Formal Derivation of the WKB Formula

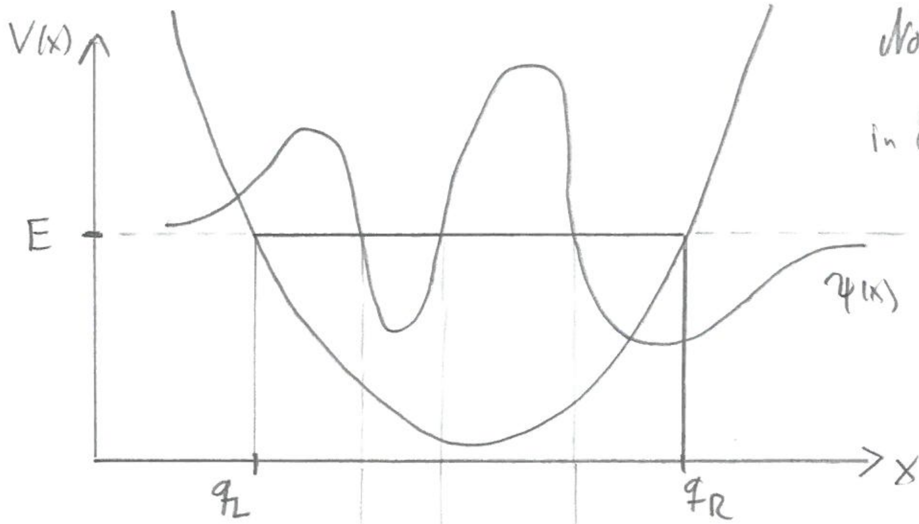
Let V be a single-well potential and

$\psi(x) = \psi_n(x)$ eigenfunction of the Schrödinger eq. with eigenvalue $E = E_n$

$$\left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x)\right)\psi(x) = E\,\psi(x) \quad , \qquad n = 0,1,2,3, \quad E_n < E_{n+1}$$

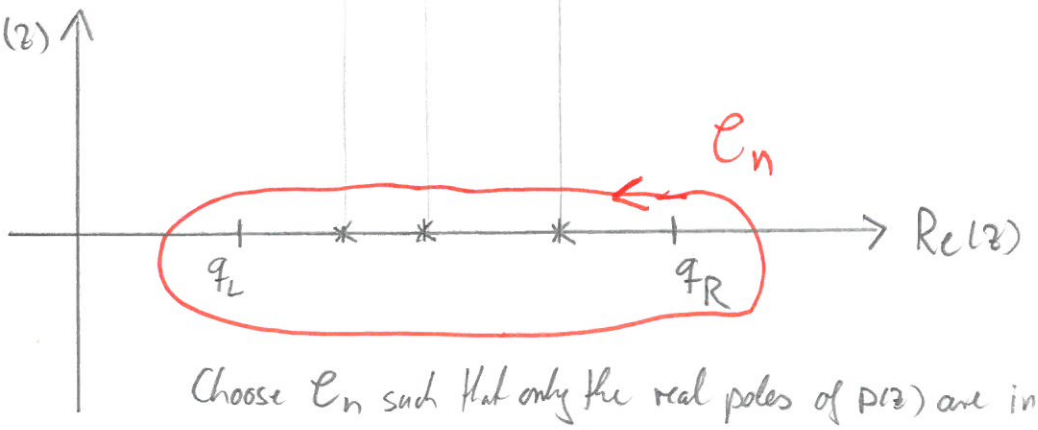
$\leadsto$ $\psi(x)$ has n simple zeros at x_i

__Def.:__ $\quad p(x) := \frac{\hbar}{i}\frac{\psi'(x)}{\psi(x)}$ has n simple poles



Note $\frac{\psi''(x)}{\psi(x)} > 0$ in classical forbidden region

Pole structure of $p(z)$ in $\mathbb{C}$



Choose $\mathcal{C}_n$ such that only the real poles of $p(z)$ are included

Consider: $\quad \frac{1}{2\pi i}\oint_{\mathcal{C}_n} dz\, p(z) = \frac{\hbar}{i}\sum_{*\,\text{in}\,\mathcal{C}_n} \operatorname{Res}\frac{\psi'(x)}{\psi(x)} = \frac{\hbar}{i}n$ $\quad$ each residuum contributes 1 !

as $\psi(x) \approx \psi(x_i) + \psi'(x_i)(x - x_i)$

Hence: $$\boxed{\oint_{\mathcal{C}_n} dz\, p(z) = 2\pi\hbar n}$$ "Quantisation Condition"

follows strictly from condition $\psi \in L^2(\mathbb{R})$

$\nearrow$ Dunham, Phys. Rev. <u>41</u> (1932) 713

Note: $\psi(x) = N \exp\left\{ \frac{i}{\hbar} \int dx\, p(x) \right\} \rightsquigarrow \psi'(x) = \frac{i}{\hbar} p(x)\psi(x)$

$$\psi''(x) = \frac{i}{\hbar}\left(p'(x)\psi(x) + \frac{i}{\hbar} p^2(x)\psi(x) \right)$$

in Schrödinger eq.:

$$-\frac{\hbar^2}{2m}\psi'' + V\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\left(-\frac{1}{\hbar^2} p^2 \cancel{\psi} + \frac{i}{\hbar} p' \cancel{\psi} \right) = E\cancel{\psi} - V\cancel{\psi}$$

$$p^2 - i\hbar p' = 2m(E - V)$$

Hence
$$\boxed{-i\hbar\, \partial_x p(x) + p^2(x) = 2m(E - V(x))} \qquad (*)$$

Remarks:
- $(*)$ is generalized Riccati equation
- R.H.S is square of classical momentum $P_0(x) := \sqrt{2m(E - V(x))}$
- Solution in general not possible
- $E = E_n$ in general depends on $\hbar$

Aim: Find quasi-classical approximation (perturbation in $\hbar$)

Ansatz: $$p(x) = \sum_{k=0}^{\infty} \hbar^k p_k(x)$$

$$\rightsquigarrow \quad p^2(x) = \sum_{k,l} \hbar^k \hbar^l p_k(x) p_l(x) = \sum_{m=0}^{\infty} \hbar^m \sum_{k=0}^{m} P_k(x) P_{m-k}(x)$$

$$= P_0^2 + 2\hbar P_0 P_1 + \hbar^2 (2P_0 P_2 + P_1^2) + \cdots$$

$$i\hbar p'(x) = i \sum_{m=1}^{\infty} \hbar^m P'_{m-1} = i\hbar P_0' + i\hbar^2 P_1' + \cdots$$

Into $(*)$ and compare coefficients of same power in $\hbar$

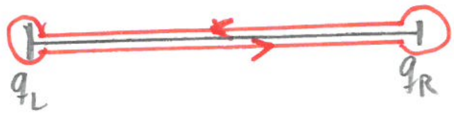
$$\boxed{\begin{aligned} P_0^2(x) &= 2m(E - V(x)) \\ \sum_{k=0}^{m} P_k(x) P_{m-k}(x) &= i P'_{m-1}(x) \end{aligned}} \qquad (**)$$

Note $P_0(x)$ cl. momentum

0. Approximation:

$p(x) = p_0(x) = \sqrt{2m(E-V(x))}$

has no poles but cut along q_L and q_R line



Quantisation condition: $\oint dz\, p(z) = 2 \int_{q_L}^{q_R} dx\, p_0(x) = 2\pi\hbar n$

$$\boxed{\int_{q_L}^{q_R} dx \sqrt{2m(E-V(x))} = \pi \hbar n}$$

Bohr-Sommerfeld-Wilson ?

1. Approximation:

$p(x) = p_0(x) + \hbar p_1(x)$

with $i p_0'(x) = 2 p_0(x) p_1(x) \Rightarrow p_1(x) = \frac{i}{2} \frac{p_0'(x)}{p_0(x)}$

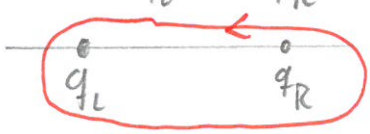
Quantisation condition: $\oint dz\, p_0(z) + \hbar \underbrace{\oint dz\, p_1(z)}_{=:I} = 2\pi\hbar n$

$$I = \oint_{\mathcal{C}_n} dz\, p_1(z) = \frac{i}{2} \oint_{\mathcal{C}_n} dz \frac{p_0'(z)}{p_0(z)} =$$

$\frac{p_0'}{p_0} = \frac{1}{2p_0^2}(-2m V'(x)) = -\frac{1}{2} \frac{V'(x)}{E-V(x)}$

$$= -\frac{i}{4} \oint_{\mathcal{C}_n} dz \frac{V'(z)}{E-V(z)}$$

Poles at q_L and q_R



$\mathcal{C}_n$

$$= -\frac{i}{4} 2\pi i \sum_{x_i \in \{q_L, q_R\}} \operatorname{Res}_{x=x_i} \frac{V'(x)}{E-V(x)}$$

Note: $V(x) \approx V(x_i) + V'(x_i)(x - x_i)$

$\rightsquigarrow$ each pole contributes -1

$$= \frac{\pi}{2}(-1-1) = -\pi$$

Hence

$$\boxed{\int_{q_L}^{q_R} dx \sqrt{2m(E-V(x))} = \pi\hbar\left(n+\frac{1}{2}\right)}$$

Wenzel-Kramers-Brillouin

WKB formula

2. Approximation: $P(x) = P_0(x) + \hbar P_1(x) + \hbar^2 P_2(x)$

with $2P_0P_2 + P_1^2 = iP_1' \rightsquigarrow P_2 = \frac{m}{4}\frac{V''}{P_0^3} + \frac{5}{8}m^2\frac{V'^2}{P_0^5}$

$$P_2(x) = \frac{1}{8\sqrt{2m}}\left(\frac{V''(x)}{(E-V(x))^{3/2}} + \frac{5}{4}\frac{V'(x)^2}{(E-V(x))^{5/2}}\right)$$

Note $\frac{d}{dx}\frac{V'}{(E-V)^{3/2}} = \frac{V''}{(E-V)^{3/2}} + \frac{3}{2}\frac{V'^2}{(E-V)^{5/2}}$

$$\rightsquigarrow \frac{5}{4}\frac{V'}{(E-V)^{5/2}} = \frac{5}{6}\frac{d}{dx}\left(\frac{V'}{(E-V)^{3/2}}\right) - \frac{5}{6}\frac{V''}{(E-V)^{3/2}}$$

Hence $P_2(x) = \frac{1}{48\sqrt{2m}}\frac{V''}{(E-V)^{3/2}} + \frac{d}{dx}(\dots)$

no contribution as $\mathcal{C}_n$ is closed loop!

$$\rightsquigarrow \oint_{\mathcal{C}_n} dz\, P_2(z) = \frac{1}{48\sqrt{2m}}\oint_{\mathcal{C}_n} dz\, \frac{V''(z)}{(E-V(z))^{3/2}}$$

$$= \frac{1}{24\sqrt{2m}}\frac{d}{dE}\oint_{\mathcal{C}_n} dz\, \frac{V''(z)}{\sqrt{E-V(z)}}$$

same cut as for 0. approx.

Hence:

$$\boxed{\int_{q_L}^{q_R} dx\, \sqrt{2m(E-V(x))} - \frac{\hbar^2}{24\sqrt{2m}}\frac{d}{dE}\int_{q_L}^{q_R} dx\, \frac{V''(x)}{\sqrt{E-V(x)}} = \pi\hbar\left(n+\tfrac{1}{2}\right)}$$

Krieger-Lewis-Rosenzweig (1967)

have also $\hbar^4$-Order!