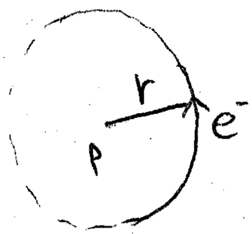
12. Semi-classical approximation (WKB):

12.1 Prelude:

8.04 Bohr quantization condition for a hydrogen atom:



(*) $$J = mvr = n\hbar \qquad n = 1, 2, 3, \ldots$$

$$\frac{mv^2}{r} = \frac{e^2}{r^2}$$

$$\Rightarrow \quad r_n = n^2 a \qquad \left(a = \frac{\hbar^2}{me^2} \right)$$

$$\underbrace{E_n = \frac{e^2}{2r_n}} \qquad n = 1, 2, \ldots$$

Exact answer!

de Broglie wave length: $\lambda = \frac{h}{p} = \frac{h}{mv}$

$$(*) \quad \Rightarrow \quad \frac{2\pi r}{\lambda} = n$$

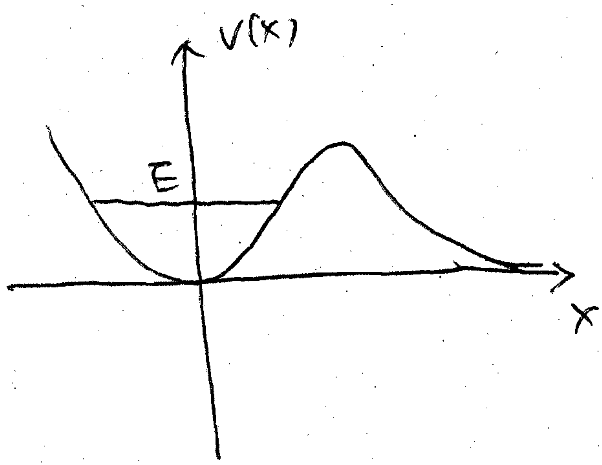
i.e. integer # of de Broglie waves fit into the classical orbit: constructive interference.

Semi-classical approximation:

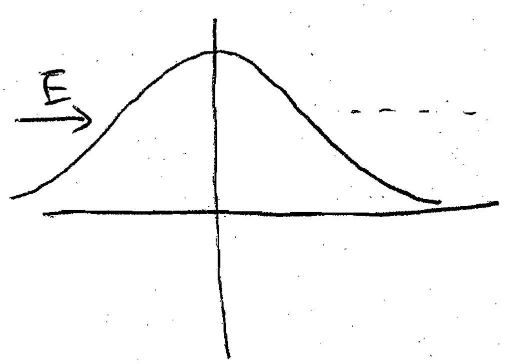
1. Systematic derivation of Bohr-type quantization condition for bound states of a general system.

(Bohr's derivation was one of those happy accidents in history of physics.)

2. Tunneling (estimate)



or



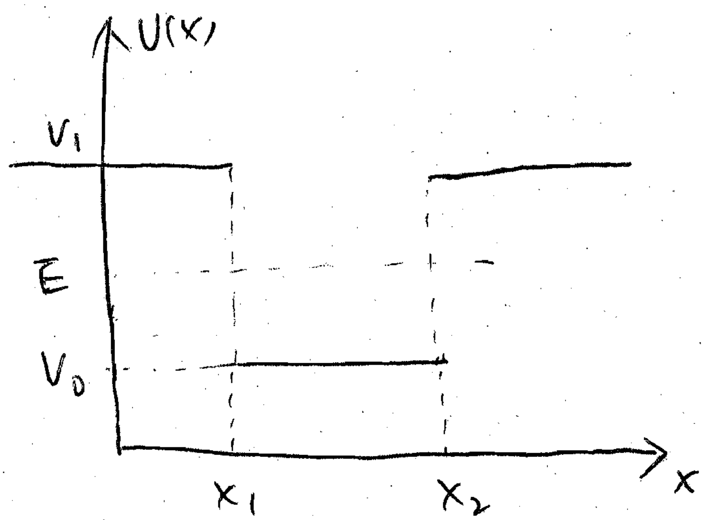
12.2 WKB approximation for wave functions:

Consider a particle moving in a 1d potential $V(x)$:

$$-\frac{\hbar^2}{2m}\partial_x^2\psi + V(x)\psi = E\psi \quad ①$$

$$\Rightarrow \quad -\partial_x^2\psi = \frac{2m(E-V(x))}{\hbar^2}\psi(x) \quad ②$$

Now consider a special example of $V(x)$:



Suppose $V_0 < E < V_1$.

1) Classical region: $(x_1 < x < x_2)$

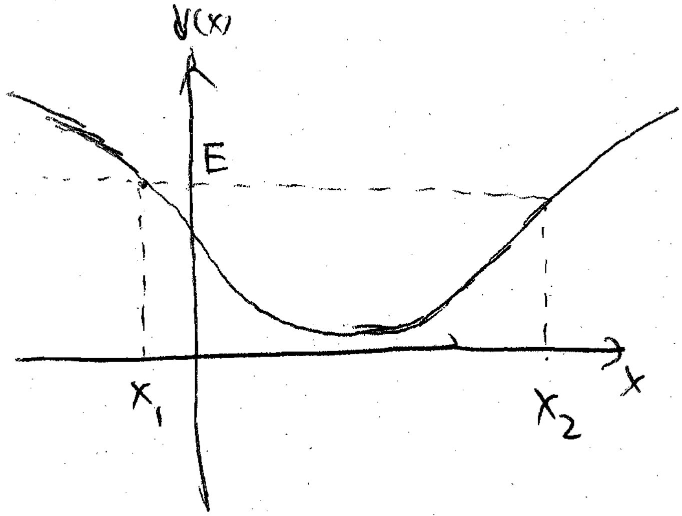
$$\psi(x) \sim A e^{\frac{ipx}{\hbar}} \quad ③$$

$$p = \sqrt{2m(E-V_0)}$$

2) Classically forbidden regions $(x > x_2$ or $x < x_1)$

$$\psi(x) \sim B e^{\pm\frac{k}{\hbar}x}, \quad k = \sqrt{2m(V_1-E)} \quad ④$$

Now consider $V(x)$ slowly varying with x:



1) first look at the classical region: $x_1 < x < x_2$

Motivated by ③, Let

$$\psi(x) = e^{\frac{iS(x)}{\hbar}} \qquad ⑤$$

and plug it into ① (with a bit algebra)

$$(\partial_x S(x))^2 - i\hbar\, \partial_x^2 S = p^2(x) \qquad ⑥$$

with

$$p(x) = \sqrt{2m(E - V(x))}$$

If $V(x)$ is constant in this region, $p(x)$ is constant and $S(x)$ is <u>linear</u> in x. $\partial_x^2 S$ term vanishes identically in ⑥.

If the potential is not exactly constant, but slowly varying, we expect $\underline{\hbar\, \partial_x^2 S}$ term in ⑥, while non-vanishing, should be small compared to other terms.

<u>Approximation:</u> ignore $i\hbar\, \partial_x^2 S$ term in ⑥

$$\Rightarrow \quad (\partial_x S)^2 \simeq p^2(x) \quad \text{⑦} \quad \Rightarrow \quad S \simeq \pm \int^x p(x')\, dx'$$

$$\Rightarrow \quad \psi(x) \simeq e^{\pm \frac{i}{\hbar} \int^x p(x')\, dx'} \qquad \text{⑧}$$

- Similarly in the classically forbidden regions ($x > x_2$ or $x < x_1$)

$$\psi(x) \simeq e^{\pm \frac{1}{\hbar} \int^x k(x')\, dx'} \qquad \text{⑨}$$

$$k(x) = \sqrt{2m(V(x) - E)} \, .$$

⑨ and ⑧: Lowest order WKB approximation.

range of validity. higher order corrections ?

- systematic treatment:

key observation: the term previously ignored in ⑥ is multiplied by $\hbar$. [thus the name semi-classical. note ⑨ and ⑧ still depend on $\hbar$].

$\Rightarrow$ Suggest we should expand S in $\hbar$ ($\hbar$ imagine small).

i.e.

$$S = S_0(x) + \hbar S_1(x) + \hbar^2 S_2(x) + \cdots \quad (10)$$

Note: $\hbar$ is dimensional.

Dimensionless expansion parameter will be transparent later

Classically allowed region: plug (10) into (6) and solve the equation order by order in $\hbar$:

$$\left(\partial_x S_0 + \hbar \partial_x S_1 + O(\hbar^2) \right)^2 - i\hbar \left(\partial_x^2 S_0 + \hbar \partial_x^2 S_1 + O(\hbar^2) \right)$$

$$= p^2(x)$$

Order $\hbar^0$: $\qquad (\partial_x S_0)^2 = p^2(x) \qquad (11)$

$\hbar^1$: $\qquad 2 \partial_x S_0 \partial_x S_1 - i \partial_x^2 S_0 = 0 \qquad (12)$

$\hbar^2$: $\qquad \ldots$

Equation (11) is simply our previous eq. (7).

$$\Rightarrow \boxed{S_0(x) = \pm \int^x p(x') \, dx'}$$

(since $\partial_x S_0 = \pm p(x)$)

Eq ⑫ $\Rightarrow$ $\quad \partial_x S_1 = \frac{i}{2} \frac{\partial_x^2 S_0}{\partial_x S_0} = \frac{i}{2} \frac{\partial_x p(x)}{p(x)}$

$$= \frac{i}{2} \partial_x \log p(x)$$

$$\Rightarrow \quad \boxed{S_1 = \frac{i}{2} \log p(x) + \text{const}}$$

Thus

$$\psi(x) = e^{\frac{i}{\hbar} S(x)} = e^{\frac{i}{\hbar} S_0 + i S_1 + O(\hbar)}$$

$$= \frac{C}{\sqrt{p(x)}} \exp\left(\pm \frac{i}{\hbar} \int^x p(x')\, dx' + O(\hbar) \right)$$

Thus we find in the classical regim $(E > V(x))$

$$\boxed{\psi(x) = \frac{c_+}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int^x p(x')\,dx'} + \frac{c_-}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int^x p(x')\,dx'}} \tag{13}$$

With $p(x) = \sqrt{2m(E - V(x))}$

Exactly parallel analysis for the classically forbidden regions, i.e. $E < V(x)$,

$$\boxed{\psi(x) = \frac{d_+}{\sqrt{k(x)}} e^{\frac{1}{\hbar}\int^x k(x')\,dx'} + \frac{d_-}{\sqrt{k(x)}} e^{-\frac{1}{\hbar}\int^x k(x')\,dx'}} \tag{14}$$

With $k(x) = \sqrt{2m(V(x) - E)}$

Remarks: (on (13) and (14))

1. As in constant potential case,

$$e^{\frac{i}{\hbar}\int^x p(x')dx'} \quad : \quad \text{right-moving wave}$$

$$e^{-\frac{i}{\hbar}\int^x p(x')dx'} \quad : \quad \text{left-moving wave}$$

$$\lambda(x) = \frac{\hbar}{p(x)} \quad \text{de Broglie wave length}$$

(spatially varying)

2. For left- or right-moving waves,

$$P = |\psi|^2 \propto \frac{1}{p(x)} \propto \frac{1}{v(x)} \quad (v(x): \text{ classical velocity})$$

Probability is larger where $v(x)$ is smaller:

a particle spends more time where it is going slow.

3. probability current:

$$J(x) = \mathrm{Im}\left(\frac{\hbar}{m}\,\psi^* \partial_x \psi\right)$$

Since $\partial_x \psi(x) = \frac{i}{\hbar}\, p(x)\, \psi(x) + \text{real} \cdot \psi(x)$

$$\Rightarrow \quad J(x) = \begin{cases} \frac{i}{m} & \text{right - moving} \\ -\frac{i}{m} & \text{left - moving} \end{cases}$$

$$= \rho\, v(x) \qquad (\rho = |\psi(x)|^2)$$

4. Range of validity.

For expansion (10) to be valid, we need

$$|\hbar S_1(x)| \ll |S_0(x)|$$

or

$$|\hbar S_1'(x)| \ll |S_0'(x)| \quad (15)$$

using eq (11) and (12) in (15), $\Rightarrow$

$$\left|\hbar \frac{p'(x)}{p(x)}\right| \ll |p(x)|$$

$$\Rightarrow \quad \left|\hbar \frac{p'(x)}{p^2(x)}\right| \ll 1 \quad (16)$$

$$\Rightarrow \quad \left|\partial_x \frac{\hbar}{p(x)}\right| \ll 1$$

$$\Rightarrow \quad \boxed{|\partial_x \lambda(x)| \ll 1} \quad (17)$$

($\lambda(x)$: de Broglie wavelength)

$\Rightarrow$ spatial variation of $\lambda(x)$ should be small.

Equation (17) can be written in an alternative way as follows:

Since $p(x) = \sqrt{2m(E - V(x))}$

$$p'(x) = -\frac{2m\, V'(x)}{p(x)} \quad (18)$$

Plug (18) into (16),

$$\Rightarrow \left| \frac{2m\hbar\, V'(x)}{p^3(x)} \right| \ll 1$$

$$\Rightarrow \left| \frac{\hbar}{p(x)} V'(x) \right| \ll \frac{p^2}{2m}$$

$$\Rightarrow \left| \lambda(x)\, V'(x) \right| \ll \frac{p^2}{2m} \quad (19)$$

Note: $\frac{p^2}{2m} = KE$ (kinetic energy)

$$\lambda(x)\, V'(x) = V(x+\lambda(x)) - V(x) = \Delta V$$

Variation of $V(x)$ over a de Broglie wavelength.

(19) $\Rightarrow$ $$\boxed{\left|\frac{\Delta V}{KE}\right| \ll 1} \quad (20)$$

Equation (20) requires:

(a) Potential $V(x)$ sufficiently smooth

or / and

(b) KE of the classical particle big.

5. For classically forbidden regions, the discussion of range of validity is completely parallel:

$$\left| d_x \frac{\hbar}{K(x)} \right| \ll 1 \qquad (21)$$

or

$$\left| \frac{\Delta V}{KE} \right| \ll 1 \qquad (22) \qquad \underline{KE = E - V(x)}$$

6. At classical turning points: x_1, x_2

where

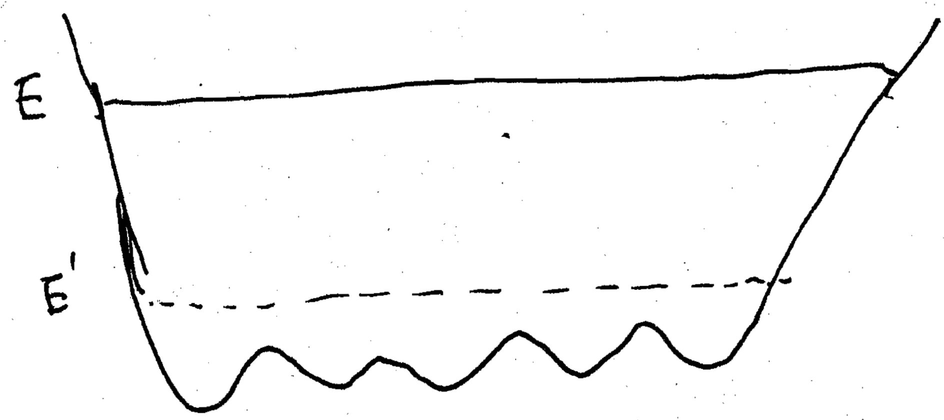
$$E = V(x)$$

i.e.

$$p(x) = K(x) = 0$$

Clearly (19) and (21) cannot be satisfied.

$\Rightarrow$ approximation breaks down. Need special treatment.



E: should be a good approximation

E': most likely not.

<u>semi-classical</u>

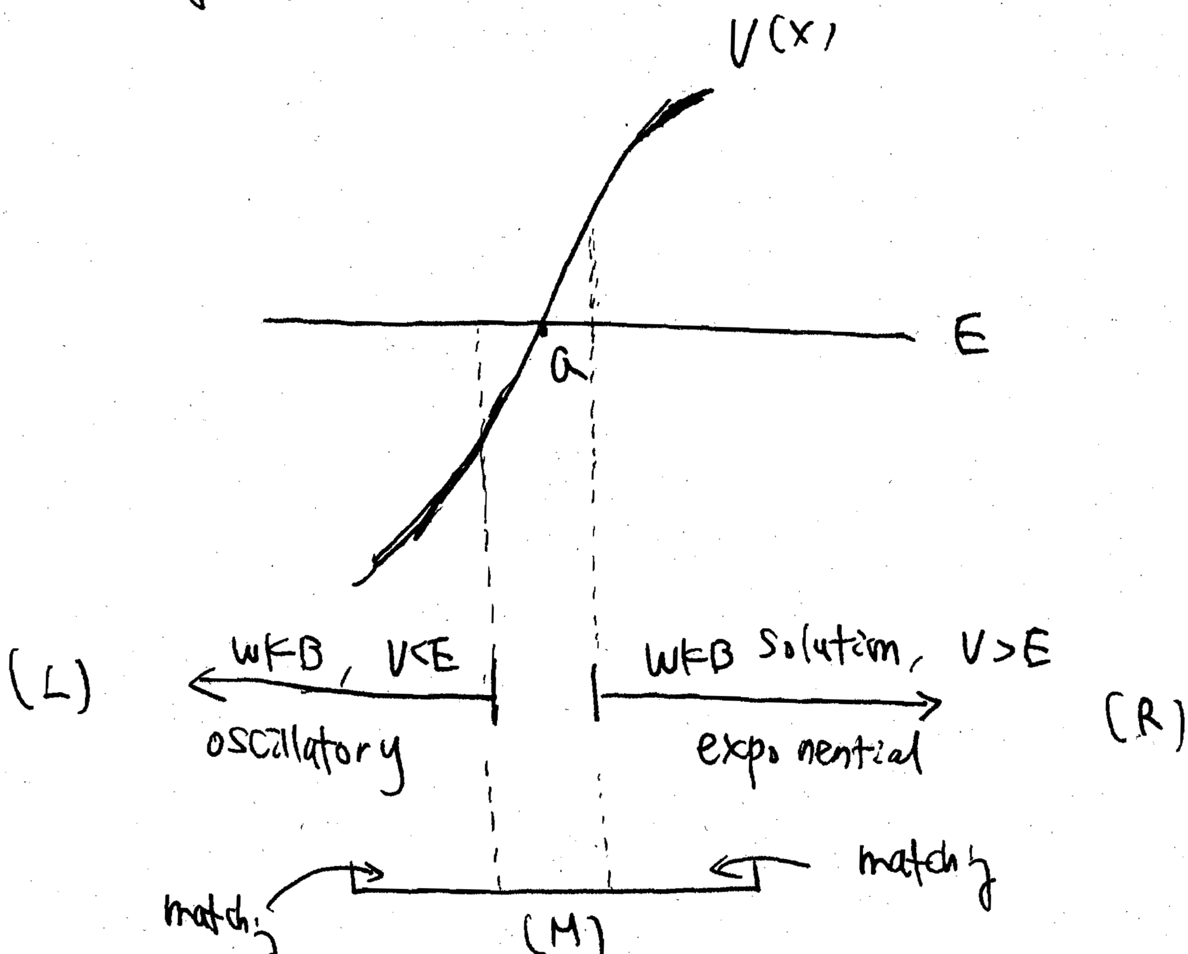
2 full board

End of lecture 14

1.3 Connection formulas:

1.3.1 Idea

Our semi-classical approximation breaks down near the turning point. To see what to do there, let us focus on the neighbourhood of one of the turning points:



approximate $\underline{V(x) = V(a) + \lambda(x-a)}$

Strategy:

1) Apply WKB approximations to regions R and L.

2) Near $x=a$, in region M, approximate $V(x)$ by

$$V(x) = V(a) + \lambda (x-a) + \underbrace{\cdots}_{\text{ignore}} \qquad (\lambda = V'(a))$$

~~Typically~~, If $V(x)$ is sufficiently smooth, M overlaps with both L and R regions.

3) Solve the schrodinger equation exactly near $x=a$ using the linear potential.

$\Rightarrow$ Airy functions

$$\psi(x) = C_1 Ai(x) + C_2 Bi(x)$$

4) Matching Airy functions with WKB solutions

in the overlap regions: $M \cap L$

$M \cap R$.

E.g. Start with $\psi_{WKB}(x)$ in the right

$$\psi_{WKB}(x) \text{ in } R \xrightarrow{M \cap R} \psi(x) = C_1 A_i + C_2 B_i(x)$$

$$\xrightarrow{M \cap L} \psi_{WKB} \text{ in } L$$

or vice versa.

Brilliant idea, but ~~to~~ in practice tedius to carry out.

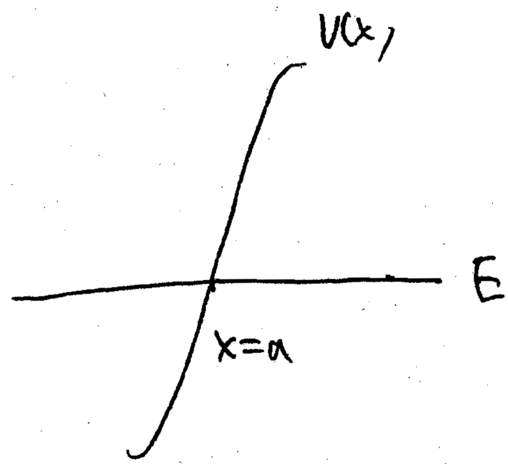
The results can be summarized in a set of rules, called connection formulas.

(3.3)2 ~~Examples~~ Cofo

Connection formulas: (On one of the back board)

See Griffiths (p. 325) for derivation.

I Forbidden region to the right

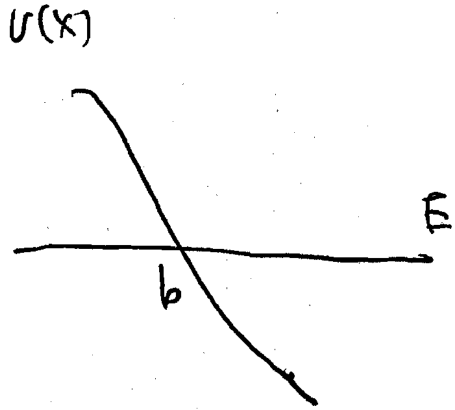


A① $$\frac{2}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_x^a p(x')\,dx' - \frac{\pi}{4}\right] \Longleftarrow \frac{1}{\sqrt{k(x)}} e^{-\frac{1}{\hbar}\int_a^x k(x')\,dx'} \qquad (1)$$

$$\frac{1}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_x^a p(x')\,dx' + \frac{\pi}{4}\right] \Longrightarrow \frac{1}{\sqrt{k(x)}} e^{\frac{1}{\hbar}\int_a^x k(x')\,dx'} \qquad (2)$$

Notation difference in Griffiths.

II Forbidden region to the left



$$\frac{1}{\sqrt{k(x)}} e^{-\frac{1}{\hbar}\int_x^b k(x')\,dx'} \Longrightarrow \frac{2}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_b^x p(x')\,dx' - \frac{\pi}{4}\right] \quad (3)$$

$$\frac{1}{\sqrt{k(x)}} e^{\frac{1}{\hbar}\int_x^b k(x')\,dx'} \Longleftarrow \frac{1}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_b^x p(x')\,dx' + \frac{\pi}{4}\right] \quad (4)$$

Remarks:

1) One can apply these formulas in both directions.
(caveat to follow).

2) Since the schrodinger equation is linear, one can simply superpose them.

12.3.3 Directions of connection formulas:

Can one apply the connection formulas in directions opposite to the arrows ?

Yes, one can replace $\Rightarrow$ by $\Leftrightarrow$

but one should be <u>very</u> carful in doing so

for equations (2) and (4).

Example : suppose in the forbidden region to the right we have

exponentially increasing (EI)

$$\psi(x) \simeq \frac{d_+}{\sqrt{k(x)}} \exp\left[\frac{1}{\hbar} \int_a^x k(x')\,dx' \right] \left(1 + O(\hbar) + \cdots\right)$$

$$+ \frac{d_-}{\sqrt{k(x)}} \exp\left[-\frac{1}{\hbar} \int_a^x k(x')\,dx' \right] \left(1 + O(\hbar) + \cdots\right)$$

exponential decreasing (ED)

If d_+ and d_- are precisely know $\Rightarrow$

Can use connection formulas in both directions.

One finds in the allowed region:

$$\psi(x) \simeq \frac{d_+}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_x^a p(x')\,dx' + \frac{\pi}{4}\right]$$

$$+ \frac{2d_-}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_x^a p(x')\,dx' - \frac{\pi}{4}\right]$$

Note: ED term is generally much smaller than EI term (exponentially small in $\hbar$ expansion). In fact ED is typically much smaller than omitted $O(\hbar)$ corrections to the EI term.

(provided d_+ is not too small compared to d_-)

Ex: $\hbar \sim 0.1$ $\quad e^{-\frac{1}{\hbar}} \sim e^{-10} \sim 4.5\times 10^{-5} \ll O(\hbar)$

Thus ED term is normally omitted, and one is left with:

$$\psi(x) \simeq \frac{d_+}{\sqrt{k(x)}} \exp\left[\frac{1}{\hbar} \int_a^x k(x')\,dx' \right] \qquad (5)$$

which is an excellent approximation.

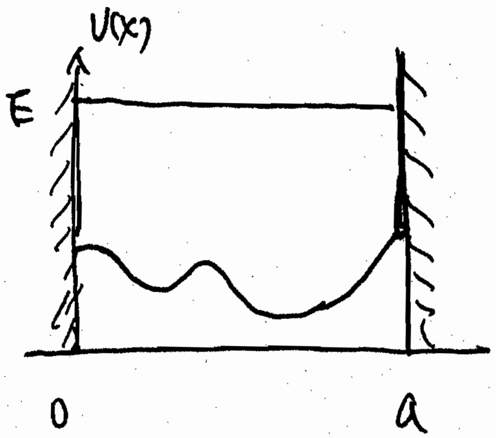
But one can NOT apply eq (2) backward to (5) any more.

Even though ED term could be tiny in the forbidden region, through connection formulas, it leads big correction in the allowed region.

13.4 WKB approximation to bound state energies

(a)

Potential well with two vertical walls:



$$\psi(x) = \frac{C_+}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar} \int_0^x dx' \, p(x') \right)$$

forced by $\psi(0) = 0$.

$$\psi(a) = 0 \Rightarrow \frac{1}{\hbar} \int_0^a dx' \, p(x') = n\pi , \quad n = 1, 2, 3, \cdots$$

$$\Rightarrow \int_0^a dx' \, p(x') = n\pi\hbar \quad n = 1, 2, \cdots$$

This quantization condition fixes bound state energies.

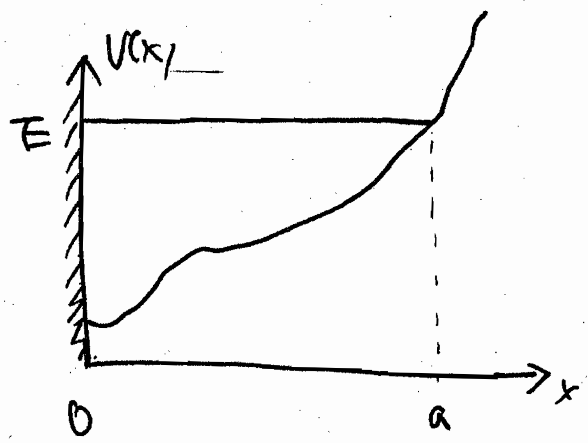
e.g. $\int_0^a dx \sqrt{2m(E - V(x))} = n\pi\hbar$

$\Rightarrow E_n$

e.g. $V=0 \Rightarrow \sqrt{2mE}\, a = n\pi\hbar$

$\Rightarrow E = \frac{n^2\pi^2\hbar^2}{2ma^2}$

(b). potential well with one vertical wall:



Solution must be ~~damped~~ exponentially damped in forbidden region.

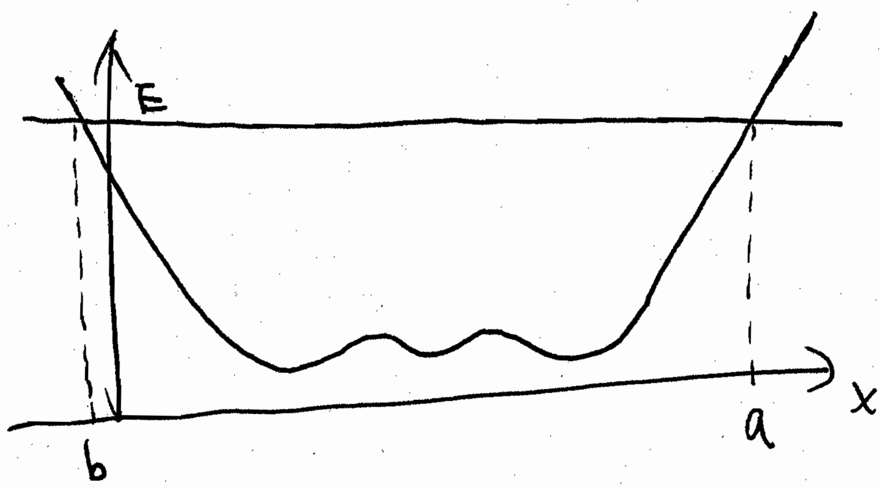
$$\Rightarrow \quad \psi(x) = \frac{2}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar} \int_x^a p(x')\,dx' - \frac{\pi}{4} \right)$$

for $\underline{\underline{x<a}}$.

$$\psi(0) = 0 \quad \Longrightarrow \quad \frac{1}{\hbar}\int_0^a p(x)\,dx - \frac{\pi}{4} = (n-\tfrac{1}{2})\pi \qquad n=1,2,3\cdots$$

$$\Rightarrow \quad \boxed{\int_0^a p(x)\,dx = (n-\tfrac{1}{4})\pi\hbar, \qquad n=1,2,\cdots}$$

(c). potential well with no vertical walls.



$x>a$:

$$\psi(x) \simeq \frac{C}{\sqrt{\kappa(x)}} e^{-\frac{1}{\hbar}\int_a^x \kappa(x')dx'}$$

$$\Rightarrow \quad \psi(x) = \frac{2C}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_x^a p(x')dx' - \frac{\pi}{4}\right] \quad (6)$$

for $b<x<a$

$x<b$: $\psi(x)$ exponential damped

$$\Rightarrow \quad \psi(x) = \frac{2C'}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar}\int_b^x p(x')dx' - \frac{\pi}{4}\right) \quad (7)$$

$$= \frac{2C'}{\sqrt{p(x)}} \cos\left(-\frac{1}{\hbar}\int_b^x p(x')dx' + \frac{\pi}{4}\right)$$

6 and 7 must be equal

$\Rightarrow$ two cos functions must be equal up to a sign
(can choose $C = +C'$ or $C = -C'$)

$$\Rightarrow \quad \frac{1}{\hbar}\int_x^a p(x')\,dx' - \frac{\pi}{4} = -\frac{1}{\hbar}\int_b^x p(x')\,dx' + \frac{\pi}{4} + n\pi$$

$$n = 0, 1, \ldots$$

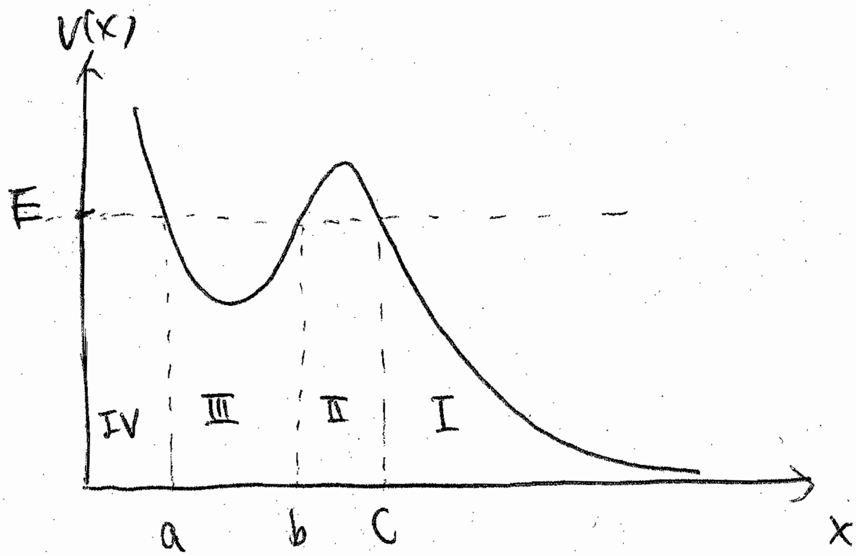
$$\Rightarrow \quad \frac{1}{\hbar}\int_b^a p(x)\,dx = (n+\tfrac{1}{2})\pi, \quad n = 0, 1, \ldots$$

$$\Rightarrow \quad \boxed{\int_b^a p(x)\,dx = (n-\tfrac{1}{2})\pi\hbar, \quad n = 1, 2, \ldots}$$

Bohr–Sommerfeld quantization

12.5 Tunneling :

Consider a particle of energy E in a potential $V(x)$ of the form :

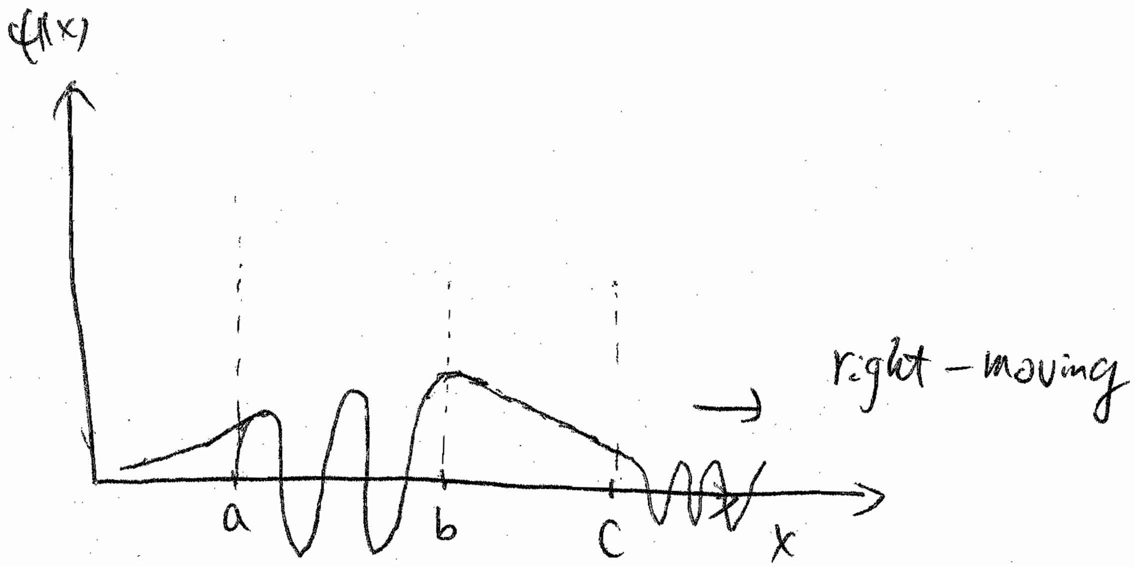


Classically : If the particle initially lies between a and b, it will periodically bounces around between a and b.

QM : can tunnel from b to c and then move to $x = +\infty$.

What is the tunneling rate ?

Qualitatively, we expect the wave function to behave:



Given a particle ~~sitting~~ at $x=b$, what is the probability it will tunnel to c:

$$\text{tunneling probability} \approx \frac{|\psi(c)|^2}{|\psi(b)|^2}$$

If we have a bunch of particles moving between a and b, how likely for them to tunnel within a given period of time?

Or ~~equa~~ equivalently, what is the probability of tunnelling per unit time?

Need to consider how often a particle collides with $x=b$.

It is $\frac{1}{T}$, where T is the classical period:

$$T = 2 \int_a^b \frac{dx}{v(x)} = 2 \int_a^b \frac{m\,dx}{p(x)}$$

$\uparrow$

it all

board

~~Tunnel~~

Tunneling rate = Prob. of tunneling per unit time

$$= \frac{|\psi(c)|^2}{|\psi(b)|^2} \frac{1}{T}$$

$$= \frac{|\psi(c)|^2}{|\psi(b)|^2} \frac{1}{2m \int_a^b \frac{dx}{p(x)}}$$

Avarage lifetime (of a particle trapped between a and b.) $= \dfrac{1}{\text{tunneling rate}}$

Now: we compute $\dfrac{|\psi(c)|^2}{|\psi(b)|^2}$ using WKB.

* Region I:

Since there is NO particle coming from $+\infty$,

in region I, ψ must be a right-moving wave,

i.e.

$$\psi(x) \simeq \frac{A}{\sqrt{p(x)}} e^{i\int_c^x p(x')\,dx'} \left(1 + O(\hbar) \cdots\right) \quad (8)$$

$$= \frac{A e^{i\frac{\pi}{4}}}{\sqrt{p(x)}} \cos\left(\int_c^x p(x')\,dx' - \frac{\pi}{4}\right) + \frac{e^{-i\frac{\pi}{4}}}{\sqrt{p(x)}} A \cos\left(\int_c^x p(x')\,dx' + \frac{\pi}{4}\right)$$

$\Longrightarrow$ (using connection formulas (3) and (4))

Region II:

$$\psi(x) \simeq \frac{e^{i\frac{\pi}{4}}}{2} \frac{A}{\sqrt{k(x)}} \exp\left(-\frac{1}{\hbar}\int_x^c k(x')\,dx'\right) \leftarrow (\text{ED})$$

$$\Uparrow$$

$$+ \frac{e^{-i\frac{\pi}{4}} A}{\sqrt{k(x)}} \exp\left(\frac{1}{\hbar}\int_x^c k(x')\,dx'\right) \leftarrow (\text{EI}) \quad (9)$$

(8) and (9) cannot be directly applied to find

$|\psi(b)|$ and $|\psi(c)|$, since WKB breaks down

there due $k(x) = p(x) = 0$ at these points.

However, we can compare

$$\left|\frac{\psi(c+\epsilon)}{\psi(b+\epsilon)}\right|^2 \simeq \exp\left[-\frac{2}{\hbar}\int_b^c k(x)\,dx\right]$$

prefactor undetermined, but it does not matter

extremely small number.

We thus find:

$$\text{tunneling rate} = \frac{\exp\left(-\frac{2}{\hbar}\int_b^c k(x)\,dx\right)}{2m\int_a^b \frac{dx}{p(x)}}$$

$$k(x) = \sqrt{2m\left(V(x)-E\right)}$$

Classical example: α- decay.

see Griffiths.

Pset: another example