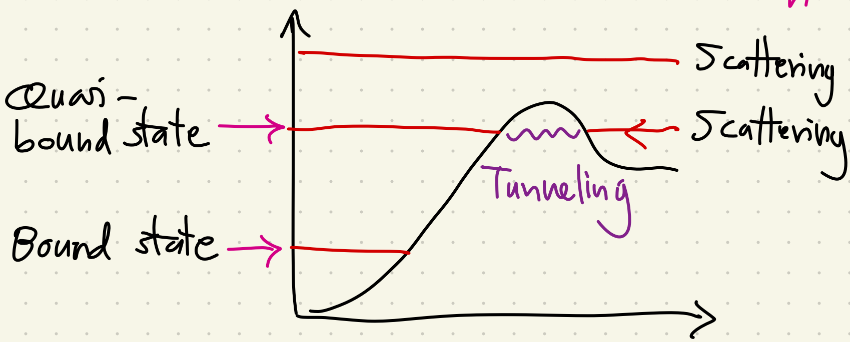
Stationary states $\varphi_n(x)$ but I drop the subscript n for convenience

TISE

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

$$\left[\frac{d^2}{dx^2} + \underbrace{\frac{2m(E-V(x))}{\hbar^2}}\right]\varphi(x) = 0 \qquad \varphi'' + k^2\varphi = 0$$

Local momentum $\quad \frac{p^2(x)}{\hbar^2} = k^2(x) = \frac{\sqrt{2m(E-V)}}{\hbar}$



(Resonance with a quasi-bound state gives stronger scattering)

Regularity conditions (Sturm-Liouville theory)

* $\varphi(x)$ is continuous and bound
* $\varphi'(x)$ is bound (continuous if $V(x)$ is regular. Not true for $V(x) = \alpha\,\delta(x)$)

Bound states are discrete. There are uncountably ∞ scattering states.

* No bound state degeneracy in 1D. The energy completely determines the trajectory. Not true in 3D. Need the energy, the angular momentum, and the projection of the angular momentum along an axis to specify a Kepler orbit. ← n, l, m for Hydrogen atom

■ $$\varphi_1'' + k^2 \varphi_1 = 0 \quad \text{①}$$

$$\varphi_2'' + k^2 \varphi_2 = 0 \quad \text{②}$$

$$\varphi_2 \text{①} - \varphi_1 \text{②} = \varphi_2 \varphi_1'' - \varphi_1 \varphi_2'' = 0$$

$$\frac{d}{dx}\underbrace{(\varphi_2 \varphi_1' - \varphi_1 \varphi_2')}_{\text{Wronskian } W(x) = \begin{vmatrix} \varphi_2 & \varphi_1 \\ \varphi_2' & \varphi_1' \end{vmatrix} = C} = 0$$

a priori C could be any constant, but since $\varphi(x) \to 0$ as $x \to \infty$, $C = 0 \Rightarrow$ Linear dependence. □

Bound state

$$\frac{\varphi_1'}{\varphi_1} = \frac{\varphi_2'}{\varphi_2}$$

$$\ln \varphi_1 = \ln \varphi_2 + c \Rightarrow \varphi_1 \propto \varphi_2$$

* # of nodes – Ground state has no node.

* $\varphi(x)$ can be chosen to be real   Time-reversal symmetry

- Since E and V are real, $\varphi'' + k^2\varphi = 0$ is satisfied by both φ and φ^*. Take the real and imaginary parts of φ to be the real solutions. $\square$

Either:

$\varphi^*(x) \propto \varphi(x)$ or: $\left.\begin{matrix} \varphi + \varphi^* \\ -i(\varphi - \varphi^*) \end{matrix}\right\}$ Degenerate real solutions

* Reflection symmetry If $V(x) = V(-x)$, then φ can be chosen to be even or odd.
  - (Should be proven using the operator formalism)

Parity operator

$\hat{\Pi}\hat{x}\hat{\Pi} = -\hat{x}$ $\hat{\Pi}^\dagger = \hat{\Pi}$ $\hat{\Pi}\,|x\rangle = |-x\rangle$, $\langle x|\hat{\Pi} = \langle x|\hat{\Pi}^\dagger = \langle -x|$

$\hat{\Pi}\hat{p}\hat{\Pi} = -\hat{p}$ $\hat{\Pi}^2 = \hat{\mathbb{1}} \Rightarrow$ Eigenvalue ± 1, Eigenfunctions $\begin{cases} \text{Even} \\ \text{Odd} \end{cases}$

$$\hat{\Pi}\psi(x) = \langle x|\hat{\Pi}|\psi\rangle = \psi(-x)$$

$V(x) = V(-x) \Longleftrightarrow [\hat{H}, \hat{\Pi}] = 0 \rightarrow$ Choose common eigenstates (Degenerate) $\square$

Bound state $\rightarrow$ $\hat{\Pi}|\varphi_n\rangle = \pm|\varphi_n\rangle$

$\varphi_n(-x) = \pm\varphi_n(x)$ either even or odd.

Either:

$\varphi(x) \propto \varphi(-x)$ or: $\left.\begin{matrix} \varphi(x) + \varphi(-x) \\ \varphi(x) - \varphi(-x) \end{matrix}\right\}$ Degenerate even and odd solutions

General strategies to solve TISE

* Piecewise-constant potential (Matching boundary conditions)
* WKB

$$k = \frac{\sqrt{2m(E-V)}}{\hbar}$$

First approach

$E > V \Rightarrow k$ real

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

or

$$= A\cos(kx) + B\sin(kx)$$

$E < V \Rightarrow k$ imaginary

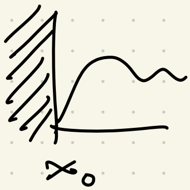
"Rho" $\rightarrow \rho = ik$

$$\varphi(x) = Ae^{\rho x} + Be^{-\rho x}$$

or

$$= A\cosh(\rho x) + B\cosh(\rho x)$$

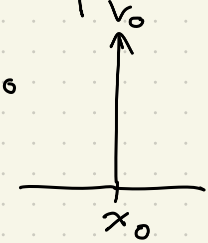
Infinite step (hard wall)



$\varphi(x) = 0,\ x \leq x_0$

φ' not continuous

δ potential (not hard wall)



φ continuous at

φ' jumps

Integrate the SE

$$\underbrace{\int_{x-\epsilon_0}^{x+\epsilon_0} dx\, \varphi''} + \int dx\, k^2 \varphi = 0$$

$$\varphi'(x_0+\epsilon) - \varphi'(x_0-\epsilon) = -\frac{2m\alpha}{\hbar^2}\int_{x-\epsilon_0}^{x+\epsilon_0} dx\, \delta(x-x_0)\,\varphi(x)$$

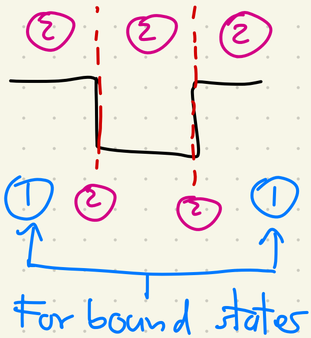
$$= -\frac{2m\alpha}{\hbar^2}\varphi(x_0)$$

* 2 constants for each piecewise potential.
* Each boundary condition eliminates 2 constants
* Normalization eliminates 1 more constant.

$E > V$ $\#$ B.C. > $\#$ Const. ⇒ Underdetermined (∞ $\#$ of solutions)

$E < V$ 2 more B.C. at $\pm\infty$ ⇒ Only certain values of E are allowed.

Cont.

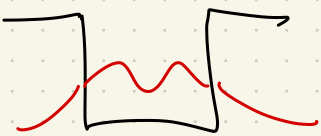


B.C.

$\#$ B.C. = $\#$ equations

$\#$ constants = $\#$ unknowns

→ See MIT 8.05 notes

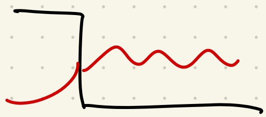


4 const. - 1 normalization = 3

4 B.C.

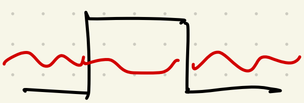
What's missing? Make E an unknown

⇒ Only certain values of E are allowed



$3 - 1 = 2$ const. = 2 B.C.

There exists a sol. for every value of energy

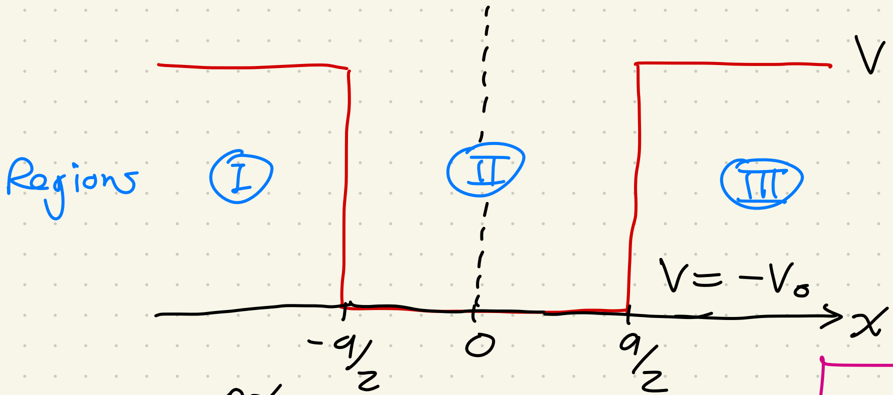


$6 - 1 = 5$ const. > 4 B.C.

Underdetermined. ⇒ Physical B.C.

(Wave coming from the left or right)

Ex Bound states in a finite well



Real

$\rho = ik$

$$\varphi_{I} = A e^{\rho x}$$

$$\rho = \frac{\sqrt{-2mE}}{\hbar} \quad (E<0)$$

$$\varphi_{II} = A' \cos(kx) + B' \sin(kx)$$

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

$$\varphi_{III} = B e^{-\rho x}$$

Match φ and φ' at the I–II interface. ($V(x)$ is symmetric so the II–III interface is the same.)

$$A e^{-\rho a/2} = A' \cos\left(\frac{ka}{2}\right) - B' \sin\left(\frac{ka}{2}\right)$$

$$\rho A e^{-\rho a/2} = +kA' \sin\left(\frac{ka}{2}\right) + kB' \cos\left(\frac{ka}{2}\right)$$

Symmetric $V(x)$ $\Rightarrow$ Can work on even and odd solutions one at a time.

Even:

$$A e^{-\rho/2} = A' \cos\left(\frac{ka}{2}\right)$$

$$\rho A e^{-\rho/2} = kA' \sin\left(\frac{ka}{2}\right)$$

Odd:

$$A e^{-\rho/2} = -B' \sin\left(\frac{ka}{2}\right)$$

$$\rho A e^{-\rho a/2} = -kB' \cos\left(\frac{ka}{2}\right)$$

Even

$$k A e^{-\rho/2} = k A' \cos\left(\frac{ka}{2}\right) \quad (1)$$

$$\rho A e^{-\rho/2} = k A' \sin\left(\frac{ka}{2}\right) \quad (2)$$

$$\frac{k}{k_0} = \sqrt{1 + \frac{E}{V_0}}$$

$(1)^2 + (2)^2$: $\underbrace{(k^2+\rho^2)} A^2 e^{-\rho/a} = k^2 A'^2$

+ Normalization = Both A and A'

$$k_0^2 \equiv \frac{2mV_0}{\hbar^2}$$

$$\boxed{\left(\frac{A}{A'}\right)^2 = \left(\frac{k}{k_0}\right)^2 e^{\rho/a}} \quad (3)$$

$(2)^2/(1)^2$:

$$\rho^2 = k^2 \tan^2\left(\frac{ka}{2}\right) = \frac{k^2}{\cos^2\left(\frac{ka}{2}\right)} - k^2$$

$$\cos^2\left(\frac{ka}{2}\right) = \left(\frac{k}{k_0}\right)^2$$

$$\boxed{\left|\cos\left(\frac{ka}{2}\right)\right| = \frac{k}{k_0}}$$

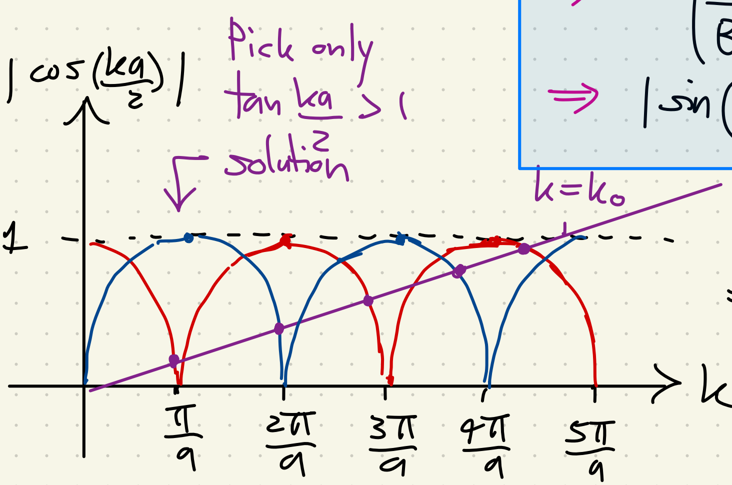
Odd

$$k B e^{\rho/2} = -k B' \sin\left(\frac{ka}{2}\right)$$

$$\rho B e^{\rho/2} = k B' \cos\left(\frac{ka}{2}\right)$$

$$\Rightarrow \left(\frac{B}{B'}\right)^2 = \left(\frac{k}{k_0}\right)^2 e^{-\rho/a}$$

$$\Rightarrow \left|\sin\left(\frac{ka}{2}\right)\right| = \frac{k}{k_0}$$



Red = Even   Blue = Odd

Bound states

$$= \left\lfloor \frac{k_0 a}{\pi} \right\rfloor + 1 = \left\lceil \frac{k_0 a}{\pi} \right\rceil$$

There alway exists at least one bound state.

Interesting limits

① Deep well

$V_0 \to \infty$ keeping a constant.

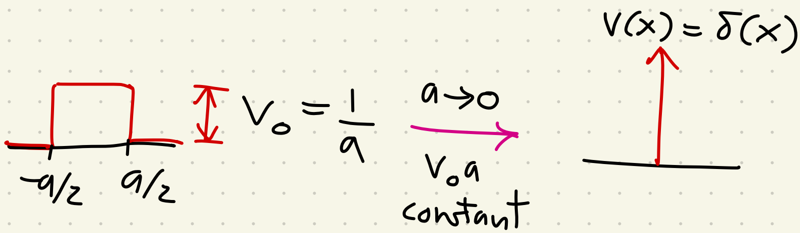
$$\frac{k_0 a}{2} \to \frac{\sqrt{2mV_0}}{2}\,a \to \infty \Rightarrow \infty \text{ \# of bound states}$$

$$k \approx \frac{n\pi}{a} \Rightarrow E + V_0 \approx \frac{n^2\pi^2\hbar^2}{2ma^2} \quad \left(\text{Infinite square well}\right)$$

② Deep, narrow well

$V_0 \to \infty$ keeping $V_0 a$ constant $\to$ (Delta potential)

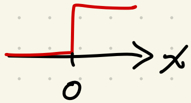
$$\frac{k_0 a}{2} = \frac{\sqrt{2mV_0}}{2}\,a = \sqrt{\frac{\overbrace{mV_0 a}^{\text{Constant}}}{2}}\,\sqrt{a} \to 0 \Rightarrow 1 \text{ bound state}$$



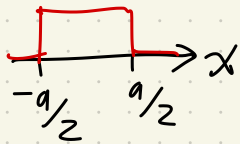
$\boxed{\text{See next page for derivation}}$ ⇒

Heaviside step function

$$H(x) = \begin{cases} 1, & x \geq 0 \\ 0, & \text{otherwise} \end{cases}$$



$$H\left(\frac{a}{2} - |x|\right) = \begin{cases} 1, & |x| \leq a/2 \\ 0, & \text{otherwise} \end{cases}$$



Representation of a delta function by the step function

$$\delta(x) = \lim_{a \to 0} \frac{1}{a} H\left(\frac{a}{2} - |x|\right)$$

$$\frac{1}{a}\int dx\, H\left(\frac{a}{2} - |x|\right) f(x) = \frac{1}{a}\int_{-a/2}^{a/2} dx\, f(x)$$

Antiderivative of f

$$= \frac{F\left(\frac{a}{2}\right) - F\left(-\frac{a}{2}\right)}{a} = \frac{1}{2}\left[\frac{F\left(0+\frac{a}{2}\right) - F(0)}{a/2} + \frac{F\left(0-\frac{a}{2}\right) - F(0)}{-a/2}\right]$$

Now take the limit $\longrightarrow \frac{1}{2}\left(F'(0) + F'(0)\right) = F'(0) = f(0)$