The Semiclassical or WKB Approximation

WKB = (Jeffreys) Wentzel - Kramers - Brillouin

- The Approximation Itself
  - Consider a particle of energy E in potential $V(x)$. What happens in classical mechanics?
    - The particle moves around in a way that respects energy conservation
      $$E = \text{constant} = p^2/2m + V(x)$$
    - On a given path, the momentum p at a point x obeys
      $$p(x) = \sqrt{2m(E - V(x))}$$
  - We want to import this into a quantum wavefunction
    - A free particle of momentum p has wavefunction $\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$
      Suggests approximating wavefunction $\psi \propto e^{i\int_{x_0}^{x} p(x')dx'/\hbar}$
    - When is this reasonable? + Free particles have constant potential and constant wavelength $\lambda = 2\pi\hbar/p$.
      + Approximation works when $|d\lambda/dx| \ll 1 \Rightarrow \left|\frac{dp}{dx}\right| \ll \frac{1}{\lambda}|p|$
      Meaning that the change in momentum over 1 wavelength is small compared to momentum
    - So think of wave function as sinusoidal with slow changes in amplitude and wavelength
  - Schrödinger Equation + Derivation (1D for now)
    - It is possible to make a rigorous expansion in the small parameter $\hbar|p'/p^2|$ ← hence "semiclassical."
      We'll take more direct approach.
    - Define
      $$\psi(x) = A(x)\, e^{i\phi(x)}, \quad A, \phi \text{ real},$$
      + for stationary state with $E > V(x)$

+ Schrödinger equation becomes

$$A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2 = -\frac{p^2}{\hbar^2} A$$

+ This is exact so far. Gives 2 real equations.

+ The imaginary part is

$$(A^2\phi')' = 0 \implies A(x) = C/\sqrt{\phi'(x)}$$

- The approximation is in the real part
  + $\phi \approx \int^x p\,dx'/\hbar$ is our guess, so $A \propto 1/\sqrt{p}$, $A' \propto P'/p\, A$,

    $$A'' \approx \pm \frac{p''}{p} A + \pm \frac{(p')^2}{p^2} A.$$ Looks small semiclassically.

  + So we have $A'' - A(\phi')^2 = -p^2/\hbar^2 A$

    Approximately $(\phi')^2 = p^2/\hbar \implies \phi(x) = \pm 1/\hbar \int dx\, p(x)$

  + Should really be a definite integral, but absorb any constants into the normalization constant C

- The total solution: $p(x) \equiv \sqrt{(E - V(x))2m}$
  + $$\psi(x) = \frac{1}{\sqrt{p(x)}}\left[C_1 e^{i\int p\,dx/\hbar} + C_2 e^{-i\int p\,dx/\hbar}\right], \quad E > V(x)$$

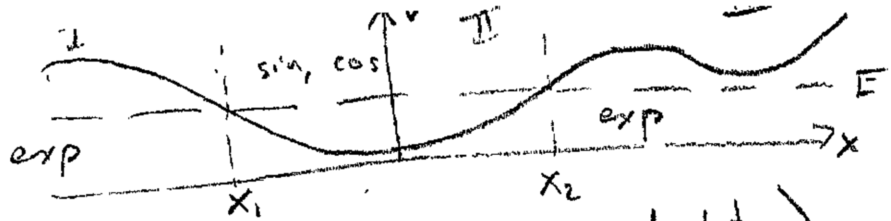
  or

  + $$\psi(x) = \frac{1}{\sqrt{p(x)}}\left[C_3 \sin\left(\int p\,dx/\hbar\right) + C_4 \cos\left(\int p\,dx/\hbar\right)\right] \quad E > V(x)$$

  + If $E < V(x)$, the solution is the same but $p(x)$ is imaginary. Define $\rho(x) = -ip(x) = \sqrt{(V(x) - E)2m}$. Then

    $$\psi(x) = \frac{1}{\sqrt{\rho(x)}}\left[D_1 \exp\left(\int \rho\,dx/\hbar\right) + D_2 \exp\left(-\int \rho\,dx/\hbar\right)\right], \quad E < V(x)$$

  + Use the appropriate formula in different regions



- Connection Formulas (to be derived later)
  + Switch from exponential to trig at <u>classical</u> <u>turning points</u> x_1 + x_2, where $E = V(x)$. Need to relate coefficients to satisfy b.c., etc
  + At downward sloping turning points

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

  + Or at upward sloping ones

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

- Applications
  - Bound States
    - Consider energy E and potential as above
      + To left of x_1, we have

$$\psi_I = A_1/\sqrt{p}\; e^{+\int_x^{x_1} dx\, p/\hbar}$$

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

      + To right of x_2, should die off

$$\psi_{III} = A_2/\sqrt{p}\; e^{-\int dx\, p/\hbar} \Longrightarrow \psi_{II} = \frac{2A_2}{\sqrt{p}} \cos\left[\left(\int_x^{x_2} dx'\, p/\hbar\right) - \pi/4\right]$$

    - We must have 2 forms of ψ_{II} match.
      + Note

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

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

+ Now note that changing $+\pi/4$ to $-\pi/4$ swaps $\sin \longleftrightarrow \cos$ (with signs). To match, we need

$$\sin\left(\int_{x_1}^{x_2} dx'\, p/\hbar\right) = \pm 1\,, \quad \cos\left(\int_{x_1}^{x_2} dx'\, p/\hbar\right) = 0$$

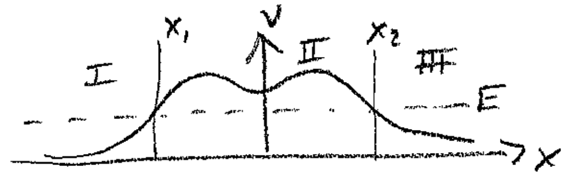
+ That leads to a <u>quantization</u> <u>condition</u> on energy

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

A lot like Bohr-Sommerfeld condition for hydrogen

- It is not hard to generalize this to a case where $V \to \infty$ at x_1 or x_2. (See HW.)

- Tunneling
  - Now we have a barrier



+ For scattering, our b. c. is

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

+ On the left

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

- You can work out transmission/reflection coefficients by working out connection formulas for complex exponentials.
  We'll make an approximation

+ Inside Region II,

$$\psi_{II} = \frac{E}{\sqrt{\rho}} \exp\left[\int_{x_1}^{x} dx'\, \rho/\hbar\right] + \frac{F}{\sqrt{\rho}} \exp\left[-\int_{x_1}^{x} dx'\, \rho/\hbar\right]$$

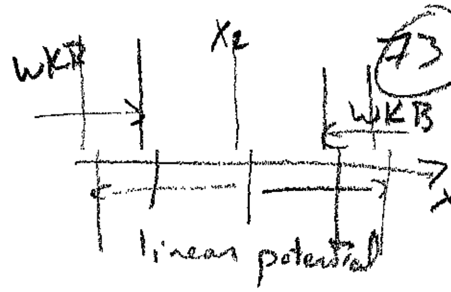
+ Mostly, the wavefunction should die off.
Therefore, assume $|B| \approx |A|$, $|C| \approx |A| \exp\left[-\int_{x_1}^{x_2} dx' \rho/\hbar\right]$
+ Just gives transmission coefficient
$$T \approx \exp\left[-2\int_{x_1}^{x_2} dx' \rho/\hbar\right]$$ See HW for more

- Example: Decay of nucleus

+ α particle bounces around in binding energy box w/ positive E.
+ Each time it hits edge of box, it has a chance to tunnel
That's once every $2x_1/v$ for speed $v = \sqrt{\frac{2}{m}(E+V_0)}$
+ The transmission coefficient is given by
$$\frac{1}{\hbar}\int_{x_1}^{x_2} dx \sqrt{\left(\frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{x} - E\right)2m} \approx \frac{\sqrt{2mE}}{\hbar}\left(\frac{\pi}{2}x_2 - 2\sqrt{x_1 x_2}\right)$$
+ Note that x_2 satisfies $E = \frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{x_2}$
So $$\Gamma_{decay} \simeq \frac{v}{2x_1}\exp\left[-\frac{a}{\sqrt{E}} + b\right]$$ works pretty well

- Deriving the Connection Formulas
  - Near the turning points, WKB is invalid as $p \to 0$.
  (Can't have $\hbar(p'/p^2) \ll 1$ then).
    - In fact, the $1/\sqrt{p}$ factors make WKB wavefunctions blow up.
    - Instead, approximate potentials by linear functions
    (for x_2) $$V(x) \approx E + g(x - x_2)$$
  + In this region
  $$\psi(x) = E A_i\left[\left(\frac{2mg}{\hbar^2}\right)^{1/3}(x-x_2)\right] + F B_i\left[\left(\frac{2mg}{\hbar^2}\right)^{1/3}(x-x_2)\right]$$
  for Airy functions A_i, B_i

- We have to match the Airy functions to WKB wave functions, where both are valid



  + Use Asymptotic expansions for Ai and Bi in terms of trig functions on left
  + The WKB integrals $\int_x^{x_L} dx' \, p/\hbar$ allow matching up
  + Similarly with real exponentials on the right
  + See textbooks for algebraic details
- A caution:
  + Must have a region where WKB approximation + linear potential approximation are both valid (almost always true)
  + Also, argument of Airy functions must become large in this region. (sometimes tricky for radial eqn in 3D)