Simple 1-D examples

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QM I _ Fall 2019

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General notes

Free particle

Potential Step

Potential Barrier & Well

Harmonic Oscillator

General Notes

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle$$

- $H|\varphi\rangle = \lambda|\varphi\rangle \Rightarrow i\hbar\frac{d}{dt}|\phi(t)\rangle = H|\phi\rangle = \lambda|\phi\rangle$

$$\Rightarrow |\phi(t)\rangle = e^{-i\lambda t/\hbar}|\phi\rangle$$

$\Rightarrow$ Given an eigenstate of H, the state would only pick up a phase.

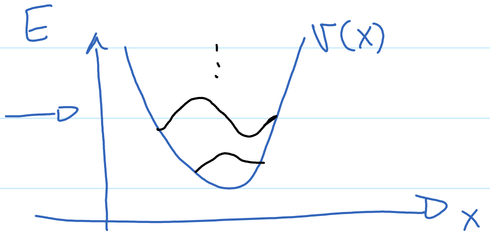
- $\{|\phi_n\rangle\} \to$ Eigenbasis of H:

$$|\psi\rangle = \sum_n c_n|\phi_n\rangle \longrightarrow |\psi(t)\rangle = \sum c_n e^{i\lambda_n t/\hbar}|\phi_n\rangle$$

$\Rightarrow$ So, one way to deal with a time-indep. Hamiltonian is to find the eigenbasis of H.

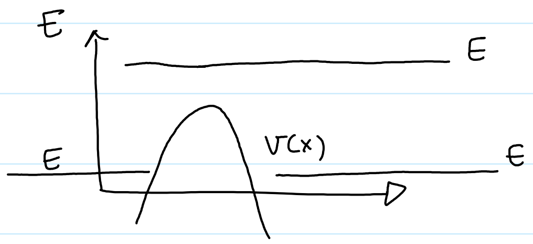
Bound State $\to$ $\lim_{x \to \pm\infty} |\psi(x)|^2 = 0$

ψ is a bound state.



Unbounded State

$\to$ Not confined



① Spectrums of bounded states are discrete.

② " , un " " " continous.

③ " " Bounded " in 1-D is non-degenerate

Ⓐ Prove that in 1-D, Bounded states are non-degenrate.

Note: Minimum energy:

(A) Prove that eigenenergies cannot be less than the minimum of the potential.

Boundary Conditions (BC)

We often need BC to specify the wavefunction $\psi(x)$.

For finite $V(x)$, $\psi(x)$ is continous as well as all of its derivatives.

(A) Prove that " .

We will deal with situations where $V(x)$ is not finite and the statement above does not hold

Symmetry

If $[S, H] = 0$ for some unitary S, then H has the corresponding symmetry.

This implies.

$$H S|\phi_n\rangle = SH|\phi_n\rangle = E_n S|\phi_n\rangle$$

* $\rightarrow S|\phi_n\rangle$ is an eigenstate with E_n.

* We can find $|\phi_n\rangle$ such that they are eige-states of S too.

Parity

Assume that $V(x) = V(-x) \rightarrow$ potential is an even function.

Then $[H, \Pi] = 0 \rightarrow H$ is even

$$H\,\Pi|\phi_n\rangle = \Pi\, H|\phi_n\rangle = E_n \Pi|\phi_n\rangle$$

$\Rightarrow \Pi|\phi_n\rangle$ is also an eigenstate with E_n.

- Non-degenerate H

$$\Pi|\phi_n\rangle = e^{i\alpha}|\phi_n\rangle \Rightarrow e^{i\alpha} = \pm 1 \rightarrow$$ Eigenvalues of parity are ± 1.

- Degenerate H: $H|\phi_{n,1}\rangle = E_n|\phi_{n,1}\rangle$
$H|\phi_{n,2}\rangle = E_n|\phi_{n,2}\rangle$

Then, $\Pi|\phi_{n,1}\rangle = \alpha|\phi_{n,1}\rangle + \beta|\phi_{n,2}\rangle \rightarrow$ check this!
$\Pi|\phi_{n,2}\rangle = -\beta|\phi_{n,1}\rangle + \alpha|\phi_{n,2}\rangle$

We can find new eigenstates of energy that are eigenstates of Π too.

(A) Find the states that are eigenstates of both H & Π, when H has degeneracy.

Free particle

$$H = \frac{P^2}{2m} \longrightarrow |\phi_p\rangle = |p\rangle$$

$$i\hbar \frac{d}{dt}|p\rangle = H|p\rangle = \frac{p^2}{2m}|p\rangle \Rightarrow |p(t)\rangle = e^{-i\frac{p^2}{2m}\frac{t}{\hbar}}|p\rangle$$

Note that $e^{-i\,p^2t/\hbar m}$ is a global phase and $|p(t)\rangle = |p\rangle$.

Alternatively, we could solve the Sch. eq. and reach plane waves

$$\psi(x,t) = A\, e^{i\left(x.p - \frac{p^2}{2m}t\right)/\hbar} = A\, e^{i\left(kx - \frac{k^2 t}{2m}\right)}$$

As we discussed before, this is not physical.

$$P(x,t) = |A|^2 dx \rightarrow \text{indep of } x.$$

(A) What is the dispersion relation corresponding the Sch. eq for a free particle.

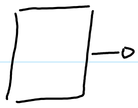
The more physical solutions are the wave packets

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \phi(k)\, e^{i(kx-\omega t)}\, dk$$

→ Add Demo

We can calculate the flux of probability:

$$J = \frac{i\hbar}{2m}\left(\psi(x)\frac{d\psi^*}{dx} - \psi^*(x)\frac{d\psi(x)}{dx}\right) = \frac{\hbar k}{m}|A|^2$$

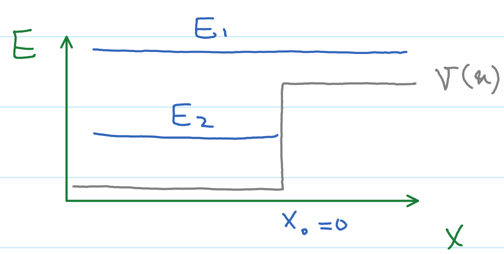


→ Flow of the probability

It seems that there's always particles coming

Step Potential

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



① $E \geq V_0$

$x < 0$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_L(x) = E\,\psi_L(x)$$

$$\frac{\partial^2}{\partial x^2}\psi_L(x) = -k^2 E\,\psi_L(x) \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi_L(x,t) = Ae^{+i(kx-\omega t)} + Be^{-i(kx+\omega t)}$$

$x \geq 0$

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

$$\psi_R(x,t) = Ce^{+i(kx-\omega t)} + De^{-i(kx+\omega t)}$$

BC

No wave is coming from right $(+\infty)$ so

* $D = 0$

* $\psi_L(0) = \psi_R(0) \Rightarrow C = A + B$

* $\frac{d\psi_L(0)}{dx} = \frac{d\psi_R(0)}{dx} \Rightarrow iqC = ik(A-B)$

$$C = \frac{2k}{k+q} A, \quad B = \frac{k-q}{k+q} A$$

Reflection

For a classical particle with $E > V_0$, there's no reflection, but we see that QM gives reflection which is consistent with the wave behaviour of the particle.

We can calculate the reflection & transmission coefficients using fluxes:

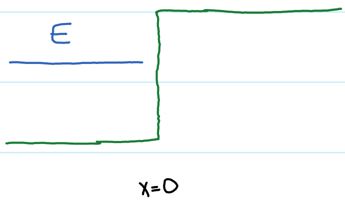
$$R = \left| \frac{J_R}{J_I} \right| = \left| \frac{\frac{\hbar k}{m} |B|^2}{\frac{\hbar k}{m} |A|^2} \right| = \left| \frac{B}{A} \right|^2 = \left(\frac{k-q}{k+q} \right)^2$$

$$T = \left|\frac{J_T}{J_I}\right| = \left|\frac{\frac{\hbar q}{m}|C|^2}{\frac{\hbar k}{m}|A|^2}\right| = \frac{q}{k}\frac{|C|^2}{|A|^2} = \left(\frac{2k}{k+q}\right)^2$$

Check that $R+T=1$.

$V_0 \geq E$

$$\frac{d^2\psi_L(x)}{dx^2} = -\overbrace{\boxed{\frac{2m}{\hbar^2}E}}^{k^2}\psi_L(x)$$



$$\frac{d^2\psi_R(x)}{dx^2} = \underbrace{\boxed{\frac{2m}{\hbar^2}(V_0-E)}}_{q^2}\psi_R(x)$$

$$\begin{cases} \psi_L(x) = Ae^{ikx} + Be^{-ikx} \\ \psi_R(x) = Ce^{-qx} + De^{qx} \end{cases}$$

BC

$D=0$. $\lim_{x\to\infty}\psi_R = \infty$

$x=0$ $\quad A+B=C$

$ik(A-B) = -qC$

$\Rightarrow B = \frac{k-iq}{k+iq}A \qquad C = \frac{2k}{k+iq}A$

What's wrong with this?

Probability of getting the particle with negative Kinetic energy.

* Measurement often would add energy

* Calculate J_{tr} $\longrightarrow J_{tr}=0$

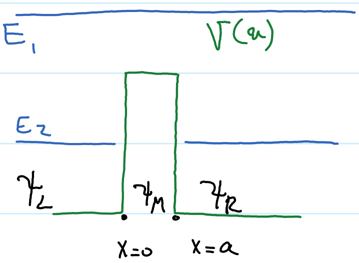
* $\psi_R(x) = Ce^{-qx}$ $\longrightarrow$ exponentialy drops

* $\psi_R(x) = C e^{-qx}$ → exponentially drops

* Similar to the evanescent light in optics

* $R = 1$ although $C \neq 0$

Potential Barrier



1) $E \geq V_0$

$$R, L: \quad \frac{d^2\psi(x)}{dx^2} = -k^2 \psi(x)$$

$$M. \quad \frac{d^2\psi(x)}{dx^2} = -q^2 \psi(x)$$

$$\psi(x) = \begin{cases} \psi_L(x) = Ae^{ikx} + Be^{-ikx} & x \leq 0 \\ \psi_M(x) = Ce^{iqx} + De^{-iqx} & 0 \leq x \leq a \\ \psi_R(x) = Ee^{ikx} & x \geq a \end{cases}$$

BC

$A + B = C + D$ $\qquad$ $ik(A-B) = iq(C-D)$

$Ce^{iqa} + De^{-iqa} = Ee^{ika}$ $\qquad$ $iq(Ce^{iqa} - De^{-iqa}) = ikEe^{ika}$

Solve for E & B

$$E = \frac{4kq\, e^{-ika}}{4kq\cos(qa) - 2i(k^2+q^2)\sin(qa)} A$$

$$T = \frac{k}{k}\frac{|E|^2}{|A|^2} = \frac{(4kq)^2}{\left(4kq\cos(qa)\right)^2 + 4(k^2+q^2)^2\sin^2(qa) \pm (4kq)^2\sin^2(qa)}$$

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

$$R = \frac{4(k^2-q^2)\sin^2(qa)}{(4qk)^2 + 4(k^2-q)^2\sin^2(qa)}$$

* $E \gg V_0 \Rightarrow k \sim q \Rightarrow R \sim 0 \longrightarrow$ Just as is classically.

* Take $\lambda = \frac{2\pi}{q} \Rightarrow a = m\lambda \Rightarrow R = 0$, Why?

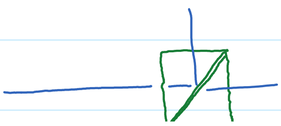
Reflections interfere destructively

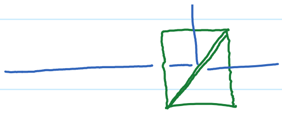
(A) Is there a situation where $T = 0$?

* $E < V_0$

Classically: A particle coming from left would change direction at the barrier and there would be no transmission.

For waves, there could be transmission.





QM

The state is similar to when $E > V_0$

except : $q \longrightarrow iq$

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x \leq 0 \\ Ce^{qx} + De^{-qx} & 0 \leq x \leq a \\ Ee^{ikx} & a \leq x \end{cases}$$

with BC we get.

$$E = \frac{4ikq \; e^{-ika}}{4ikq \cos(iqa) - 2i\,(k^2 - q^2)\sin(iqa)} \; A$$

$$T = \frac{(4kq)^2}{(4kq\cosh(qa))^2 + 4(k^2-q^2)^2\sinh^2(qa)} = \frac{1}{1 + \left(\frac{k^2+q^2}{2kq}\right)^2 \sinh^2(qa)}$$

$$R = \frac{\left(\frac{k^2+q^2}{2kq}\right)^2 \sinh^2(qa)}{1 + \left(\frac{k^2+q^2}{2kq}\right)^2 \sinh^2(qa)}$$

* R & T are not periodic functions of a

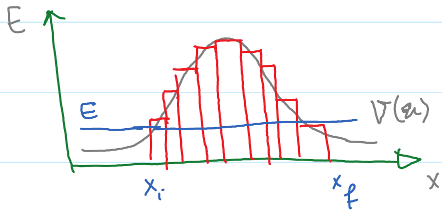
* For $E \ll V_0$

$$T \simeq 16E \; (V_0 - E) \; e^{-2aq}$$

$$T \simeq \frac{16E}{V_0^2}(V_0 - E)\, e^{-2aq}$$

(A) Show the eq. above.

For an arbitrary potential like



$$T = T_1 T_2 \cdots T_n$$

$$\sim e^{-a_1 q_1} e^{-a_2 q_2} \cdots e^{-a q_n}$$

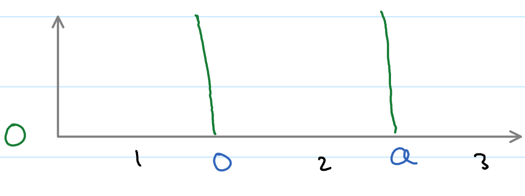
$$\sim e^{-\int_{x_i}^{x_f} q(x)\,dx} \longrightarrow T$$

Note that this only gives the scaling.
There's a factor of $\frac{16E(V_0(x) - E)}{V_0(x)}$
that changes for each T_1, but does not
affect the scaling

→ More on this when we get
to WKB.

Potential Well

$$V(x) = \begin{cases} \infty & x > a \;\&\; x < 0 \\ 0 & 0 \leq x \leq a \end{cases}$$



$V(x)\,\psi(x) \to \infty$ for (1,3) unless $\psi(x) = 0$

For (2) $\quad \dfrac{d^2\psi(x)}{dx^2} = -k^2\psi(x) \Rightarrow \psi(x) = A e^{ikx} + B e^{-ikx}, \quad k = \sqrt{\frac{2m}{\hbar}E}$

$x = 0 \quad \psi(x) = 0 \Rightarrow \psi(x) = A' \sin(kx)$

$x = a \quad \psi(x) = 0 \Rightarrow \psi(a) = A' \sin(ka) = 0 \Rightarrow ka = m\pi$

$$k = \frac{m\pi}{a} = \sqrt{\frac{2m}{\hbar^2}E}$$

$$\Rightarrow \boxed{E_m = m^2 \frac{\pi\hbar^2}{2ma^2}}$$

* $m = 0 \Rightarrow \psi = 0 \to$ Not acceptable (is not normal)

* E is not continous !

* $m = 1 \to$ Lowest energy level $\to E_{min} = \dfrac{\pi\hbar^2}{2ma^2}$

Classically this should be zero, but is not in QM.

Why?

$\Delta x \leq a \Rightarrow \Delta p \geq \dfrac{\hbar}{2a} \Rightarrow \Delta p^2 > 0$

$\langle P \rangle = 0 \to$ check this!

$\hookrightarrow \Delta P^2 = \langle P^2 \rangle = 2m\langle H \rangle = 2mE$

$\to \Delta P^2 = \langle P^2 \rangle > 0 \Rightarrow E_{min} > 0$

(A) For the potential well, calculate

$\langle \hat{x} \rangle \quad \langle \hat{p} \rangle \quad \langle x^2 \rangle \quad \langle p^2 \rangle$

Ⓐ For the potential well, calculate

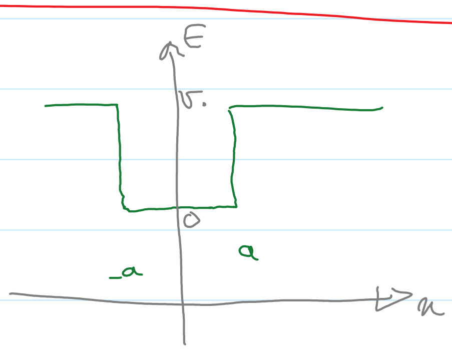
$\langle \hat{x} \rangle$, $\langle \hat{p} \rangle$, $\langle x^2 \rangle$, $\langle p^2 \rangle$

and $\Delta \hat{x}$ & $\Delta \hat{p}$

and check that the E_{min} is compatible with Δp^2.

Finite Potential Well

$$V(x) \begin{cases} V_0 & |x| > a \\ 0 & |x| \leq a \end{cases}$$



$E \geq V_0$: Scattering

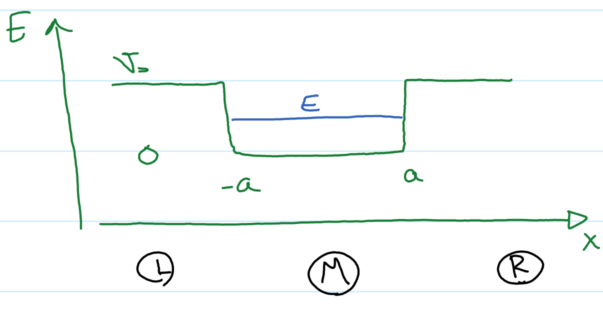
$$\begin{cases} A e^{iqx} + B e^{-iqx} \\ C e^{ikx} + D e^{-ikx} \\ E e^{-iqx} \end{cases}$$

Ⓐ Do the calculation and show that B is non-zero.

Calculate the reflection coefficient

$E \leq V$

$$\frac{d^2 \psi_L(x)}{dx^2} = q^2 \psi_L(x) \rightarrow \psi_L(x) = A e^{-qx} + B e^{qx}$$



Similarly $\psi_R(x) = A' e^{-qx} + B' e^{qx}$

BC $x \to \pm\infty \Rightarrow \psi_L(x) = A e^{qx}$

$$\psi_R(x) = B e^{-qx}$$

$$\frac{d^2\psi_M(x)}{dx^2} = -k^2 \psi_M(x) \Rightarrow \psi_M(x) = C' e^{ikx} + D' e^{-ikx}$$

But since H is symmetric, i.e $[\hat{H}, \hat{\Pi}] = 0$, ψ should be either odd

$$\psi_M^o(x) = C \sin(kx)$$

or even

$$\psi_M^e(x) = D \cos(kx)$$

Ⓐ But do all values of k satisfy the BC?

BC

Odd. $x = a \Rightarrow$

$$C \sin(ka) = B e^{-qa}$$

$$k C \cos(ka) = -qB e^{-qa}$$

$$/ \quad k \cot(ka) = -q \qquad k = \sqrt{\frac{2m}{\hbar^2} E}, \quad q = \sqrt{\frac{2m}{\hbar^2}(V - E)}$$

$\times a$

$$(ka) \cot(ka) = -qa$$

$ka = x$

$$qa = \sqrt{\frac{2ma^2}{\hbar^2} V - x^2}$$

$$\kappa a = x$$

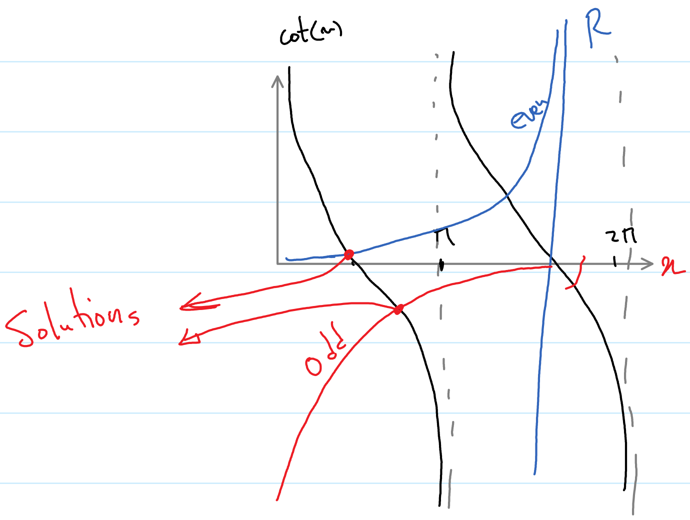
$$qa = \sqrt{\frac{2ma^2}{\hbar^2}V - x^2}$$

$$R = \sqrt{\frac{2m}{\hbar^2}V a^2}$$

$$\Rightarrow -x \cot x = \sqrt{R^2 - x^2} \Rightarrow \cot(x) = -\sqrt{\frac{R^2 - x^2}{x^2}}$$

Similarly for $\psi^e_\mu(x)$

$$x\,tg(x) = \sqrt{R^2 - x^2} \Rightarrow \cot(x) = \sqrt{\frac{x^2}{R^2 - x^2}}$$



* Solutions x_n gives E_n that can fullfil the BC.

* There are finite number of solutions.

* $R \uparrow \equiv V \uparrow$ or $a \uparrow$

$\Rightarrow$ # solutions $\uparrow$

* There's at least one even solution. (If $R < \pi/2$, that's the only ")

* There's a penetration that depends on $q = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$

$V_0 \to \infty \Rightarrow q \to \infty \Rightarrow$ No penetration.

Also $\quad tg(x) = 0 \xrightarrow{\text{odd}} x = n\pi \Rightarrow E_n = \dfrac{n^2 \pi^2 \hbar^2}{2ma^2}$

$\cot(x) = 0 \xrightarrow{\text{even}} x = (n + 1/2)\pi \Rightarrow E_n = \dfrac{(n+1/2)^2 \pi^2 \hbar^2}{2ma^2}$