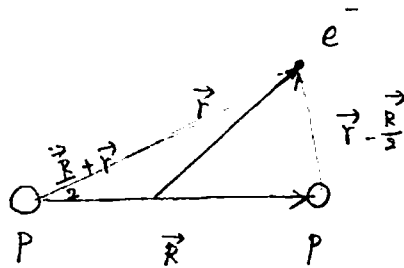


8. 分子構造

(Gasiorowicz Ch. 20)

8.1. Born - Oppenheimer 近似

最も単純な分子: H_2^+



$$H = -\frac{\hbar^2}{2\mu} \nabla_R^2 - \frac{\hbar^2}{2m} \nabla_r^2 + V_0(R) + V_c(\vec{r} + \frac{\vec{R}}{2}) + V_c(\vec{r} - \frac{\vec{R}}{2})$$

$$\mu = \frac{m_p}{2} \approx \frac{940}{2} \text{ MeV} \approx 500 \text{ MeV}$$

$$m = m_e = 0.5 \text{ MeV}$$

$$V_0(R) = e^2/R \quad (p-p)$$

$$V_c(r) = -e^2/r \quad (p-e)$$

- $\mu \gg m_e \rightarrow$ 陽子の運動に比べて電子の運動は急速
 \rightarrow 各瞬間で電子は基底状態を“探し出す”時間がある
 (断熱過程)
 $\rightarrow R$ を固定して電子に対する Schrödinger 方程式
 を解く (ボーン-オッペンハイマー近似)

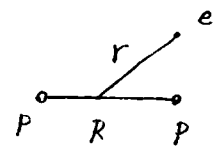
$$i) \quad \left[-\frac{\hbar^2}{2m} \nabla_r^2 + V_c(\vec{r} + \frac{\vec{R}}{2}) + V_c(\vec{r} - \frac{\vec{R}}{2}) \right] \psi_n(r; R) = \epsilon_n(R) \psi_n(r; R)$$

$$ii) \quad \left[-\frac{\hbar^2}{2\mu} \nabla_R^2 + V_0(R) + \epsilon_0(R) \right] \Psi(R) = E \Psi(R)$$

8.2. LCAO 法

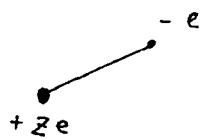
$$\left[-\frac{\hbar^2}{2m} \nabla_r^2 - \frac{e^2}{|r+\frac{R}{2}|} - \frac{e^2}{|r-\frac{R}{2}|} \right] \psi_0(r; R) = \epsilon_0(R) \psi_0(r; R)$$

ある与えられた R での基底状態,



LCAO 法による近似計算:

(note) hydrogen-like atom:



$$\psi_{1s}(\vec{r}) = \sqrt{\frac{Z}{\pi a_0^3}} e^{-Zr/a_0}$$

$$a_0 = \frac{\hbar}{m c \alpha}$$

$$E_{1s} = -\frac{m c^2}{2} (Z\alpha)^2$$

LCAO (Linear Combination of Atomic Orbitals)

$$\psi_0(r; R) = \left(\text{---} \oplus \text{---} \right) \pm \left(\text{---} \ominus \text{---} \right)$$

$$= C_{\pm}(R) \left\{ \underbrace{\frac{1}{\sqrt{\pi a_0^3}} e^{-|r-\frac{R}{2}|/a_0}}_{\psi_1(r, R)} \pm \underbrace{\frac{1}{\sqrt{\pi a_0^3}} e^{-|r+\frac{R}{2}|/a_0}}_{\psi_2(r, R)} \right\}$$

↑ gerade
↓ ungerade

Normalization:

$$1 = \langle \psi_0 | \psi_0 \rangle_{\vec{r}}$$

$$= C_{\pm}^2 \langle \psi_1 \pm \psi_2 | \psi_1 \pm \psi_2 \rangle_{\vec{r}}$$

$$= C_{\pm}^2 \left\{ 2 \pm 2 \underbrace{\int d\vec{r} \psi_1(\vec{r}, \vec{R}) \psi_2(\vec{r}, \vec{R})}_{\substack{||| \\ S(R)}} \right\}$$

$$\downarrow \quad C_{\pm}(R)^2 = \frac{1}{2(1 \pm S(R))}$$

$$S(R) = \int d\vec{r} \frac{1}{\pi a_0^3} e^{-|\vec{r} + \frac{\vec{R}}{2}|/a_0} e^{-|\vec{r} - \frac{\vec{R}}{2}|/a_0}$$

$$= \dots = \left(1 + \frac{R}{a_0} + \frac{R^2}{3a_0^2} \right) e^{-R/a_0}$$

Hamiltonian :

$$\begin{aligned}
 \langle H \rangle_{g,u} &= \frac{1}{2[1 \pm S(R)]} \langle \psi_1 \pm \psi_2 | H_e | \psi_1 \pm \psi_2 \rangle_{\vec{r}} \\
 &= \frac{1}{2[1 \pm S(R)]} \left\{ \langle \psi_1 | H_e | \psi_1 \rangle + \langle \psi_2 | H_e | \psi_2 \rangle \right. \\
 &\quad \left. \pm \langle \psi_1 | H_e | \psi_2 \rangle \pm \langle \psi_2 | H_e | \psi_1 \rangle \right\} \\
 &= \frac{1}{1 \pm S(R)} \left\{ \underline{\langle \psi_1 | H_e | \psi_1 \rangle} \pm \underline{\langle \psi_1 | H_e | \psi_2 \rangle} \right\}
 \end{aligned}$$

$$\begin{aligned}
 \langle \psi_1 | H_e | \psi_1 \rangle &= \int d\vec{r} \psi_1^*(\vec{r}, \vec{R}) \left(T_e - \frac{e^2}{|\vec{r} - \frac{\vec{R}}{2}|} - \frac{e^2}{|\vec{r} + \frac{\vec{R}}{2}|} \right) \\
 &\quad \times \psi_1(\vec{r}, \vec{R}) \\
 &= E_{1s} - \int d\vec{r} \frac{1}{\pi a_0^3} \left(e^{-|\vec{r} - \frac{\vec{R}}{2}|/a_0} \right)^2 \frac{e^2}{|\vec{r} + \frac{\vec{R}}{2}|} \\
 &= \dots = E_{1s} + \frac{e^2}{R} \left(1 + \frac{R}{a_0} \right) e^{-2R/a_0} - \frac{e^2}{R}
 \end{aligned}$$

$$\begin{aligned}
 \langle \psi_1 | H_e | \psi_2 \rangle &= \int d\vec{r} \psi_1^*(\vec{r}, \vec{R}) \left(T_e - \frac{e^2}{|\vec{r} - \frac{\vec{R}}{2}|} - \frac{e^2}{|\vec{r} + \frac{\vec{R}}{2}|} \right) \\
 &\quad \times \psi_2(\vec{r}, \vec{R}) \\
 &= E_{1s} \cdot S(R) - e^2 \int d\vec{r} \psi_1^*(\vec{r}, \vec{R}) \psi_2(\vec{r}, \vec{R}) \frac{1}{|\vec{r} + \frac{\vec{R}}{2}|} \\
 &= \dots = E_{1s} \cdot S(R) - \frac{e^2}{a_0} \left(1 + \frac{R}{a_0} \right) e^{-R/a_0}
 \end{aligned}$$

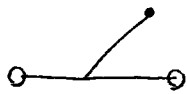
$$E_n = -\frac{1}{2} \mu c^2 \frac{(Z\alpha)^2}{n^2}$$

$$(ii) \left[-\frac{\hbar^2}{2\mu} \nabla_R^2 + V_0(R) + \epsilon_g(R) \right] \Psi(\vec{R}) = E \Psi(\vec{R})$$

$$\epsilon_g(R) = \langle \psi_1 + \psi_2 | He | \psi_1 + \psi_2 \rangle$$



(note)

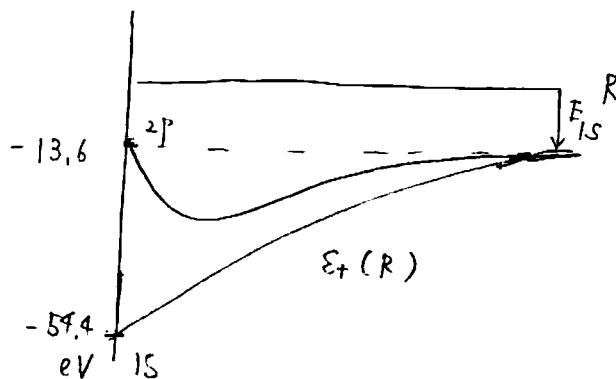


reflection symmetry \rightarrow parity

$$\Psi_{\pm}(\vec{r}, \vec{R}) = \frac{1}{\sqrt{2}} \{ \phi(\vec{r}) \pm \phi(\vec{r}') \}$$

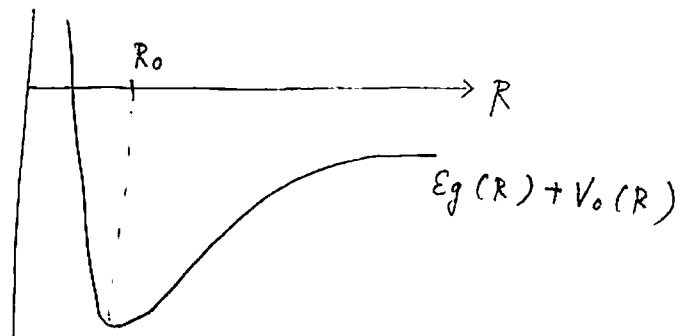
↑
一般形

$$\epsilon_{\pm}(\vec{R}) = \langle \Psi_{\pm} | He | \Psi_{\pm} \rangle$$



$$\Psi_{+} \xrightarrow{R \rightarrow 0} \Psi_{1S}$$

$$\Psi_{-} \xrightarrow{R \rightarrow 0} \Psi_{2P}$$



第 0 近似

$$\Psi(\vec{r}, \vec{R}) = \delta(R - R_0) \cdot \varphi_0(\vec{r}; R_0)$$

第 1 近似

$$\Psi(\vec{r}, \vec{R}) = \int dR f(R) \varphi_0(\vec{r}; R)$$

$$E_g(R) + V_0(R) \sim E_g(R_0) + V_0(R_0) + \frac{1}{2} M \omega^2 (R - R_0)^2$$

と近似すると

$$f(R) \sim \left(\frac{M\omega}{\pi\hbar}\right)^{1/4} e^{-M\omega R^2/2\hbar}$$

6. 半古典論 (WKB 近似)

- 近似解が比較的簡単に求まる (← 解の定性的な振る舞い)
- 古典描像との対応
↳ 解の物理的解釈
: 直観的理解

6.1. WKB 波動関数

$$\frac{d^2}{dx^2} \psi(x) + \underbrace{\frac{2m}{\hbar^2} (E - V(x))}_{k^2(x)} \psi(x) = 0$$

(note) if $V(x) = \text{const.}$ $\rightarrow \psi(x) \propto e^{\pm ikx}$

WKB Ansatz: $\psi(x) = \exp\left(i \int^x \eta(x') dx'\right)$

↓

$$\begin{aligned} \psi' &= i\eta \psi \\ \Rightarrow \psi'' &= i(\eta' \psi + \eta \psi') \\ &= i\eta' \psi - \eta^2 \psi = -k^2 \psi \end{aligned}$$

↷

$$\eta^2 = k^2 + i\eta'$$

半古典近似: η : ゆっくりと変化する関数
 $\Leftrightarrow |\eta'| \ll |\eta|^2$

↓

$$\eta_0^2(x) \sim k^2(x) \quad \rightarrow \quad \eta_0(x) = \pm k(x)$$

↓

$$\begin{aligned} \eta^2(x) &\sim \eta_0^2(x) + i\eta_0'(x) \\ &= k^2(x) \pm i k'(x) \\ &= k^2(x) \left(1 \pm i \frac{k'(x)}{k^2(x)} \right) \end{aligned}$$

↓

$$\begin{aligned} \eta(x) &\sim \pm k(x) \left(1 \pm \frac{i}{2} \frac{k'(x)}{k^2(x)} \right) \\ &= \pm k(x) + \frac{i}{2} \frac{k'(x)}{k(x)} \end{aligned}$$

(note) $e^{i \int^x dx' \frac{i}{2} \frac{k'(x')}{k(x')}} = e^{-\frac{1}{2} \int^x \frac{k'(x')}{k(x')} dx'}$
(log k)'

$$= c \cdot e^{-\frac{1}{2} \log k(x)} = c k(x)^{-\frac{1}{2}}$$

↓

$$\Psi(x) = \frac{c_1}{\sqrt{k(x)}} e^{i \int^x k(x') dx'} + \frac{c_2}{\sqrt{k(x)}} e^{-i \int^x k(x') dx'}$$

(note) 古典的に許されない領域 ($E < V(x)$)

$$k(x) = i \gamma(x) \quad \text{or} \quad \gamma(x) = \frac{2m}{\hbar^2} (V(x) - E)$$

$$\downarrow \quad \psi(x) = \frac{\tilde{C}_1}{\sqrt{\gamma(x)}} e^{-\int^x \gamma(x') dx'} + \frac{\tilde{C}_2}{\sqrt{\gamma(x)}} e^{+\int^x \gamma(x') dx'}$$

• WKB近似の妥当性

$$|n'| \ll |n|^2 \quad \Downarrow \quad |k'(x)| \ll |k(x)|^2$$

\Downarrow

$$\left| \frac{d\gamma(x)}{dx} \right| \ll 1 \quad \left(\gamma(x) = \frac{1}{k(x)} \right)$$

\Downarrow 波長の変化量が非常に大なるゆへ

\Downarrow - 波長内でポテンシャルの変化が非常に大なるゆへ.

\Leftrightarrow high E , a/o large m

$$(note) \quad k'(x) = \frac{\frac{2m}{\hbar^2} V'(x)}{2k(x)} = \frac{m}{\hbar^2} \gamma(x) V'(x)$$

$$\Downarrow \quad |\gamma(x) V'(x)| \ll \frac{k^2(x) \hbar^2}{m} = \frac{P(x)^2}{m}$$

\Downarrow - 波長内のポテンシャルの変化が

局所運動エネルギーに比べて充分小さい.

6.2. WKB 接続公式

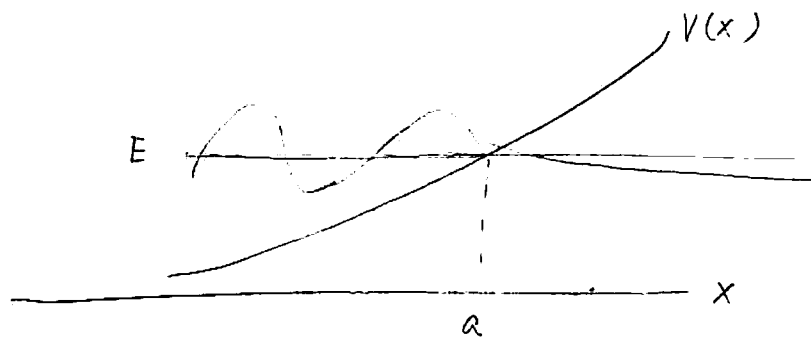
WKB 近似: 古典的転回点, ($E=V(x)$) のまわりでは
成り立たない。 $\rightarrow \frac{1}{\sqrt{k(x)}}$: 発散

\leadsto WKB 近似は実際には役に立たないか?

\downarrow

WKB 接続公式

(転回点のまわりをうまく繋げる)



$$x \gg a: \psi(x) \sim \frac{1}{2} C r(x)^{-1/2} e^{-\int_a^x r(x') dx'}$$

$$x \ll a: \psi(x) \sim k(x)^{-1/2} \left\{ C_1 e^{i \int_a^x k(x') dx'} + C_2 e^{-i \int_a^x k(x') dx'} \right\}$$

C_1, C_2 は C とどのように関連するか?

6.2. WKB 接続公式

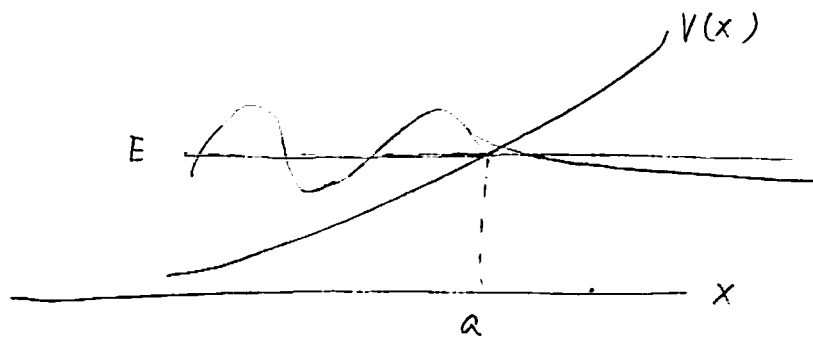
WKB 近似: 古典的転回点, ($E=V(x)$) のまわり τ' は
成り立たない。 $\rightarrow \frac{1}{\sqrt{k(x)}}$: 発散

\sim WKB 近似は実際には役に立たないか?



WKB 接続公式

(転回点のまわりをうまく避ける)



$$x \gg a: \psi(x) \sim \frac{1}{2} C \gamma(x)^{-1/2} e^{-\int_a^x \gamma(x') dx'}$$

$$x \ll a: \psi(x) \sim k(x)^{-1/2} \left\{ C_1 e^{i \int_a^x k(x') dx'} + C_2 e^{-i \int_a^x k(x') dx'} \right\}$$

C_1, C_2 は C とどのように関連するの?

(i) Airy 関数法

$x = a$ の周りで $V(x)$ を展開:

$$\begin{aligned} V(x) &\sim V(a) - F_0 \cdot (x-a) \\ &= E - F_0 \cdot (x-a) \end{aligned}$$

$$F_0 = -V'(a)$$

↓

Schrödinger 方程式

$$\frac{d^2}{dx^2} \psi(x) + \frac{2m}{\hbar^2} \cdot F_0 \cdot (x-a) \psi(x) = 0$$

(note) $z = \left(\frac{2m}{\hbar^2} F_0\right)^{1/3} (x-a)$

↓ $\frac{d^2}{dz^2} \psi + z \psi = 0$

Solution: $\boxed{\psi(z) = Ai(-z)}$

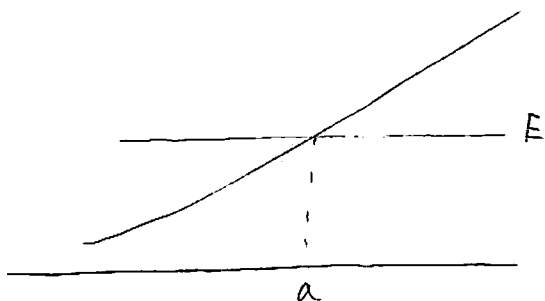
↓

$Ai(-z)$ (の漸近形) と WKB 解を比較する。

↓

$$\begin{cases} \psi(x) = \frac{1}{2} C \gamma^{-1/2} e^{-\int_a^x \gamma(x') dx'} & (x > a) \\ \psi(x) = C k(x)^{-1/2} \cos\left(\int_x^a k(x') dx' - \frac{\pi}{4}\right) & (x < a) \end{cases}$$

(ii) 解析接続法



$$E - V(x) \sim F_0 \cdot (x-a)$$

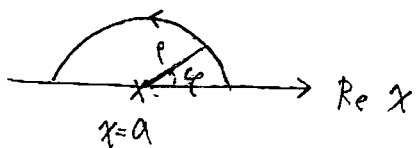
↓

$x > a$ の WKB 波動関数:

$$\psi(x) = \frac{C}{2} \cdot \frac{1}{\left(\frac{2m}{\hbar^2} F_0\right)^{1/4}} \cdot \frac{1}{(x-a)^{1/4}} \cdot e^{-\int_a^x \sqrt{\frac{2m}{\hbar^2} F_0(x'-a)} dx'}$$

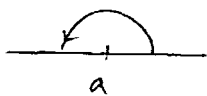
この関数を複素変数の関数とみなし、複素平面上を半径 ρ の円に沿って関数をまわす:

↳ 上半面に沿って 1 回回る場合



$$x-a = \rho e^{i\varphi} \quad (\varphi: 0 \rightarrow \pi)$$

$$\begin{aligned} \int_a^x \sqrt{x'-a} dx' &= \int_0^\rho (\rho' e^{i\varphi})^{1/2} e^{i\varphi} d\rho' \\ &= \frac{2}{3} \rho^{3/2} e^{i\frac{3}{2}\varphi} \end{aligned}$$



at $\varphi = \pi$:

$$\int_a^x \sqrt{x'-a} dx' \rightarrow \left(\frac{2}{3}\right) \rho^{\frac{3}{2}} \cdot (-i) = +i \int_a^x \sqrt{a-x'} dx'$$

(note) $\int_a^x \sqrt{a-x'} dx'$ ($x < a$)
 $\xrightarrow{a-x' = \rho} -\int_0^{\rho} \rho'^{1/2} d\rho' = -\frac{2}{3} \rho^{\frac{3}{2}}$

$$(x-a)^{1/4} \rightarrow \rho^{1/4} e^{i\pi/4} = (a-x)^{1/4} e^{i\pi/4}$$

↓

$$\frac{c}{2} \frac{1}{\left(\frac{2m}{\hbar^2} F_0\right)^{1/4}} \frac{1}{(x-a)^{1/4}} e^{-\int_a^x \sqrt{\frac{2m}{\hbar^2} F_0(x'-a)} dx'}$$

$$\rightarrow \frac{c}{2} \frac{1}{\left(\frac{2m}{\hbar^2} F_0\right)^{1/4}} \frac{1}{(a-x)^{1/4}} e^{-i \int_a^x \sqrt{\frac{2m}{\hbar^2} F_0(a-x')} dx' - i\pi/4}$$

・ 下半面に沿って 7 回巻くと

$$e^{+i \int_a^x \sqrt{\frac{2m}{\hbar^2} F_0(a-x')} dx' + i\pi/4}$$

を得る。

↓

2つの解をあわせて:

$$\psi(x) = \begin{cases} \frac{1}{2} c \gamma^{-1/2} e^{-\int_a^x \gamma(x') dx'} & (x > a) \\ c k(x)^{-1/2} \cos\left(\int_x^a k(x') dx' - \frac{\pi}{4}\right) & (x < a) \end{cases}$$

- 一般式

$$\frac{C}{2} \gamma(x)^{-1/2} e^{-\left| \int_a^x \gamma(x') dx' \right|} + D \gamma(x)^{-1/2} e^{+\left| \int_a^x \gamma(x') dx' \right|}$$

($E < V(x)$)

$$\leftrightarrow C k(x)^{-1/2} \cos \left(\left| \int_a^x k(x') dx' \right| - \frac{\pi}{4} \right)$$

$$- D k(x)^{-1/2} \sin \left(\left| \int_a^x k(x') dx' \right| - \frac{\pi}{4} \right)$$

($E > V(x)$)

[複習]

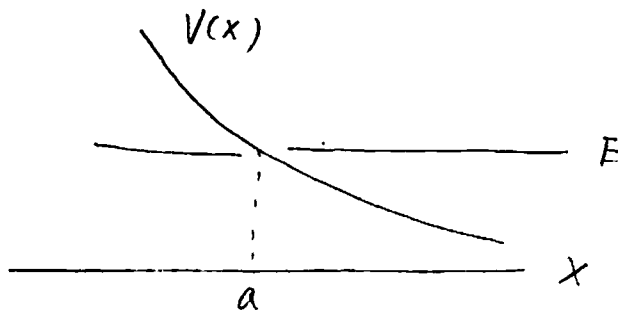
$$\frac{d^2}{dx^2} \psi(x) + k^2(x) \psi(x) = 0$$

$$k^2(x) = \frac{2m}{\hbar^2} (E - V(x))$$

$$|k'(x)| \ll |k(x)|^2$$

WKB 波動関数 : $\psi(x) \sim \frac{1}{\sqrt{k(x)}} e^{\pm i \int^x k(x') dx'}$

WKB 接続公式



$$\frac{C}{2} \frac{1}{\sqrt{\delta(x)}} e^{-\left| \int_a^x \delta(x') dx' \right|} + D \frac{1}{\sqrt{\delta(x)}} e^{+\left| \int_a^x \delta(x') dx' \right|}$$

$$(E < V(x))$$

$$\leftrightarrow \frac{C}{\sqrt{k(x)}} \cos \left(\left| \int_a^x k(x') dx' \right| - \frac{\pi}{4} \right)$$

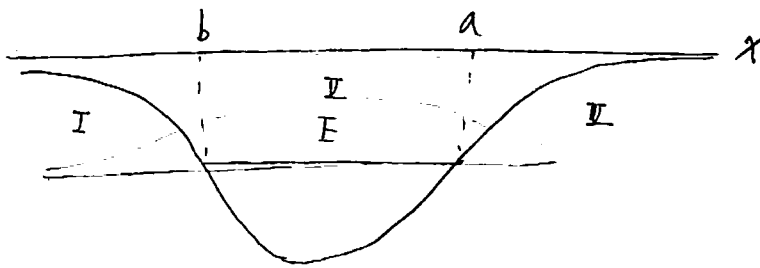
$$- \frac{D}{\sqrt{k(x)}} \sin \left(\left| \int_a^x k(x') dx' \right| - \frac{\pi}{4} \right)$$

$$(E > V(x))$$

$$\cos x = \sin(x + \frac{\pi}{2}) = -\sin(x - \frac{\pi}{2})$$

$$\sin x = \cos(x - \frac{\pi}{2}) = -\cos(x + \frac{\pi}{2})$$

求 γ -
 6.3. $\psi'' > \gamma$ 及 $\psi < 0$ の WKB 量子化条件
 (束縛状態への応用)



Region I :

$$\psi(x) = \frac{1}{\sqrt{\gamma(x)}} e^{-\int_x^b \gamma(x') dx'} \quad (x < b)$$

→ Region II :

$$\begin{aligned} \psi(x) &= \frac{2}{\sqrt{k(x)}} \cos\left(\int_b^x k(x') dx' - \frac{\pi}{4}\right) \quad (b < x < a) \\ &= \frac{2}{\sqrt{k(x)}} \cos\left(\int_b^a k(x') dx' - \int_x^a k(x') dx' - \frac{\pi}{4}\right) \\ &= -\frac{2}{\sqrt{k(x)}} \cos\left(\int_b^a k(x') dx'\right) \sin\left(\int_x^a k(x') dx' - \frac{\pi}{4}\right) \\ &\quad + \frac{2}{\sqrt{k(x)}} \sin\left(\int_b^a k(x') dx'\right) \cos\left(\int_x^a k(x') dx' - \frac{\pi}{4}\right) \end{aligned}$$

→ Region III :

$$\begin{aligned} \psi(x) &= +\frac{2}{\sqrt{\gamma(x)}} \cos\left(\int_b^a k(x') dx'\right) e^{+\int_a^x \gamma(x') dx'} \\ &\quad + \frac{1}{\sqrt{\gamma(x)}} \sin\left(\int_b^a k(x') dx'\right) e^{-\int_a^x \gamma(x') dx'} \quad (x > a) \end{aligned}$$

↓

Region II τ'' exp. 的に解が小さくなるためには

$$\cos \left(\int_b^a k(x') dx' \right) = 0 \quad \text{が「必要」}$$

↓

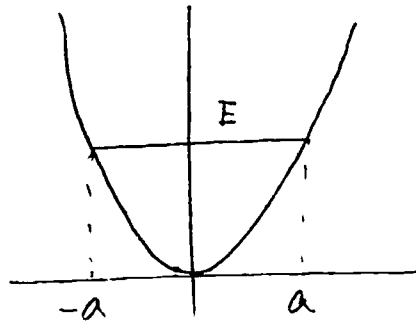
$$\int_b^a k(x') dx' = \left(n + \frac{1}{2} \right) \pi \quad (n=0, 1, \dots)$$

↓

$$\int P(x) dx = \left(n + \frac{1}{2} \right) \cdot \left(2\pi \frac{h}{k} \right)$$



(note) 調和振動子: $V(x) = \frac{1}{2} m \omega^2 x^2$



$$a = + \sqrt{\frac{2E}{m\omega^2}}$$

$$\int_{-a}^a k(x) dx = \int_{-a}^a \sqrt{\frac{2m}{\hbar^2} \left(E - \frac{1}{2} m \omega^2 x^2 \right)} dx$$

$$= \sqrt{\frac{2mE}{\hbar^2}} \int_{-a}^a \sqrt{1 - \frac{x^2}{a^2}} dx$$

$$y = \frac{x}{a}$$

$$= \sqrt{\frac{2mE}{\hbar^2}} \int_{-1}^1 \sqrt{1-y^2} \cdot a dy$$

$$= \frac{2E}{\hbar\omega} \underbrace{\int_{-1}^1 \sqrt{1-y^2} dy}_{\parallel}$$

$$\int_0^\pi \sin^2 \theta d\theta = \int_0^\pi \frac{1}{2} (1 - \cos 2\theta) d\theta = \frac{\pi}{2}$$

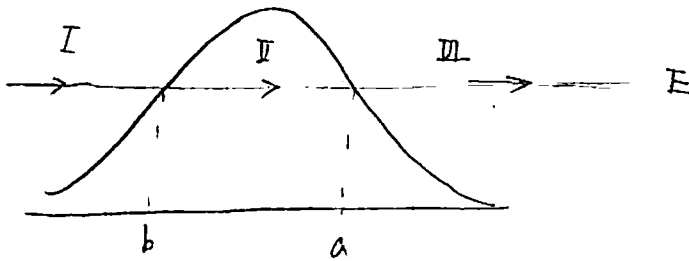
↓

$$\boxed{E = \left(n + \frac{1}{2}\right) \hbar \omega}$$

調和振動子に對しては WKB 近似は exact

cf. 経路積分

6.4. トンネリング



$$\text{Region III: } \psi(x) = \frac{+i \cdot c}{\sqrt{k(x)}} e^{i \int_a^x k(x') dx' - \frac{i}{4} \pi}$$

$$= \frac{+i c}{\sqrt{k(x)}} \left\{ \cos \left(\int_a^x k(x') dx' - \frac{\pi}{4} \right) + i \sin \left(\int_a^x k(x') dx' - \frac{\pi}{4} \right) \right\}$$

$$\text{Region II: } \psi(x) = \frac{c}{\sqrt{\delta(x)}} e^{\int_x^a \delta(x') dx'} + \frac{i c}{2} \frac{1}{\sqrt{\delta(x)}} e^{-\int_x^a \delta(x') dx'}$$

$$= \frac{c}{\sqrt{\delta(x)}} e^{\int_b^a \delta(x') dx' - \int_b^x \delta(x') dx'}$$

$$\text{Region I: } \psi(x) = \frac{2c}{\sqrt{k(x)}} e^{\int_b^a \delta(x') dx'} \cos \left(\int_x^a k(x') dx' - \frac{\pi}{4} \right)$$

$$= \frac{c}{\sqrt{k(x)}} e^{\int_b^a \delta(x') dx'} \left\{ e^{i \int_x^a k(x') dx' - \frac{i}{4} \pi} + e^{-i \int_x^a k(x') dx' + \frac{i}{4} \pi} \right\}$$

トンネル確率: 入射フラックスと透過フラックスの比

$$\downarrow \boxed{P = e^{-2 \int_b^a \gamma(x) dx}} = e^{-2 \int_b^a \sqrt{\frac{2m}{\hbar^2} (V(x) - E)} dx}$$

↓ . m が大きいと P は ↓

(note) a と b が近いと接続公式が破綻

→ 一様近似

$$P = \frac{1}{1 + e^{2 \int_b^a \gamma(x) dx}}$$

(note) $E > V_b$ ても一様近似は成立

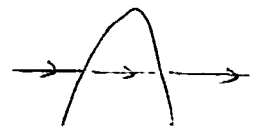
→ a, b は複素数

$$E = V_0 - \frac{1}{2} m \omega^2 x^2$$

$$x = \pm \sqrt{\frac{2}{m \omega^2} (V_0 - E)}$$

(note) $V(x) = V_0 - \frac{1}{2} m \omega^2 x^2$ のとき

$$P = \frac{1}{1 + e^{-\frac{2\pi}{\hbar \omega} (E - V_b)}}$$



↔ P_{WKB} と一致