· Método variacional.

Ref.: Sec. 18.I, Messiah

considerar, e.g. o problema de autovalores p/ um sistema 1-D

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \qquad (85.1)$$

hipótese: $\exists$ funcional $Q[\psi]$ tal que

$$\delta Q[\psi] = 0 \;\leftrightarrow\; \text{Eq. } (85.1). \qquad (85.2)$$

i.e., a condição $Q[\psi]$ estacionário é equivalente ao problema de autovalores (85.1)

considerar: sol. Eq. (85.1) $\psi(x) \in \tilde{F}$: espaço de funções
e $\phi(x) \in F' \subset \tilde{F}$; i.e., F': subespaço $\tilde{F}$;

↳ ideia método variacional de Ritz: determinar $\phi(x)$ tal que
$\delta Q[\phi] = 0$;
como $\phi \in F'$: subespaço soluções (85.1)
↳ solução aproximada do problema de autovalores (85.1)!

em particular, se $\phi = \phi(x, a, b, c)$; a, b, c: parâmetros contínuos;

$$Q[\phi(x, a, b, c)] = q(a, b, c) : \text{função de } a, b, c$$

e $q(a_0, b_0, c_0)$: extremo função $q(a, b, c)$

↳ $\phi_0(x, a_0, b_0, c_0)$: solução aproximada Eq. (85.1).

considerar: $\psi_0(x)$: solução exata Eq. (85.1)

$\Phi_0(x)$: " aproximada "

e $\delta\psi = \Phi_0 - \psi_0$: variação ; temos que

$$\delta Q[\psi_0] = Q[\psi_0 + \delta\psi] - Q[\psi_0] = Q[\Phi_0] - Q[\psi_0]$$

$$= \int dx \underbrace{\frac{\delta Q}{\delta\psi}}_{=0} \delta\psi(x) + \int dx\, dx' \frac{\delta^2 Q}{\delta\psi(x)\delta\psi(x')} \delta\psi(x)\delta\psi(x') + \dots,$$

$= 0$: condição $Q[\psi_0]$ estacionário

i.e. $Q[\Phi_0] - Q[\psi_0]$: 2ª ordem variação $\delta\psi$!

· método variacional p/ estados ligados.

inicial: dois resultados importantes.

(1) Teorema: seja H : hamiltoniano sistema quântico e

$$E[\psi] = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \quad \text{: valor esperado energia do sistema : funcional } \psi \qquad (86.1)$$

se ψ_0 é tal que $\delta E[\psi_0] = 0 \leftrightarrow H|\psi_0\rangle = E|\psi_0\rangle$ e $E = E[\psi_0]$

Dem.: temos que,

$$\delta E = \delta\left(\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}\right) = \frac{\delta(\langle\psi|H|\psi\rangle)}{\langle\psi|\psi\rangle} - \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle^2}\delta(\langle\psi|\psi\rangle)$$

$$\hookrightarrow \langle\psi|\psi\rangle^2 \delta E = \langle\psi|\psi\rangle\left(\langle\delta\psi|H|\psi\rangle + \langle\psi|H|\delta\psi\rangle\right)$$

$$- \underbrace{\langle\psi|H|\psi\rangle}_{E\langle\psi|\psi\rangle}\left(\langle\delta\psi|\psi\rangle + \langle\psi|\delta\psi\rangle\right)$$

$\hookrightarrow \langle\psi|\psi\rangle\,\delta E = \langle\delta\psi|H-E|\psi\rangle + \langle\psi|H-E|\delta\psi\rangle$

como $0 < \langle\psi|\psi\rangle < +\infty$, a condição $\delta E = 0$ é equivalente a

$$\langle\delta\psi|H-E|\psi\rangle + \langle\psi|H-E|\delta\psi\rangle = 0 \qquad (87.1)$$

como $\langle\psi|\psi\rangle = cte \rightarrow \langle\delta\psi|\psi\rangle + \langle\psi|\delta\psi\rangle = 0$: $|\delta\psi\rangle$ e $\langle\delta\psi|$ não são, em princípio, independentes;

entretanto, considerando $|\delta\psi\rangle$ e $\langle\delta\psi|$ independentes

~ considerar partes Re e Im separadamente -> Eq. (87.1) OK

se $\langle\delta\psi|H-E|\psi\rangle = \langle\psi|H-E|\delta\psi\rangle = 0$

$\hookrightarrow (H-E)|\psi\rangle = 0$ e $\langle\psi|(H-E) = 0$, pois $|\delta\psi\rangle$ e $\langle\delta\psi|$ são arbitrários;

como $H = H^\dagger$ e $E \in \mathbb{R}$ -> as duas condições acima são equivalentes

e $\delta E[\psi] = 0 \rightarrow H|\psi\rangle = E|\psi\rangle$ (IDA: OK)

(VOLTA): se $H|\psi\rangle = E|\psi\rangle \rightarrow E\langle\psi|\psi\rangle = \langle\psi|H|\psi\rangle$

ou $E = \dfrac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = cte \rightarrow \delta E = \delta\left(\dfrac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}\right) = 0$.

(2) Lema: se $|\psi\rangle$: estado do sistema

$$\hookrightarrow E[\psi] \geq \underbrace{E_0}_{\text{energia estado fundamental}} \qquad (87.1)$$

Dem.: considerar: $H|n,i\rangle = E_n|n,i\rangle$; H espectro discreto; $E_0 < E_1 < E_2 < \dots$

e P_n : projetor subespaço autovalor E_n.

como $\sum_n P_n = 1$ e $H = \sum_n E_n P_n$, temos que

$$H - E_0 = \sum_{n \geq 0} E_n P_n - E_0 \sum_{n \geq 0} P_n = \sum_{n \geq 1} (E_n - E_0) P_n$$

$$\hookrightarrow E[\psi] - E_0 = \frac{\langle \psi | H - E_0 | \psi \rangle}{\langle \psi | \psi \rangle} = \sum_{n \geq 1} \underbrace{(E_n - E_0)}_{\geq 0} \underbrace{\frac{\langle \psi | P_n | \psi \rangle}{\langle \psi | \psi \rangle}}_{\geq 0} \geq 0$$

· sobre o método variacional,

considerar: $H|\psi\rangle = E|\psi\rangle$ e $|\psi\rangle \in \mathcal{F}$; (88.1)

estado arbitrário $|\Phi\rangle \in \mathcal{F}' \subset \mathcal{F}$

e P: projetor subespaço $\mathcal{F}'$: $P|\Phi\rangle = |\Phi\rangle$; temos que

$$E[\Phi] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \frac{\langle \Phi | P H P | \Phi \rangle}{\langle \Phi | \Phi \rangle} \equiv \frac{\langle \Phi | H_P | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

notar: $H_P = PHP$: projeção H no subespaço $\mathcal{F}'$

Teorema (1): $\delta E[\Phi] = 0 \leftrightarrow H_P|\Phi\rangle = E|\Phi\rangle$ e $E = E[\Phi]$,

i.e., a determinação da solução aproximada $|\Phi\rangle$ é equivalente à solução do problema de autovalores (88.1) restrito ao subespaço $\mathcal{F}'$!

· notar: se $H = H_0 + V$;

$\mathcal{F}'$: subespaço autovalor não perturbado E_0^0

e $\langle \Phi | \Phi \rangle = 1$, temos que

$$E[\Phi] = \langle\Phi|PHP|\Phi\rangle = \underbrace{\langle\Phi|PH_0P|\Phi\rangle}_{E_s^0} + \langle\Phi|PVP|\Phi\rangle \; : \qquad (89.1)$$

: energia em 1ª ordem teoria de perturbação, Eq (41.1)

Ex. 1: estado fundamental átomo H.

ideia: determinar variacionalmente a função de onda do estado fundamental átomo H;

como os autoestados do hamiltoniano do sistema são " dos ops. L^2 e L_z, vamos considerar funções tentativas do tipo:

$$\Phi(\vec{r}) = \frac{1}{\sqrt{a_0^3}} \frac{1}{\rho} u(\rho) Y_\ell^m(\theta,\varphi) \qquad (89.2)$$

onde: $a_0 = \frac{\hbar^2}{me^2}$: raio de Bohr e $\rho = \frac{r}{a_0}$

Lembrar que: $E_0 = \frac{1}{2}\left(\frac{e^2}{\hbar c}\right)^2 mc^2 = \frac{me^4}{2\hbar^2} = \frac{1}{2}\frac{e^2}{a_0}$

e $-E_0$: energia estado fundamental átomo H

notar: • $\langle\Phi|\Phi\rangle = \int d^3r\, |\Phi(\vec{r})|^2 =$

$$= \frac{1}{a_0^3} \underbrace{\int r^2 dr \frac{1}{\rho^2} |u(\rho)|^2}_{a_0^3 \int d\rho\, |u(\rho)|^2} \underbrace{\int d\Omega\, Y_\ell^m(\theta,\varphi)^* Y_\ell^m(\theta,\varphi)}_{1}$$

$$\cdot \langle \Phi | H | \Phi \rangle = \int d^3r \; \Phi^*(\vec{r}) \langle \vec{r} | H | \Phi \rangle$$

como (veja Eq. (12.4), Merzbacher)

$$\langle \vec{r} | H | \Phi \rangle = \frac{-\hbar^2}{2mr^2} \partial_r \left(r^2 \partial_r \Phi \right) + \frac{L^2}{2mr^2} \Phi - \frac{e^2}{r} \Phi . \qquad (90.1)$$

verifica-se que o funcional de energia assume a forma (exercício):

$$E[\Phi] = E[u] = -E_0 \int_0^\infty d\rho \; u^* \left(\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2} + \frac{2}{\rho} \right) u \Big/ \int_0^\infty d\rho \, |u|^2$$

$$(90.2)$$

considerar: estados-s ($\ell = m = 0$) e as seguintes funções radiais:

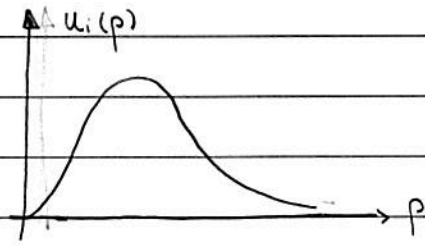
$$u_1(\rho, b) = \rho e^{-b\rho} ; \qquad u_2(\rho, b) = \frac{\rho}{b^2 + \rho^2} ; \qquad u_3(\rho) = \rho^2 e^{-b\rho} \qquad (90.3)$$

notar:

(i) $u_i(\rho, b)$ depende apenas parâmetro b;

↳ Eq. (90.2) : $E[\Phi] \equiv f(b) \to \delta E = 0 \sim \frac{df}{db} = 0$

(ii) qualitativamente:



: ou p/ estado fundamental: $u_i(\rho)$ não possui raízes p/ $\rho > 0$!

verifica-se que (p/ detalhes, veja tabela 18.1, Messiah)

	u_1	u_2	u_3	
b_{MIN}	1	$\pi/4$	$3/2$	
E_{VAR}	$-E_0$	$-0.81E_0$	$-0.75E_0$	$\geq -E_0$: OK Eq. (87.1)
ϵ	0	0.21	0.05	

onde $\epsilon = 1 - |\langle \psi_0 | \psi_{VAR} \rangle|^2$

Obs.: apesar funções radiais $u_i(\rho)$ serem qualitativamente similares, elas apresentam comportamentos distintos p/ $\rho \approx 0$ e $\rho \gg 1$ (veja Fig. 18.1, Messiah)
↳ diferenças valores E_{VAR} !

Ex. 2: estado fundamental átomo He,
similar Ex. 1, pg. 10;
considerar: sistema - núcleo (massa $m \to \infty$), carga Ze
⊕ 2 elétrons;
hamiltoniano:

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{Ze_1^2}{r_1} - \frac{Ze_2^2}{r_2} + \frac{e^2}{r_{12}} \qquad (91.1)$$

$$= T_1 + T_2 + V_1 + V_2 + V_{12}$$

onde $\vec{r}_i$: posição elétron i ; $r_{12} = |\vec{r}_1 - \vec{r}_2|$
$\vec{p}_i$: momento " "

ideia: determinar variacionalmente a energia do estado fundamental.

considerar: função de onda tentativa p/ estado fundamental:

$$\Phi_a(\vec{r}_1, \vec{r}_2) = \varphi_a(\vec{r}_1)\,\varphi_a(\vec{r}_2) = \frac{1}{\pi a^3}\, e^{-(r_1+r_2)/a} \qquad (92.1)$$

Eq. (92.1): similar autoestado não-perturbado (10.2), porém

$a \neq \frac{a_0}{Z}$ e a: parâmetro variacional.

temos que:

$$\cdot\ \langle \Phi_a | \Phi_a \rangle = \int d^3r_1\, d^3r_2\, |\Phi(\vec{r}_1, \vec{r}_2)|^2 :$$

$$= \int dr_1\, dr_2\, r_1^2 r_2^2 \frac{1}{\pi^2 a^6} e^{-2(r_1+r_2)/a} \int d\Omega_1 \int d\Omega_2$$

$$= \left(\frac{4\pi}{\pi a^3} \underbrace{\int_0^\infty dr_1\, r_1^2 e^{-2r_1/a}}_{a^3/4} \right)^2 = 1$$

$$\cdot\ \langle \Phi_a | H | \Phi_a \rangle = \sum_{i=1}^{2} \langle \varphi_a | T_i | \varphi_a \rangle + \langle \varphi_a | V_i | \varphi_a \rangle + \langle \Phi_a | V_{12} | \Phi_a \rangle ;$$

notar:

(i) $\langle \varphi_a | p^2/2m | \varphi_a \rangle = \int d^3r\, \varphi_a^*(r) \langle \vec{r} | p^2/2m | \varphi_a \rangle$

$$= -\frac{\hbar^2}{2m} \underbrace{\int dr \frac{r^2}{r^2} \varphi_a^*(r)\, \partial_r \left(r^2 \varphi_a(r) \right)}_{-\frac{1}{\pi a^4} \underbrace{\int dr \left(2r - \frac{r^2}{a}\right) e^{-2r/a}}_{\frac{a^2}{4}}} \underbrace{\int d\Omega}_{4\pi} = \frac{\hbar^2}{2ma^2} = \left(\frac{a_0}{a}\right)^2 \underbrace{\frac{\hbar^2}{2ma_0^2}}_{\frac{e^2}{2a_0}}$$

Eq. (90.1) p/ $\ell = 0$

Definição: $Z' = a_0/a$; $a_0 = \hbar^2/me^2$: raio de Bohr

tilibra

$\hookrightarrow \langle \varphi_a | T_i | \varphi_a \rangle = Z'^2 \dfrac{e^2}{2a_0} = Z'^2 E_H$ (93.1)

(ii) $\langle \varphi_a | -Ze^2/r | \varphi_a \rangle = -\dfrac{Ze^2}{\pi a^3} \underbrace{\int dr\, r^2 \frac{1}{r} e^{-2r/a}}_{a^2/4} \underbrace{\int d\Omega}_{4\pi}$

$= -\dfrac{Ze^2}{a} = -2Z\left(\dfrac{a_0}{a}\right)\dfrac{e^2}{2a_0} = -2ZZ'E_H$ (93.2)

(iii) $\langle \Phi_a | V_{12} | \Phi_a \rangle = \dfrac{5}{8}\dfrac{e^2}{a} = \dfrac{5}{4}\left(\dfrac{a_0}{a}\right)\dfrac{e^2}{2a_0} = \dfrac{5}{4} Z' E_H$ (93.3)

Eq. (11.5)

Dessa forma,

$E[\Phi_a] = E(a) = E(Z') = \left(2Z'^2 - 4ZZ' + \dfrac{5}{4}Z'\right) E_H$ (93.4)

$\hookrightarrow \dfrac{dE}{dZ'} = 0 : \; 4Z' - 4Z + \dfrac{5}{4} = 0 \rightarrow Z' = Z - \dfrac{5}{16}$

$\hookrightarrow E_{VAR} = E\left(Z' = Z - 5/16\right) = -2\left(Z - 5/16\right)^2 E_H$: energia estado fundamental (93.5)

Obs. 1: Eq. (93.5) similar energia do estado fundamental não-perturbada (10.2) : $E^0 = -2Z^2 E_H$

$\hookrightarrow$ interpretação (93.4) : elétrons se movimento sob ação potencial núcleo, carga efetiva $(Z - 5/16)e$

blindagem!

Obs. 2: Eq. (11.1): $E_{pert} = -2Z^2 E_H + \frac{5}{4} Z E_H$: 1ª ordem

↳ $E_{VAR} - E_{pert} = -\frac{25}{128} E_H < 0 \rightarrow E_{VAR} < E_{pert}$.

De fato, temos que (veja tabela 16.1, Messiah)

$E_{exp} < E_{VAR} < E_{pert}$!

Obs.: veja Sec. 18.5, Messiah p/ discussão sobre uso método variacional no estudo de estados excitados.

Approximation methods

1. WKB
2. Time-independent perturbation theory
3. Variational method
4. Time-dependent perturbation theory

1. WKB (Wentzel, Kramers, Brillouin)

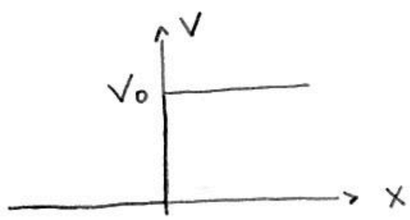
Ref. : chap. 7, Merzbacher

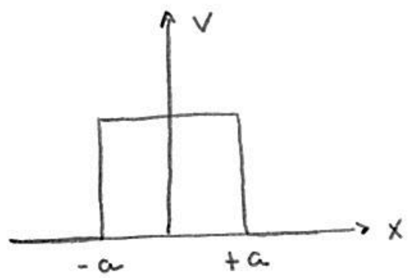
chap. 2, Sakurai

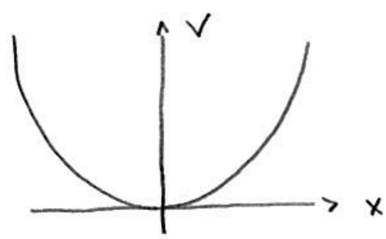
Consider the (1-D) Schrödinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \qquad (1.1)$$

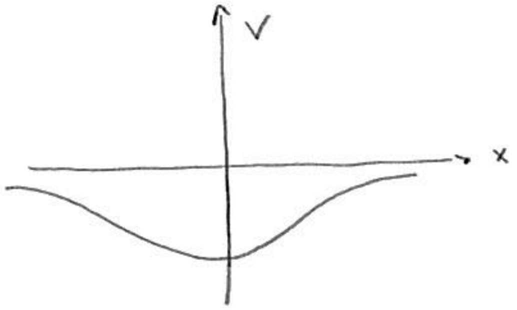
So far : (exact) solution for sectionally constant potentials, harmonic oscillator

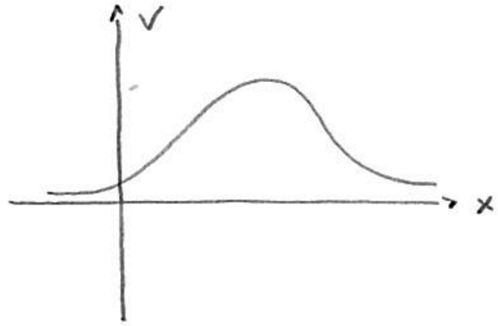






we want to consider:





We will focus on $V = V(x)$ that "slowly varies" with x (*)

Idea WKB: to determine approximated solutions for Eq. (1.1) under the <u>assumption</u> (*).

Recall:

if $V = cte \longrightarrow \psi(x) = e^{\pm i k x}$; $k = cte$

$$\text{since } V = V(x) \xrightarrow[\text{ansatz}]{} \psi(x) = e^{i u(x)} \tag{2.1}$$

Let's determine $u = u(x)$!

Defining:

$$k(x) = \left(\frac{2m}{\hbar^2} (E - V(x)) \right)^{1/2} , \quad E > V(x)$$

$$k(x) = -i \left(\frac{2m}{\hbar^2} (V(x) - E) \right)^{1/2} = -i \bar{k}(x) , \quad E < V(x)$$

$\hookrightarrow$ Eq. (1.1):
$$\frac{d^2\psi}{dx^2} + k^2(x)\, \psi(x) = 0 \tag{2.2}$$

(2.1) in (2.2) (exercise) :

$$i \frac{d^2 u}{dx^2} - \left(\frac{du}{dx}\right)^2 + K^2(x) = 0 \qquad (3.1)$$

note : (3.1) is equivalent to (2.2), but
(2.2) is a linear differential eq. while (3.1) is a nonlinear one.

idea : use nonlinearity of (3.1) and solve it within an iteration procedure.

- If $V = cte \longrightarrow u(x) = K = cte \longrightarrow \frac{d^2u}{dx^2} = 0$

if $V = V(x)$ slowly varies with $x \xrightarrow[\text{expect}]{\text{we}} |u''|^2 \ll (u')^2$

$\hookrightarrow$ (3.1) : $(u')^2 \simeq K^2(x)$

$$\hookrightarrow u_0(x) = \pm \int^x dx' \, K(x') + C_0 \quad : \text{Zero-order approx. for } u = u(x) \qquad (3.2)$$

- First order approximation,

Eq. (3.1) : $\left(\frac{du}{dx}\right)^2 = K^2(x) + i \frac{d^2u}{dx^2}$

$\hookrightarrow (u_1')^2 = K^2 + i u_0''$

solution:

$$u_1(x) = \pm \int^{x} dx' \left(K^2(x') + i\, u_0''(x') \right)^{1/2} + C_1 \qquad (4.1)$$

$$= \pm \int^{x} dx' \left(K^2(x') \pm i\, K'(x') \right)^{1/2} + C_1$$

· (n+1)-th order approximation,

$$u_{n+1}(x) = \pm \int^{x} dx' \left(K^2(x') + i\, u_n''(x') \right)^{1/2} + C_{n+1}$$

note: the iteration procedure $\longrightarrow u(x)$ if $u_1(x) \simeq u_0(x)$ or

$$|K'(x)| \ll |K^2(x)| \qquad (4.2)$$

condition (4.2)

$$\hookrightarrow \quad u_1(x) = \pm \int^{x} dx'\, K(x') \underbrace{\left(1 \pm i \frac{K'}{K^2} \right)^{1/2}}_{\simeq\, 1 \pm \frac{i}{2} \frac{K'}{K^2}} + C_1$$

$$\simeq \pm \int^{x} dx' \left[K(x') \pm \frac{i}{2} \frac{K'}{K} \right] + C_1$$

$$= + \frac{i}{2} \ln K(x) \pm \int^{x} dx'\, K(x') + C_1 \;:$$

$\hookrightarrow$ to be included in the normal. etc

$$\hookrightarrow \psi(x) = e^{iu_1(x)} = \frac{1}{\sqrt{K(x)}} \exp\left(\pm i \int^x dx' \, K(x')\right) \qquad (5.1)$$

Eq. (5.1) : wavefunction within the WKB approximation !

- More about condition (4.2) :

consider $E > V(x)$,

one can define an effective wavelength $\lambda(x) = \frac{2\pi}{K(x)}$

$$\hookrightarrow \lambda' = -\frac{2\pi}{K^2} K' \quad \rightarrow \quad |\lambda'| \sim \frac{|K'|}{|K^2|} \ll 1$$

: λ slowly varies with x !

$$K^2 \sim (E - V) \quad \rightarrow \quad 2KK' \sim -\frac{dV}{dx}$$

$$\hookrightarrow \frac{1}{K}\left|\frac{dV}{dx}\right| \sim \frac{|K'|}{K^2} K^2 \ll K^2 = E_{KINETIC}$$

$$\hookrightarrow \left|\frac{dV}{d(x/\lambda)}\right| \ll E_{KINETIC}$$

: change V over one λ is much smaller than $E_{KINETIC}$.

- Note :
  - if $E > V(x)$: classically accessible region :

    solution (1.1) : two independent propagating waves

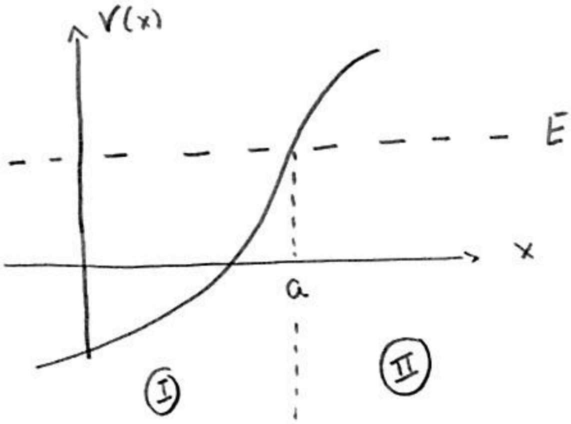
  - if $E < V(x)$: nonclassical region :

    rewriting eq. (5.1) :

$$\psi(x) = \frac{1}{\sqrt{\bar{k}(x)}} \exp\left(\pm \int^{x} dx' \, \bar{k}(x') \right) \qquad (6.1)$$

Recall : form solutions (1.1) for potentials sectionally ctes.

So far :



Region I : solution = (5.1), in general

$$\psi(x) \approx \frac{A}{\sqrt{k(x)}} \exp\left(+i \int_a^x dx' \, k(x') \right) + \frac{B}{\sqrt{k(x)}} \exp\left(-i \int_a^x dx' \, k(x') \right) \qquad (6.2)$$

Region II : solution = (6.1), in general

$$\psi(x) \approx \frac{C}{\sqrt{\bar{k}(x)}} \exp\left(- \int_a^x dx' \, \bar{k}(x') \right) + \frac{D}{\sqrt{\bar{k}(x)}} \exp\left(\int_a^x dx' \, \bar{k}(x') \right) \qquad (6.3)$$

* In fact, (6.2) and (6.3) are ok only if $|x-a| \gg 1$,

since close to the <u>classical</u> <u>turning point</u> $x=a$:

$E \approx V(x) \rightarrow k(x) \approx 0 \rightarrow$ condition (4.2) breaks down !

- Recall sectionally cte potentials in 1-D:

we require: $\psi(x)$ and $\psi'(x)$ continuous at potentials discontinuities $\longrightarrow$ connection solutions regions I and II.

- Within WKB (see Sec. 7.2, Merzbacher, for details),

idea: analysis eq. (1.1) with $V(x)$ linearized around $x = a$.

assumption: $V(x) - E \approx g(x-a)$

$$(1.1): \quad -\frac{\hbar}{2m}\frac{d^2\psi}{dx^2} + g(x-a)\psi = 0 \tag{7.1}$$

defining : $z = \left(2mg/\hbar^2\right)^{1/3}(x-a)$

$$(7.1) \longrightarrow \frac{d^2\psi}{dz^2} - z\psi = 0$$

solution: Airy functions $Ai(z)$ and $Bi(z)$

* Analysis asymptotic behaviour $\left(|z| \gg 1\right)$ $Ai(z)$ and $Bi(z)$

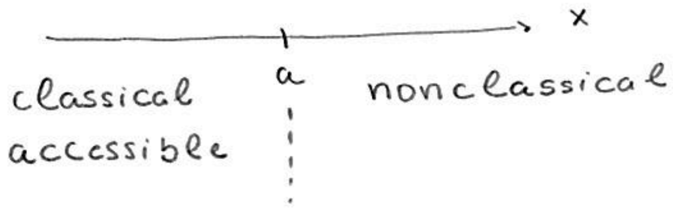
↳ connection formulas:

$$\frac{2A}{\sqrt{k(x)}}\cos\left(\int_x^a k(x')\,dx' - \frac{\pi}{4}\right) - \frac{B}{\sqrt{k(x)}}\sin\left(\int_x^a k(x')\,dx' - \frac{\pi}{4}\right)$$

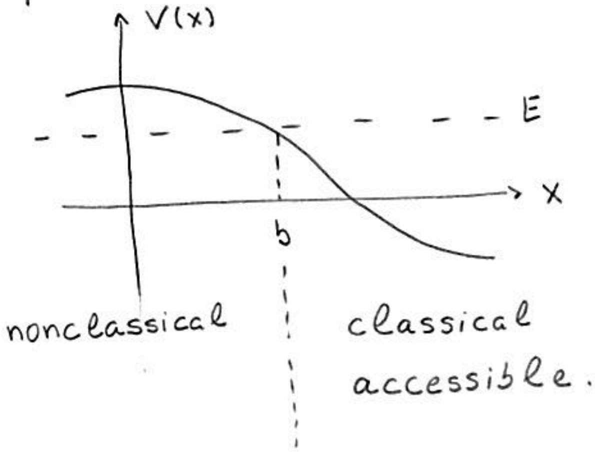
$$\longleftrightarrow \frac{A}{\sqrt{\bar{k}(x)}}\exp\left(-\int_a^x \bar{k}(x')\,dx'\right) + \frac{B}{\sqrt{\bar{k}(x)}}\exp\left(\int_a^x \bar{k}(x')\,dx'\right) \tag{7.2}$$

Eq. (7.2) : - note limits integrals and coefficients sin, cos, and exp functions

- turning point as in Fig on pg. 6 :



It's useful to write (7.2) for the case

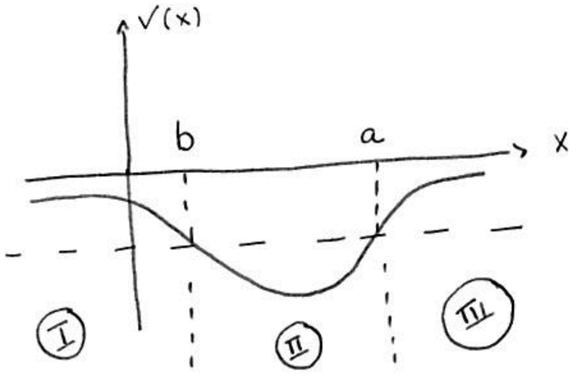


$$\frac{A}{\sqrt{\bar{\kappa}(x)}} \exp\left(- \int_x^b \bar{\kappa}(x')\,dx' \right) + \frac{B}{\sqrt{\bar{\kappa}(x)}} \exp\left(+ \int_x^b \bar{\kappa}(x')\,dx' \right) \longleftrightarrow$$

$$\frac{2A}{\sqrt{\kappa(x)}} \cos\left(\int_b^x \kappa(x')\,dx' - \frac{\pi}{4} \right) - \frac{B}{\sqrt{\kappa(x)}} \sin\left(\int_b^x \kappa(x')\,dx' - \frac{\pi}{4} \right) \quad (8.1)$$

Ex. 1 : Bound states $V = V(x)$

consider particle mass $\underline{m}$, energy $\underline{E}$, under $V = V(x)$



idea: to determine energy bound states within the WKB approximation.

solution (1.1), region I:

$$\psi_I(x) \approx \frac{1}{\sqrt{\bar{\kappa}(x)}} \exp\left(-\int_x^b \bar{\kappa}(x')\,dx'\right) \quad ; \quad x' < b \qquad (9.1)$$

using the connection formula (8.1):

$$\psi_{II}(x) \approx \frac{2}{\sqrt{\kappa(x)}} \cos\left(\int_b^x \kappa(x')\,dx' - \frac{\pi}{4}\right) \quad ; \quad b < x < a \qquad (9.2)$$

In order to determine $\psi_{III}(x)$, it's necessary to rewritte (9.2). It's possible to show that (exercise):

$$\psi_{II}(x) \approx \frac{-2}{\sqrt{\kappa(x)}} \cos\left(\int_b^a \kappa(x')\,dx'\right) \sin\left(\int_x^a \kappa(x')\,dx' - \frac{\pi}{4}\right)$$

$$+ \frac{2}{\sqrt{\kappa(x)}} \sin\left(\int_b^a \kappa(x')\,dx'\right) \cos\left(\int_x^a \kappa(x')\,dx' - \frac{\pi}{4}\right) \qquad (9.2)$$

Since

$$\psi_{III}(x) \sim \exp\left(-\int_a^x \bar{\kappa}(x')\,dx'\right)$$

connection formula (7.2) $\longrightarrow$ only second term (9.2) $\neq 0$!

$$\hookrightarrow \cos\left(\int_b^a \kappa(x')\,dx'\right) = 0$$

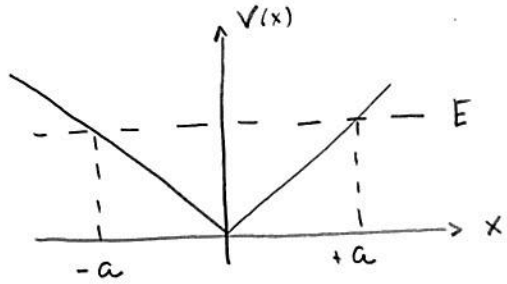
$\hookrightarrow \displaystyle\int_b^a dx\, K(x) = \int_b^a dx \sqrt{\frac{2m}{\hbar^2}\left(E - V(x)\right)} = (n + 1/2)\,\pi,$ (10.1)

$n = 0, 1, 2, \ldots$

- defining $p(x) = \pm \hbar K(x)$,

$\hookrightarrow \displaystyle\oint p(x)\,dx = 2\hbar \int_b^a K(x)\,dx = (n + 1/2)\,h$: apart from 1/2 factor, <u>Sommerfeld quantization rule</u> (old quantum theory)

- Let's consider, in particular, $V(x) = g|x|$, $g > 0$



classical turning points

$E = V(a) = ga \rightarrow a = \frac{E}{g}$

(10.1) :

exercise !

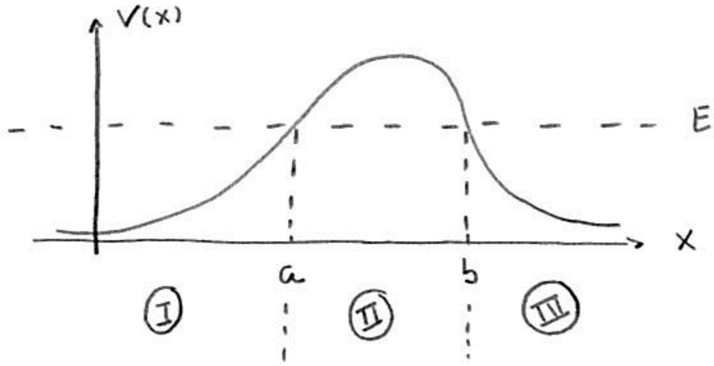
$$2\int_0^a dx \sqrt{\frac{2m}{\hbar^2}\left(E - gx\right)} = \sqrt{\frac{8mE^3}{\hbar^2 g}}\ \underbrace{\int_0^1 dy\,\sqrt{1-y}}_{2/3} = (n + 1/2)\,\pi$$

$$\hookrightarrow E^3_{WKB} = \frac{9\pi^2}{32}\cdot\frac{\hbar^2 g^2}{m}\,(n + 1/2)^2$$

Obs.: See Sec. 7.3, Merzbacher for comparison between WKB and <u>exact</u> results.

Ex. 2 : Transmission through a barrier,

consider particle mass $\underline{\underline{m}}$ under potential



solution (1.1) within the WKB approximation

$$\psi_I(x) = \frac{A}{\sqrt{k(x)}} \exp\left(i \int_a^x k(x')\,dx' \right) + \frac{B}{\sqrt{k(x)}} \exp\left(-i \int_a^x k(x')\,dx' \right)$$

$$\psi_{II}(x) = \frac{C}{\sqrt{\bar{k}(x)}} \exp\left(- \int_a^x \bar{k}(x')\,dx' \right) + \frac{D}{\sqrt{\bar{k}(x)}} \exp\left(\int_a^x \bar{k}(x')\,dx' \right)$$

$$\psi_{III}(x) = \frac{F}{\sqrt{k(x)}} \exp\left(i \int_b^x k(x')\,dx' \right) + \frac{G}{\sqrt{k(x)}} \exp\left(-i \int_b^x k(x')\,dx' \right)$$

Using the connection formulas, it's possible to show that (exercise) :

$$\begin{pmatrix} A \\ B \end{pmatrix} = M \begin{pmatrix} F \\ G \end{pmatrix}$$

where

$$M = \frac{1}{2} \begin{pmatrix} a & ib \\ -ib & a \end{pmatrix} \quad ; \quad a = 2\theta + \frac{1}{2\theta} \quad ; \quad b = 2\theta - \frac{1}{2\theta}$$

$$\theta = \exp\left(\int_a^b \bar{k}(x)\,dx \right)$$

$\theta = \theta(E)$: measurement height and width barrier !

Recall sectionally cte potentials, <u>transmission</u> <u>coef.</u>:

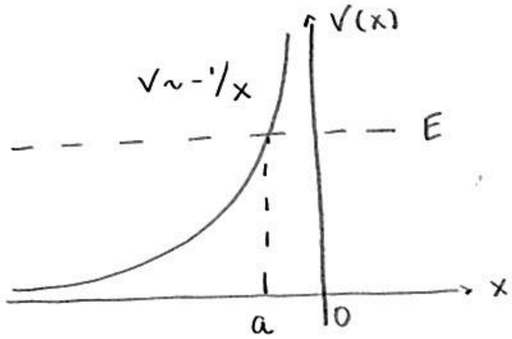
$$T = \frac{|\psi_{TRANS}\sqrt{k_{TRANS}}|^2}{|\psi_{INC}\sqrt{k_{INC}}|^2} = \frac{|F|^2}{|A|^2}$$

if $G=0$ (no particle incident from the right),

$$T = \frac{1}{|M_{11}|^2} = \frac{4}{(2\theta + 1/2\theta)^2} \xrightarrow[\theta \gg 1]{} T \simeq \frac{1}{\theta^2} = \exp\left(-2\int_a^b \bar{k}(x)\,dx\right)$$

(high and broad barrier)

· Let's calculate T for a particle charge $Z_1 e$ to penetrate nucleus charge $Z_2 e$: <u>1-D repulsive Coulomb barrier</u>



$$V(x) = -\frac{Z_1 Z_2 e^2}{x}$$

classical turning point: $V(a) = E = -\frac{Z_1 Z_2 e^2}{a} \rightarrow Ea = -Z_1 Z_2 e^2$

↳ $V(x) = Ea/x$

note!

$$\int_a^b \bar{k}(x)\,dx = \int_a^{b=0} dx\sqrt{\frac{2mE}{\hbar^2}\left(\frac{a}{x}-1\right)} = (-a)\sqrt{\frac{2mE}{\hbar^2}}\underbrace{\int_0^1\sqrt{\frac{1}{u}-1}\,du}_{\pi/2}$$

$$= \frac{Z_1 Z_2 e^2}{\hbar v}\pi$$

exercise!

where $v = \sqrt{\dfrac{2E}{m}}$: classical particle velocity at $x \to +\infty$.

$$\hookrightarrow \quad T \simeq \frac{1}{\theta^2} = \exp\left(-2\pi \frac{Z_1 Z_2 e^2}{\hbar v}\right) \text{ : } \underline{\text{penetrability}}.$$

Application : alpha decay.