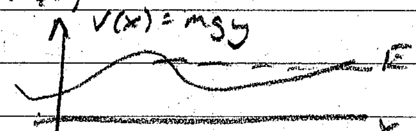
Semi-classical or WKB Approximation

WKB = (Jeffreys) Wentzel - Kramers - Brillouin

Approximation

- Classical Mechanics w/ energy conservation
  - Particle of energy E in potential $V(x)$
    - Like rolling on a hill $y(x)$



  - Conservation of energy
    - $$E = \text{const} = \frac{p^2}{2m} + V(x)$$
    - On a trajectory of energy E, momentum is a function of position
      $$p(x) = \sqrt{2m\,(E - V(x))}$$
- Use this in quantum wavefunction
  - A free particle ($V(x) = \text{const}$) of definite momentum has
    $$\psi(x) = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \qquad (\text{in 1D})$$
    Suggests approximating
    $$\psi(x) \approx e^{i\int_{x_0}^{x} dx'\, p(x')/\hbar} \qquad \text{for any potential}$$
  - When should this work?
    - Free particle wavefunction has constant (de Broglie) wavelength $\lambda = 2\pi\hbar/p$
    - The approximation is good when it changes slowly
      $$|d\lambda/dx| \ll 1 \implies \lambda\,|dp/dx| \ll |p|$$
      (The change in $p(x)$ over a wavelength is small compared to p)
  - The WKB wavefunction (when valid) is sinusoidal (complex exponential) with slowly varying wavelength and also amplitude. (Think about radio)

- Derivation from Schrödinger Eqn (1D)
  - One derivation is ~~to~~ expand in powers of a small parameter $\hbar|p'/p^2| \ll 1$
    - This is semi-classical b/c it works when $\hbar \to 0$.
    - We will use a different approach.

- Consider an energy e'state with $E > V(x)$
  - + Define the wavefunction as $\psi(x) = A(x)\exp(i\phi(x))$ with $A(x)$, $\phi(x)$ real
  - + The Schr. eqn is
$$A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2 = \frac{-p^2}{\hbar^2}A$$
    This is 2 real eqns. No approximations yet.
  - + The imaginary part is
$$(A^2\phi')' = 0 \implies A(x) = \text{const}/\sqrt{\phi'(x)}$$
- We make our approximation in the real part.
  - + Let's assume $\phi(x) \approx \int^x dx'\, p(x')/\hbar$ (and confirm later)
  - + Then $A \propto 1/\sqrt{p}$, $A'(x) \propto p'/p\, A$, $A'' \sim \frac{p''}{p}A,\ (p'/p)^2 A$
  - + Now recall we assumed WKB works for
$$\hbar|p'| \ll p^2 \implies \hbar|p''| \ll |p'p| \ll |p^3|/\hbar$$
    Comparing terms in real part of Schr eqn
$$A'' \sim p''A/p,\ (p'/p)^2 A \ll (p^2/\hbar^2)A$$
  - + Therefore, we approx have
$$(\phi')^2 = p^2/\hbar^2 \implies \phi(x) = \pm\frac{1}{\hbar}\int dx\, p(x)$$
  - + This should really be a definite integral, but changing a limit just changes the coefficient in the total wavefunction (the const. in $A(x)$)

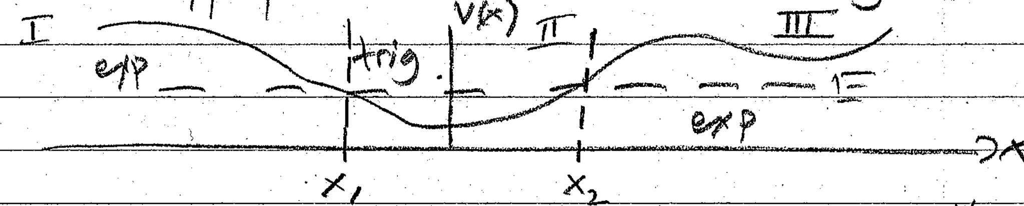
- The final approximate wavefunction
  - +
$$\psi(x) = \frac{1}{\sqrt{p(x)}}\left[C_1 e^{i\int dx\, p(x)/\hbar} + C_2 e^{-i\int dx\, p(x)/\hbar}\right]$$
  - + for $E > V(x)$ where $p(x) = \sqrt{2m(E - V(x))}$

    or alternately
$$\psi(x) = \frac{1}{\sqrt{p(x)}}\left[C_3 \sin\left(\int dx\, p(x)/\hbar\right) + C_4 \cos\left(\int dx\, p(x)/\hbar\right)\right]$$
  - + Where $E < V(x)$, the derivation is the same but $p(x)$ is imaginary

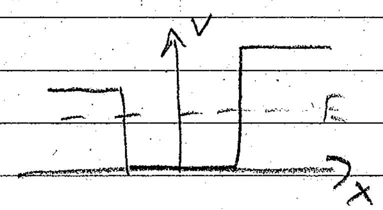
    Define
$$\rho(x) = -ip(x) = \sqrt{2m(V(x) - E)}$$

$$\Rightarrow \psi(x) = \frac{1}{\sqrt{p(x)}}\left[D_1 \exp\left(\int dx\, p(x)/\hbar\right) + D_2 \exp\left(-\int dx\, p(x)/\hbar\right)\right]$$

+ Use the appropriate solution in different regions



- Connection formulas (derived later)
  + We need to know how to relate exp to trig solutions at *classical turning points* x_1 & x_2 where $E = V(x)$. This is like having b.c. at jumps in square well potentials



  + We can use the following *connection formulas* to relate coefficients in solutions

  + At down-ward sloping turning points like x_1,

$$\psi = \begin{cases} \frac{A}{\sqrt{p}}\exp\left[-\int_x^{x_1} dx'\, p(x')/\hbar\right] + \frac{B}{\sqrt{p}}\exp\left[\int_x^{x_1} dx'\, \frac{p(x')}{\hbar}\right] & x < x_1 \\ \frac{2A}{\sqrt{p}}\cos\left[\left(\int_{x_1}^{x} dx'\, p(x')/\hbar\right) - \frac{\pi}{4}\right] - \frac{B}{\sqrt{p}}\sin\left[\left(\int_{x_1}^{x} dx'\, \frac{p(x')}{\hbar}\right) - \frac{\pi}{4}\right] & x > x_1 \end{cases}$$

  + At an upward-sloping turning point x_2

$$\psi = \begin{cases} \frac{2A}{\sqrt{p}}\cos\left[\left(\int_x^{x_2} dx'\, p/\hbar\right) - \frac{\pi}{4}\right] - \frac{B}{\sqrt{p}}\sin\left[\left(\int_x^{x_2} dx'\, \frac{p}{\hbar}\right) - \frac{\pi}{4}\right] & x < x_2 \\ \frac{A}{\sqrt{p}}\exp\left[-\int_{x_2}^{x} dx'\, p/\hbar\right] + \frac{B}{\sqrt{p}}\exp\left[\int_{x_2}^{x} dx'\, \frac{p}{\hbar}\right] & x > x_2 \end{cases}$$

  + No, the signs and factors of 2 are not mistakes

Applications

– Bound States

- Consider particle energy E in potential $V(x)$ as in the figure. Classically it stays in region II.

+ In region I, ψ must die off to the left

$$\psi_I = \frac{A_1}{\sqrt{p}} \exp\left(-\int_x^{x_1} dx'\, p/\hbar\right)$$

$$\Rightarrow \psi_{II} = \frac{2A_1}{\sqrt{p}} \cos\left[\left(\int_{x_1}^{x} dx'\, p/\hbar\right) - \pi/4\right]$$

by connection formula

+ In region III, it must die off to the right

$$\psi_{III} = \frac{A_2}{\sqrt{p}} \exp\left(-\int_{x_2}^{x} dx'\, p/\hbar\right)$$

$$\Rightarrow \psi_{II} = \frac{2A_2}{\sqrt{p}} \cos\left[\left(\int_{x}^{x_2} dx'\, p/\hbar\right) - \pi/4\right]$$

- We have 2 versions of the wavefunction in classically allowed region II. How are they the same?

+ To check if the cosines are the same, note

$$\int_{x_1}^{x_2} dx'\, p/\hbar = \int_{x_1}^{x} dx'\, p/\hbar + \int_{x}^{x_2} dx'\, \frac{p}{\hbar}$$

+ Then

$$\cos\left[\int_{x_1}^{x} dx'\, p/\hbar - \frac{\pi}{4}\right] = \cos\left[\int_{x_1}^{x_2} dx'\, p/\hbar - \int_{x}^{x_2} dx'\, p/\hbar - \frac{\pi}{4}\right]$$

$$= \cos\left(\int_{x_1}^{x_2} dx'\, \frac{p}{\hbar}\right) \cos\left[\left(\int_{x}^{x_2} dx'\, \frac{p}{\hbar}\right) + \frac{\pi}{4}\right] + \sin(\cdots)\sin[\cdots]$$

+ Remember that shifting the argument by $\pi/2$ to change $+\pi/4 \rightarrow -\pi/4$ for matching wavefunctions swaps $\cos[\cdots] \Longleftrightarrow \sin[\cdots]$

+ Therefore, 2 forms of wavefunctions match if

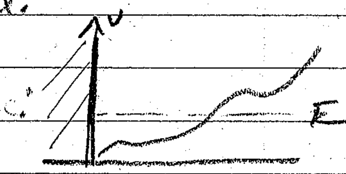
$$\cos\left(\int_{x_1}^{x_2} dx\, \frac{p}{\hbar}\right) = 0 \Longleftrightarrow \sin\left(\int_{x_1}^{x_2} dx\, \frac{p}{\hbar}\right) = \pm 1 \text{ and } A_1 = \pm A_2$$

- Quantization Condition
  + This matching requirement gives a quantization condition

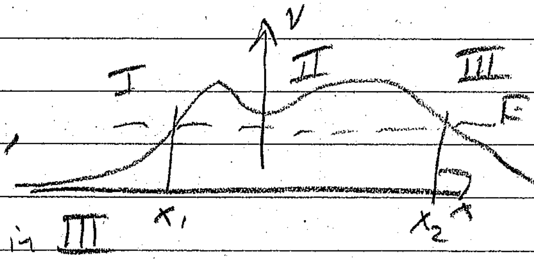
$$\int_{x_1}^{x_2} dx\, p(x) = (n+\tfrac{1}{2})\pi\hbar, \quad n=0,1,2,\ldots$$

x_1, x_2, p depend on energy →

  + This is a lot like the Bohr-Sommerfeld condition used in the Bohr model.
  + It's not hard to generalize to a case where $V \to \infty$ [illegible]. Use the connection formula & make the wavefunction vanish at the wall.



- Tunneling
  - Consider a potential barrier
    + As usual for 1D scattering, there are an incoming + reflected wave in I and outgoing wave in III



  + On the right,

$$\psi_{III} = \frac{C}{\sqrt{p}} \exp\left[i\int_{x_2}^{x} dx'\, p/\hbar\right] \quad \text{(right-moving)}$$

  + On the left

$$\psi_I = \frac{A}{\sqrt{p}} \exp\left[-i\int_{x}^{x_1} dx'\, p/\hbar\right] + \frac{B}{\sqrt{p}} \exp\left[i\int_{x}^{x_1} dx'\, \frac{p}{\hbar}\right]$$

The 1st term is right-moving (incident) b/c the phase increases (gets less negative) as x increases — you can compare to $e^{ipx/\hbar}$

- Get transmission/reflection coefficients by matching the wavefunction through the barrier
  + In principle, you use real exp. WKB wavefunctions and then connection formulas to relate coefficients. Instead, we'll use an extra approximation

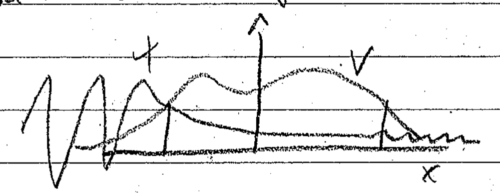
+ Normally, we think of the wavefunction in the barrier as dying off, so we keep only that term (extra approx)

$$\psi_{II} \approx \frac{F}{\sqrt{p}} \exp\left[-\int_{x_1}^{x} dx' \frac{p}{\hbar}\right]$$

This is good for wide (+ high) barriers

+ Then $|A| \approx |B|$, $|A| \approx |F|$

$$|C| \approx |F| \exp\left[-\int_{x_1}^{x_2} dx' \frac{p}{\hbar}\right]$$

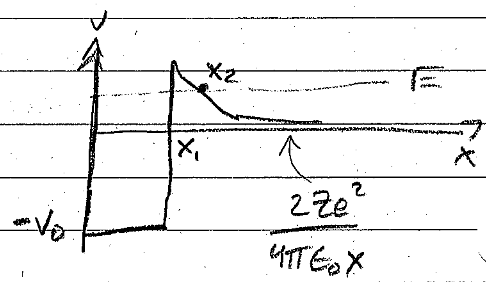


+ Transmission coefficient

$$T = |F/A|^2 \approx \exp\left[-2\int_{x_1}^{x_2} dx\, p/\hbar\right]$$

• Example: Decay of Nucleus

+ Model the decaying nucleus as α particle w/energy E in a potential given by square well with Coulomb repulsion outside



$$V = \begin{cases} \infty, & x < 0 \\ -V_0, & 0 < x < x_1 \\ 2Ze^2/4\pi\epsilon_0 x, & x > x_1 \end{cases}$$

+ Each time the α reaches x_1, it has a probability to escape given by transmission coeff. The classical speed in the nucleus is $v = \sqrt{2(E+V_0)/m}$ so the "time between tunneling attempts" $= 2x_1/v$

+ The transmission coeff. is given by the integral

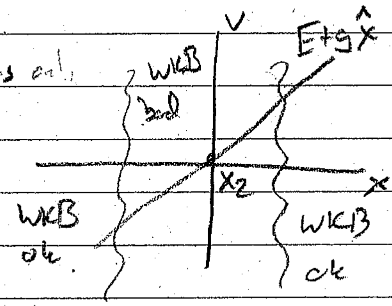
$$\int_{x_1}^{x_2} dx \sqrt{2m\left(\frac{2Ze^2}{4\pi\epsilon_0 x} - E\right)} \approx \sqrt{2mE}\left(\frac{\pi}{2} x_2 - 2\sqrt{x_1 x_2}\right)$$

where $E = \frac{1}{4\pi\epsilon_0} \frac{2Ze^2}{x_2}$

+ Folding constants together, $T = \exp\left[-a/\sqrt{E} + b\right]$
and the decay rate is $\Gamma = T/(2x_1/v)$

Deriving Connection Formulas

- The WKB approximation breaks down near the classical turning points
  - The reason is $p(x) \to 0$ there
    + The validity of the approximation is $\left|\frac{d\lambda}{dx}\right| = +2\pi\hbar\frac{|p'|}{p^2} \ll 1$
      which is badly wrong when $p = 0$
    + The WKB wavefunctions $\propto 1/\sqrt{p(x)}$ $\left(\alpha \propto 1/\sqrt{|p(x)|}\right)$
      blow up at the turning points
- Matching Across
  - But close to turning points, we can Taylor expand the potential
    + Look near an upward sloping turning point
      $V(x) \simeq V(x_2) + V'(x_2)(x - x_2) + \cdots$
      $\equiv E + g(x - x_2)$ ← keep linear terms only
      and define $\hat{x} = x - x_2$



    + We want a region where both the linear + WKB approximations are valid
    + In the region where both approximations work,
      $p(x) = \sqrt{2mg|\hat{x}|}$, $\rho(x) = \sqrt{2mg\hat{x}}$, so WKB integrals are
      $$\int_x^{x_2} dx'\, p(x') = \frac{2}{3}\sqrt{2mg}\,|\hat{x}|^{3/2}, \quad \int_{x_2}^{x} dx'\, \rho(x') = \frac{2}{3}\sqrt{2mg}\,\hat{x}^{3/2}$$

  - But the Schr. eqn. with linear potential is solved by Airy functions A_i + B_i

$$\psi(x) = a\, A_i\left[\left(\frac{2mg}{\hbar^2}\right)^{1/3}\hat{x}\right] + b\, B_i\left[\left(\frac{2mg}{\hbar^2}\right)^{1/3}\hat{x}\right]$$

+ "Far" left where $z \equiv \left(\frac{2mg}{\hbar^2}\right)^{1/3} \hat{x} \ll -1$,

$$Ai \approx \frac{1}{\sqrt{\pi}|z|^{1/4}} \sin\left(\frac{2}{3}|z|^{3/2} + \frac{\pi}{4}\right), \quad Bi = \frac{1}{\sqrt{\pi}|z|^{1/4}} \cos\left(\frac{2}{3}|z|^{3/2} + \frac{\pi}{4}\right)$$

(cos shift by $\pi/2$)

+ To the right $z \gg 1$, these look like exponential WKB wavefunctions

+ Matching coefficients gives connection formulas

- Caution:
  - There must be a region where both the WKB & linear approximations are both valid.
  - And the Airy function arguments must become large in this region
  - These aren't always true, esp. the 2nd one for the radical eqn. in 3D