Semiclassical Quantum Mechanics

Given a Hamiltonian $H = \frac{p^2}{2m} + V(x)$, the semiclassical ansatz for the wavefn $\psi(x,t)$ takes the form $\psi = e^{i\theta(x,t)/\hbar}$. The reason for this form will become apparent below.

Substituting this ansatz into the time-dependent Schrodinger's eqn, one finds,

$$\frac{\partial \theta}{\partial t} + \frac{1}{2m}\left(\frac{\partial \theta}{\partial x}\right)^2 + V(x) = \frac{-\hbar}{i}\frac{1}{2m}\frac{\partial^2 \theta}{\partial x^2} \qquad (1)$$

Contrast this with the Hamilton Jacobi eqn for the <u>classical</u> action S_{cl}:

$$\frac{\partial S_{cl}}{\partial t} + \frac{1}{2m}\left(\frac{\partial S_{cl}}{\partial x}\right)^2 + V(x) = 0 \qquad (2)$$

Comparing to (1) above, θ resembles S_{cl} if $\frac{\partial^2 \theta}{\partial x^2}$ term on the RHS of (1) can be neglected.

So if $\theta = S_{cl}$ + small corrections, then one requires that $\left(\frac{\partial S_{cl}}{\partial x}\right)^2 \gg \hbar\left|\frac{\partial^2 S_{cl}}{\partial x^2}\right|$

$$\Rightarrow \quad p^2(x) \gg \hbar\,|\partial p/\partial x|$$

or, $\left|\frac{d\lambda}{dx}\right| \ll 1$ where $\lambda = \frac{h}{p}$ is the debroglie wavelength.

This is semiclassical regime of quantum mechanics.

For a quantum system confined in a length scale L, $p \simeq \frac{nh}{L} \Rightarrow p^2 \simeq \frac{n^2h^2}{L^2}$

where n is the eigenenergy index ($n=1$ corresponds to the ground state). Similarly, $\frac{dp}{dx} \simeq \frac{nh}{L^2}$

Therefore if $p^2(x) \gg \hbar\left|\frac{dp}{dx}\right|$

$$\Rightarrow \frac{n^2h^2}{L^2} \gg \frac{nh^2}{L^2}$$

$$\Rightarrow \boxed{n \gg 1}.$$

A different way to state the same result is to write the time-independent Schrodinger's eqn for eleven n as.

$$\left(\frac{\hbar^2}{2mL^2}\right)\Big/E_n \quad \frac{d^2\psi_n}{d\tilde{x}^2} = \left(\frac{V(x)-E_n}{E_n}\right)\psi_n$$

where $\tilde{x} = x/L$. Since $E_n \gg \hbar^2/2mL^2$ when $n \gg 1 \Rightarrow$ This equation has the form

$\epsilon^2\, d^2y/dx^2 = Q(x)\,y$, the which is subject of WKB analysis.

Correspondence principle (to be derived using WKB soon)

$$\int_A^B p(x)\, dx = \hbar\left(n+\frac{1}{2}\right)\pi$$

$$\int_A^B \sqrt{2m\left(E_n - V(x)\right)} = \hbar\left(n+\frac{1}{2}\right)\pi$$

differentiating w.r.t. n:

$$\int_A^B \sqrt{2m}\, \frac{dx}{2\sqrt{E_n - V(x)}}\, \frac{dE_n}{dn} = \hbar\pi$$

$$\Rightarrow \frac{dE_n}{dn} \int_A^B \underbrace{\frac{dx}{\left[p(x)/m\right]}}_{\text{velocity}} = \pi\hbar$$

$$\Rightarrow \frac{dE_n}{dn} \underbrace{\frac{\pi}{\omega}}_{\text{Half-period time}} = \pi\hbar$$

$$\Rightarrow \boxed{\frac{dE_n}{dn} = \hbar\omega}$$

Example :

$$V(x) = |x|$$

$$\int_{-E}^{E} \sqrt{[E-|x|]} \, dx \sim \left(n+\frac{1}{2}\right)\pi$$

$$\Rightarrow \quad \frac{4}{3} E^{3/2} \sim \left(n+\frac{1}{2}\right)\pi$$

$$\Rightarrow \quad E \sim \left[\frac{3\pi}{4}\left(n+\frac{1}{2}\right)\right]^{2/3}$$

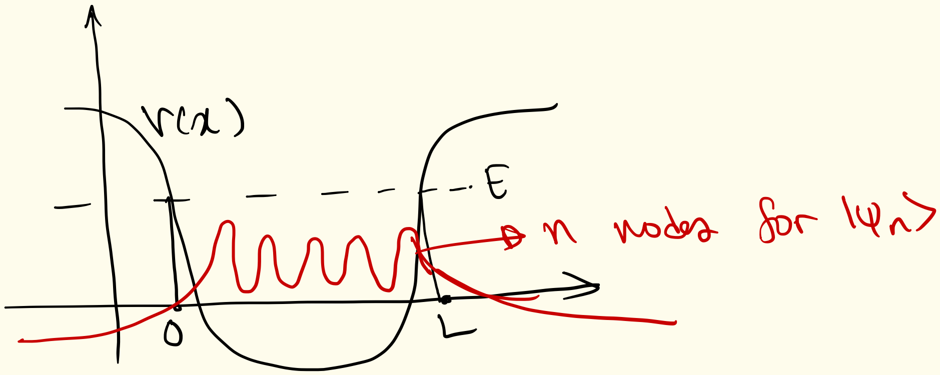
Heuristic :

$$E \sim \frac{n^2}{L^2} + L$$

$$\Rightarrow \quad L \sim n^{2/3}$$

and $\boxed{E \sim n^{2/3}}$

More Examples of Semiclassical Quantization.



Approximate way to find eigenenergies:

$$\lambda \sim \frac{1}{p} \sim \frac{1}{\sqrt{2(E-V)}} \sim \frac{1}{\sqrt{2E}}$$

semiclassical

$E \gg V$

$$L(E_n) = \frac{n\lambda}{2}$$

Ex1: Harmonic oscillator

$$\frac{1}{2}\omega^2 L_n^2 \sim E_n \Rightarrow L_n \sim \sqrt{\frac{E_n}{\omega^2}}$$

$$h(E_n) \sim n\lambda \sim \frac{n}{\sqrt{E_n}} \sim \sqrt{\frac{E_n}{\omega^2}}$$

$$\Rightarrow \quad E_n \sim n\omega$$

$$\boxed{E_n = c_1 n \omega}$$

correspondence principle:

$$\frac{dE_n}{dn} = \text{classical frequency}$$

$$\Rightarrow c_1 = 1$$

Ex2: Hydrogen atom

Consider $l = 0$, arbitrary n.

$$E \sim \frac{n^2}{L^2} - \frac{Z}{h}$$

$$\Rightarrow \quad h \sim \frac{n^2}{Z}$$

$$\Rightarrow \boxed{E_n \sim -\frac{Z^2}{n^2}}$$

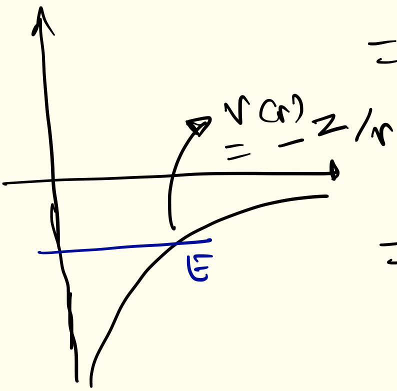
write $E = -\dfrac{cZ^2}{n^2}$

To find c, again use correspondence principle:

$$\frac{dE_n}{dn} = \omega_{classical} = \frac{2\pi}{T}$$

$$T_{classical} = 2\int \frac{dr}{v(r)}$$

$$= 2\int_0^{-Z/E_n} \frac{dr\,\sqrt{m}}{\sqrt{2\left(E_n + \frac{Z}{r}\right)}}$$



$$= \frac{2\pi Z}{(-2E_n)^{3/2}}$$

$$\Rightarrow \boxed{E_n = -\frac{Z^2}{2n^2}}$$

$v = \dfrac{p}{m}$ $\qquad p^2/2m = E - V$

WKB Method

(Bender and Orszag, Gottfried, Migdal).

The Schrodinger's eqn is:

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

We want to study this equation semiclassically, i.e. in the limit $\hbar \to 0$. So let's study differential eqns. of the form

$$\varepsilon^2 y'' = Q(x)\, y \quad \text{in the limit } \varepsilon \to 0.$$

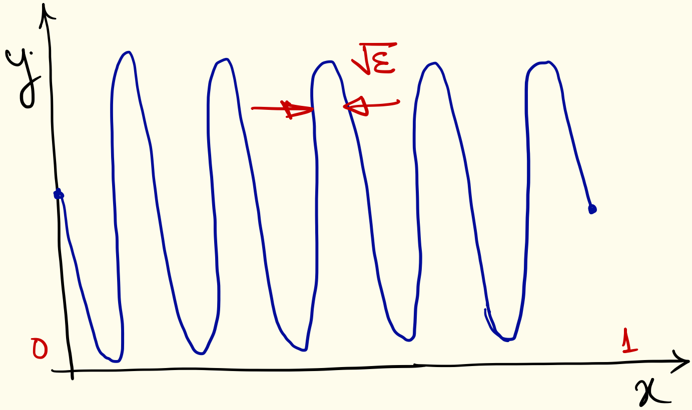
"Small highest derivative"

an example: $\varepsilon y'' + y = 0$, $y(0) = 0$, $y(1) = 1$

Soln: $$y = \frac{\sin(x/\sqrt{\varepsilon})}{\sin(1/\sqrt{\varepsilon})}$$

with $\varepsilon \neq n^2\pi^2$

Note that as $\varepsilon \to 0$, the soln. becomes wildly oscillating for the whole region $0 \leq x \leq 1$. This is the hallmark of WKB: there exist regions of $O(1)$ size where the fn oscillates wildly.



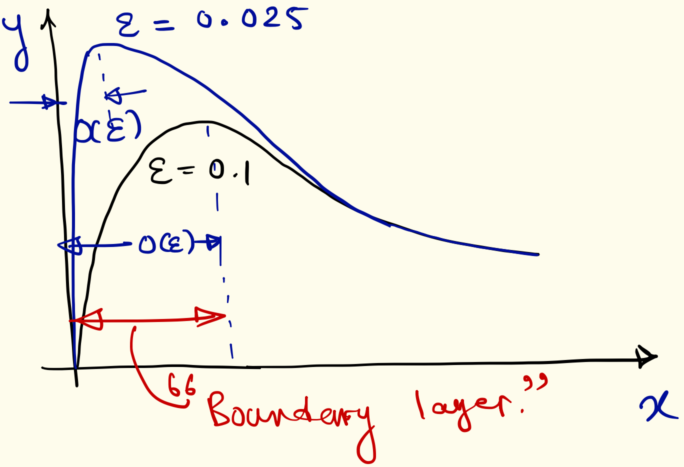
Contrast this with the following eqn:

$$\varepsilon y'' + (1+\varepsilon) y' + y = 0$$

$$y(0) = 0, \quad y(1) = 1.$$

Soln:
$$y = \frac{e^{-x} - e^{-x/\varepsilon}}{e^{-1} - e^{-1/\varepsilon}}$$

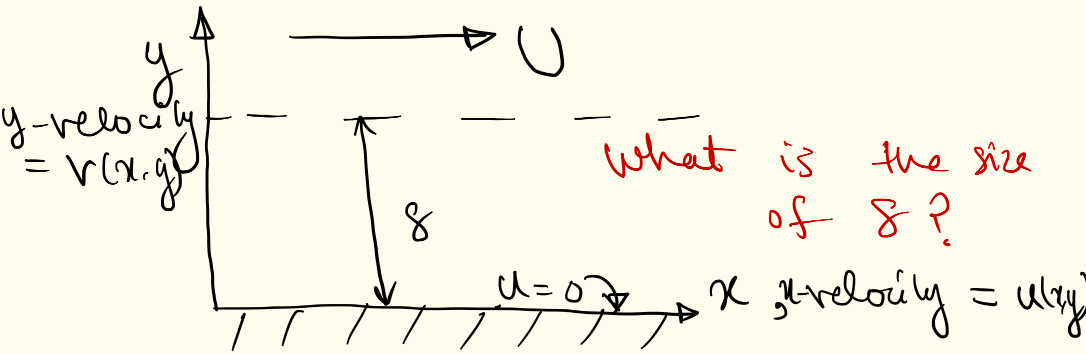
For $1 \gg x \gg \varepsilon$, the soln. is just $\dfrac{e^{-x}}{e^{-1}}$.
The soln. is rapidly varying only for $0 < x \lesssim \varepsilon$.



Thus, here one can solve in the region $x \gtrsim \varepsilon$ without encountering any singular behavior. The region $x \lesssim \varepsilon$ is called boundary layer, inspired by its applications in fluid dynamics.

A short detour:

Consider the fluid flow



Boundary layer emerges in large Reynolds number limit.

$$\vec{\nabla}\cdot\vec{v} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$ Continuity for incompressible fluid.

$$\frac{\partial u}{\partial x} \sim \frac{U}{L} \Rightarrow \frac{V}{\delta} \sim \frac{U}{L}$$

$$\Rightarrow V = \frac{U\delta}{L}$$

$$\vec{v}\cdot\vec{\nabla}\vec{v} = \nu\,\vec{\nabla}\cdot(\vec{\nabla}v)$$ (Newton's law)

$$\Rightarrow \underbrace{u\frac{\partial u}{\partial x}}_{\sim \frac{U^2}{L}} + \underbrace{v\frac{\partial u}{\partial y}}_{\frac{U\delta}{L}\frac{U}{\delta} \sim \frac{U^2}{L}} = \nu\left(\underbrace{\frac{\partial^2 u}{\partial x^2}}_{\frac{\nu U}{L^2}} + \underbrace{\frac{\partial^2 u}{\partial y^2}}_{\frac{\nu U}{\delta^2}}\right)$$

Thus, $\frac{\partial^2 u}{\partial y^2} \gg \frac{\partial^2 u}{\partial x^2}$. By matching dominance

$$\frac{\nu U}{\delta^2} \sim \frac{U^2}{L} \Rightarrow \delta = \sqrt{\frac{\nu L}{U}}$$

$\Rightarrow$ Fractional size of the boundary layer $= \dfrac{\delta}{L} \sim \sqrt{\dfrac{\nu}{UL}} \sim \dfrac{1}{\sqrt{\text{Reynolds number}}}$.

Back to WKB:

WKB like equations have strong oscillations, thus, natural to try soln. of the form

$$y(x) \sim e^{S(x)/\delta} \quad \text{where}$$

$\delta \to 0$ as $\varepsilon \to 0$.

Consider Schrodinger's eqn:

$$\varepsilon^2 y'' = Q(x)\, y$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (V - E)\,\psi$$

$$\varepsilon^2 = \frac{\hbar^2}{2m}$$

$$Q(x) = V(x) - E$$

writing $y(x) = e^{S(x)/\delta}$

and perform a taylor series expansion for $S(x)$:

$$S(x) = \sum_{n=0}^{\infty} \delta^n S_n(x).$$

i.e. $$y(x) = \exp\left(\sum_{n=0}^{\infty} \delta^{n-1} S_n(x) \right)$$

$$\frac{dy}{dx} = \left[\sum_{n=0}^{\infty} \delta^{n-1} S_n'(x) \right] \exp\left(\sum_{n=0}^{\infty} \delta^{n-1} S_n(x)\right)$$

$$= \frac{1}{\delta} \left[\sum_{n=0}^{\infty} \delta^n S_n'(x) \right] y(x)$$

$$\frac{d^2y}{dx^2} = \frac{1}{\delta^2} \left\{ \sum_{n=0}^{\infty} \left[\delta^n S_n'(x) \right] \right\}^2 y(x)$$

$$+ \frac{1}{\delta} \sum_{n=0}^{\infty} \delta^n S_n''(x) \; y(x)$$

Matching terms on both sides of

$$\varepsilon^2 \frac{d^2y}{dx^2} = Q(x)\, y$$

$$\Rightarrow \quad \frac{\varepsilon^2}{\delta^2} (S_0')^2 + \frac{2\varepsilon^2}{\delta} S_0' S_1' + \frac{\varepsilon^2}{\delta} S_0''$$

$$+ \varepsilon^2 (S_1')^2 + \varepsilon^2 S_1'' + \dots = Q(x)$$

Matching terms order by order in $\frac{1}{\delta}$:

$$\frac{\varepsilon^2}{\delta^2} S_0'^2 = Q(x)$$

$$\frac{\varepsilon^2}{\delta}\left[2 S_0' S_1' + S_0''\right] = 0$$

$$2 S_0' S_n' + S_{n-1}'' + \sum_{j=1}^{n-1} S_j' S_{n-j}' = 0$$
$$(n \geq 2)$$

We can set $\delta = \varepsilon$ so that S_0 is independent of ε.

$$\Rightarrow \quad S_0(x) = \pm \int_0^x \sqrt{Q(x')}\, dx' + \text{const.}$$

$$2 S_0' S_1' = -S_0''$$

$$\Rightarrow \quad S_1' = -\frac{S_0''}{2 S_0'}$$

$$\Rightarrow \quad dS_1 = -\frac{1}{2} d\left[\log(S_0')\right]$$

$$= -\frac{1}{4} \log\left[Q(x)\right]$$

$$\Rightarrow \quad S_1(x) = -\frac{1}{4} \log\left[Q(x)\right]$$

Substituting these back into the schrodinger's eqn:

$$y(x) \sim c_1 \exp \frac{1}{\epsilon}\left[\int_a^x \sqrt{Q(x')}\, dx' - \frac{\epsilon}{4}\log Q(x) + \ldots\right]$$

$$+ c_2 \exp \frac{1}{\epsilon}\left[-\int_a^x \sqrt{Q(x')}\, dx' - \frac{\epsilon}{4}\log Q(x) + \ldots\right]$$

$$\sim \frac{c_1}{[Q(x)]^{1/4}} \exp\left[\frac{1}{\epsilon}\int_a^x \sqrt{Q(x')}\, dx'\right]$$

$$+ \frac{c_2}{[Q(x)]^{1/4}} \exp\left[-\frac{1}{\epsilon}\int_a^x \sqrt{Q(x')}\, dx'\right]$$

(See Bender. Orszag for the explicit form of higher-order terms.)