

$$\hbar\text{-展開} : S(x) = S_0(x) + \hbar S_1(x) + \dots$$

$$O(\hbar^0) : -(S_0')^2 = -p(x)^2$$

$$\Downarrow S_0(x) = \pm \int^x dx' p(x')$$

$$O(\hbar^1) : i S_0'' - 2 S_0' S_1' = 0$$

$$\Downarrow S_1' = \frac{i}{2} \frac{S_0''}{S_0'} = \frac{i}{2} (\ln |S_0'|)'$$

$$\Downarrow S_1 = \frac{i}{2} \ln |S_0'| + \text{const.}$$

$$\Downarrow \psi(x) \sim \pm \frac{1}{\hbar} \int^x p(x') dx' e^{-\frac{1}{2} \ln |S_0'|} \times \text{const.}$$

$$= \frac{C}{\sqrt{|S_0'|}} e^{\pm i \int^x k(x') dx'}$$

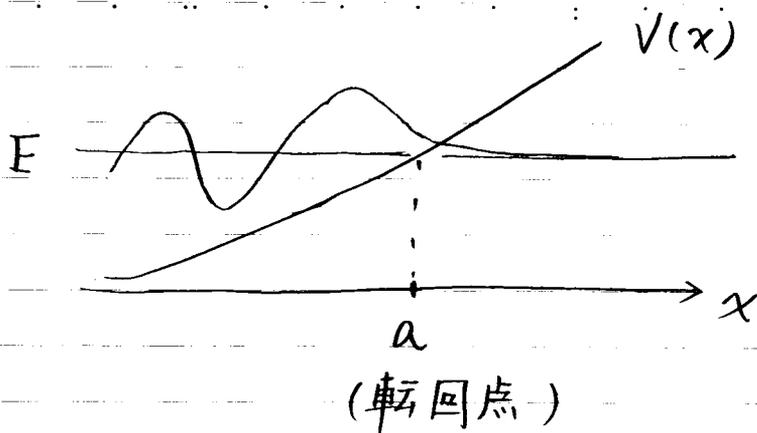
$$= \frac{C'}{\sqrt{k(x)}} e^{\pm i \int^x k(x') dx'}$$

## 4.2. 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。

( $k(x) \sim 0$  だが  $|k'(x)| \ll k(x)^2$  と仮定)。  
( $1/\sqrt{k(x)}$  は発散)

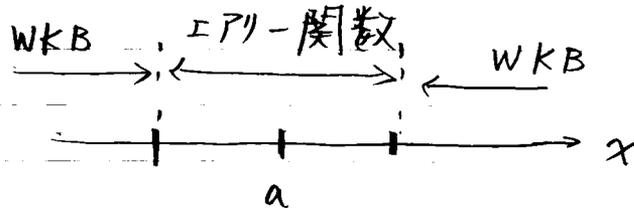
→ WKB 接続公式で転回点をうまく避けることで WKB 近似を有用に使える



$x = a$  のまわりでポテンシャルを展開:

$$V(x) \sim V(a) + \underbrace{V'(a)}_{\text{Airy関数}} (x-a)$$

↓  
解はエアリ-関数



エアリ-関数の漸近形と一致するように  $x = a$  の右側と左側の関数をつなぐ。

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

(note) エアリ-関数

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

$z \rightarrow \infty$  で指数関数的に減衰する解

$$Ai(z) = \frac{1}{\pi} \int_0^{\infty} \cos\left(\frac{t^3}{3} + zt\right) dt$$

$$\rightarrow \begin{cases} \frac{1}{\sqrt{\pi} |z|^{1/4}} \cos\left(\frac{2}{3} |z|^{3/2} - \frac{\pi}{4}\right) & (z \rightarrow -\infty) \\ \frac{1}{2\sqrt{\pi} z^{1/4}} \exp\left(-\frac{2}{3} z^{3/2}\right) & (z \rightarrow \infty) \end{cases}$$

一般に

$$\frac{C}{2} \gamma(x)^{-1/2} e^{-\left|\int_a^x \gamma(x') dx'\right|} \quad (E < V(x))$$

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

$$D \gamma(x)^{-1/2} e^{+\left|\int_a^x \gamma(x') dx'\right|} \quad (E < V(x))$$

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

• 解析接続の方法

$$\psi(x) = \frac{C}{2\sqrt{\gamma(x)}} e^{-\int_a^x \gamma(x') dx'} \quad (x > a)$$

例 3.  $x \sim a$  附近  $V(x) \sim V(a) + V'(a)(x-a)$

↓

$$\gamma(x) \sim \sqrt{\frac{2m}{\hbar^2} (V(a) + V'(a)(x-a) - E)}$$

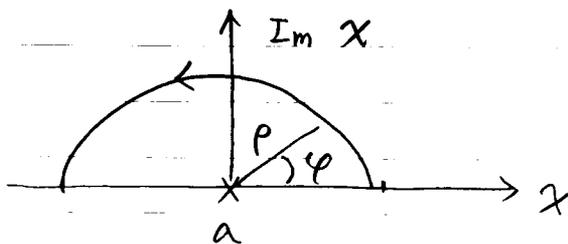
$$= \underbrace{\left( \sqrt{\frac{2m}{\hbar^2} V'(a)} \right)}_{\beta} \sqrt{x-a}$$

≡

$\beta$

↓

$$\psi(x) \sim \frac{C}{2\sqrt{\beta} (x-a)^{1/4}} e^{-\beta \int_a^x \sqrt{x'-a} dx'}$$



$$x-a = \rho e^{i\varphi} \quad \text{と解析接続.}$$

$$(\varphi = 0 \rightarrow \pi)$$

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

$$(x-a)^{1/2} \rightarrow (a-x)^{1/2} e^{i\pi/2} = i(a-x)^{1/2}$$

$$\begin{aligned} \Downarrow \\ \psi(x) &\rightarrow \frac{c e^{-i\pi/4}}{2\sqrt{\beta} (a-x)^{1/4}} e^{-i\beta \int_a^x \sqrt{a-x'} dx'} \\ &\sim \frac{c e^{-i\pi/4}}{2\sqrt{k(x)}} e^{-i \int_a^x k(x') dx'} \end{aligned}$$

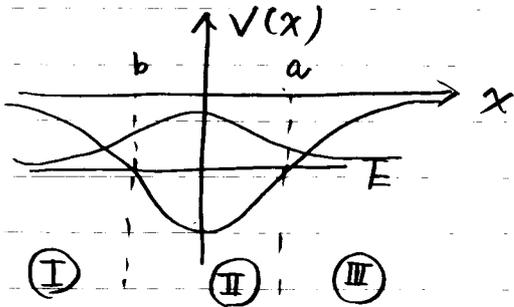
下半面の経路をとると

$$\psi(x) \rightarrow \frac{c e^{i\pi/4}}{2\sqrt{k(x)}} e^{+i \int_a^x k(x') dx'}$$

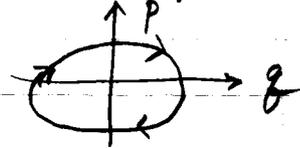
両者の線形結合をとると

$$\begin{aligned} \psi(x) &\rightarrow \frac{c}{\sqrt{k(x)}} \cos \left( \int_a^x k(x') dx' + \frac{\pi}{4} \right) \\ &= \frac{c}{\sqrt{k(x)}} \cos \left( - \int_a^x k(x') dx' - \frac{\pi}{4} \right) \\ &= \frac{c}{\sqrt{k(x)}} \cos \left( \int_x^a k(x') dx' - \frac{\pi}{4} \right) \end{aligned}$$

4.3. ホルン-ポテンシャル-フェルトの量子化条件



cf. ホルン-ポテンシャル原子模型



$$\oint p dq = n\hbar = 2\pi n\hbar$$

領域 I ( $x < b$ ):

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

→ 領域 II ( $b \leq x < a$ ) に接続:

$$\psi_{II}(x) = \frac{2}{\sqrt{k(x)}} \cos\left(\underbrace{\int_b^x k(x') dx'}_{\int_b^a dx' - \int_x^a dx'} - \frac{\pi}{4}\right) \quad (b \leq x < a)$$

$$= \frac{2}{\sqrt{k(x)}} \cos\left(\int_b^a dx' k(x')\right) \cos\left(\int_x^a dx' k(x') + \frac{\pi}{4}\right) + \frac{2}{\sqrt{k(x)}} \sin\left(\int_b^a dx' k(x')\right) \sin\left(\int_x^a dx' k(x')\right)$$

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

$$\cos\theta = \sin\left(\theta + \frac{\pi}{2}\right) = -\sin\left(\theta - \frac{\pi}{2}\right)$$

$$\sin\theta = \cos\left(\theta - \frac{\pi}{2}\right)$$

→ 領域 III ( $x \geq a$ )  $\wedge$

$$\psi_{III}(x) = \frac{2}{\sqrt{\gamma(x)}} \cos\left(\int_b^a dx' k(x')\right) \underbrace{e^{\int_a^x \gamma(x') dx'}}_{\text{---}} + \frac{1}{\sqrt{\gamma(x)}} \sin\left(\int_b^a dx' k(x')\right) e^{-\int_a^x \gamma(x') dx'}$$

↪ 領域 IV 7" 解が exponential 的に  $\psi < 0$  になるため

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

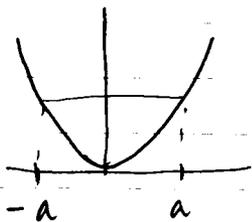
$$\int_b^a dx k(x) = \left(n + \frac{1}{2}\right) \pi \quad (n=0, 1, \dots)$$

$$\oint p(x) dx = \left(n + \frac{1}{2}\right) \cdot \underbrace{2\pi \hbar}_{\hbar}$$

↑  
 $p(x) = k(x)\hbar$



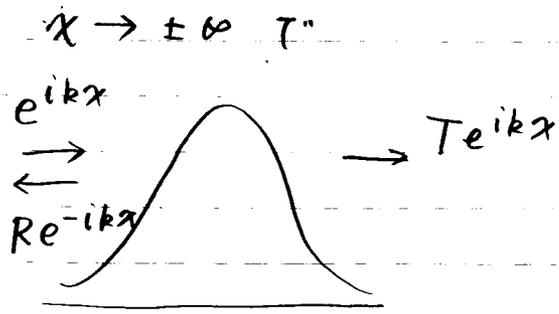
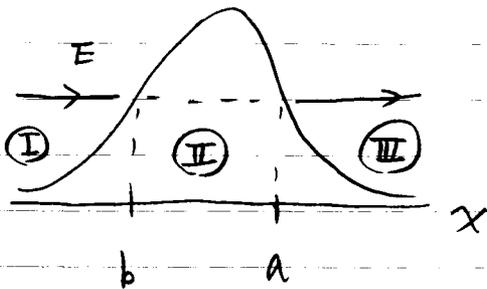
cf. 調和振動子  $V(x) = \frac{1}{2} m \omega^2 x^2$



$$\int_{-a}^a dx k(x) = \dots = \frac{\pi E}{\hbar \omega}$$

$$\rightarrow E = \left(n + \frac{1}{2}\right) \hbar \omega \quad (\text{exact})$$

4.4. トネリ>7"



$$\psi_{III}(x) = \frac{iC}{\sqrt{k(x)}} e^{i\left(\int_a^x k(x') dx' - \frac{\pi}{4}\right)} \quad (x \geq a)$$

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

→ 領域 II

$$\psi_{II}(x) = \frac{C}{\sqrt{\gamma(x)}} e^{\int_x^a \gamma(x') dx'} + \frac{iC}{2} \frac{1}{\sqrt{\gamma(x)}} e^{-\int_x^a \gamma(x') dx'}$$

$$\sim \frac{C}{\sqrt{\gamma(x)}} e^{\int_b^a \gamma(x') dx' - \int_b^x \gamma(x') dx'}$$

→ 領域 I

$$\psi_{I}(x) = \frac{2C}{\sqrt{k(x)}} e^{\int_b^a \gamma(x') dx'} \cos\left(\int_x^b k(x') dx' - \frac{\pi}{4}\right)$$

$$= \frac{C}{\sqrt{k(x)}} \left[ e^{\int_b^a \gamma(x') dx'} \left( e^{i\int_x^b k(x') dx' - \frac{i\pi}{4}} + e^{-i\int_x^b k(x') dx' + \frac{i\pi}{4}} \right) \right]$$

$$\Downarrow \quad P(E) = \frac{J_{III}}{J_I} = e^{-2\int_b^a \gamma(x') dx'} = e^{-2\int_b^a \sqrt{\frac{2m}{\hbar^2} (V(x) - E)} dx}$$

→ Eが関数 <math>E < V(x)</math> exp. 的,  $m$ が大きいほど  $P(E)$ は小,

## 4.5. 経路積分と半古典近似

### 経路積分

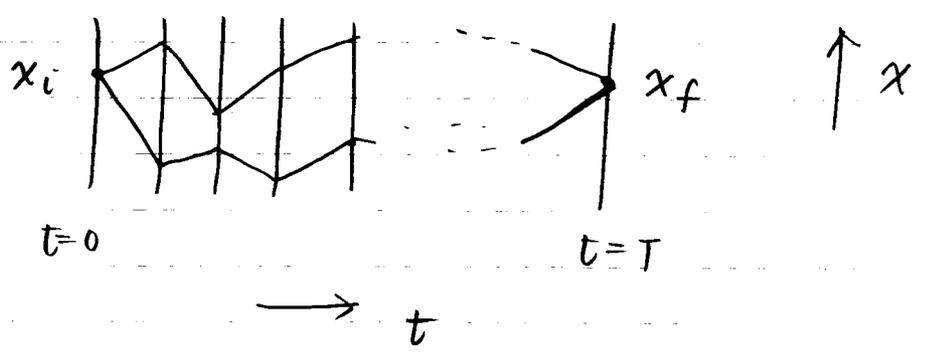
座標  $x_i$   $\xrightarrow{\text{時間 } T}$   $x_f$  の遷移

$$K(x_f, x_i; T) = \langle x_f | e^{-i\hat{H}T/\hbar} | x_i \rangle$$

時間インターバルを  $N$  等分

$$\downarrow e^{-i\hat{H}T/\hbar} = \underbrace{e^{-i\hat{H}\Delta t/\hbar} e^{-i\hat{H}\Delta t/\hbar} \dots e^{-i\hat{H}\Delta t/\hbar}}_{N \text{ 回}} \quad (\Delta t = \frac{T}{N})$$

$$= \left( \int dx_N |x_N\rangle \langle x_N| \right) e^{-i\hat{H}\Delta t/\hbar} \left( \int dx_{N-1} |x_{N-1}\rangle \langle x_{N-1}| \right) e^{-i\hat{H}\Delta t/\hbar} \dots \left( \int dx_1 |x_1\rangle \langle x_1| \right) e^{-i\hat{H}\Delta t/\hbar} \\ \times \left( \int dx_0 |x_0\rangle \langle x_0| \right)$$



$x_i$  と  $x_f$  を結ぶすべての経路を足し合わせる。

$$\downarrow$$

$$K(x_f, x_i; T) = \dots = \lim_{N \rightarrow \infty} \sqrt{\frac{m}{2\pi\hbar \cdot i\Delta t}} \prod_{i=1}^{N-1} \int \left( \sqrt{\frac{m}{2\pi\hbar \cdot i\Delta t}} dx_i \right) \\ \times e^{\frac{i}{\hbar} \Delta t \left( \frac{m}{2} \left( \frac{x_i - x_{i-1}}{\Delta t} \right)^2 - V\left(\frac{x_i + x_{i-1}}{2}\right) \right)}$$

$$= \int_{x(0)=x_i}^{x(T)=x_f} dl[x(t)] e^{\frac{i}{\hbar} S(x, T)} \quad (\text{経路積分})$$

$$S(x, T) = \int_0^T dt L(x, \dot{x}) = \int_0^T dt \left( \frac{m}{2} \dot{x}^2 - V(x) \right)$$

(note) 古典力学

最小作用の原理  $\frac{\delta}{\delta x} S = 0$

$$\rightarrow \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) = \frac{\partial L}{\partial x}$$

・半古典近似

$\hbar \rightarrow 0$  時は  $e^{iS/\hbar}$  は激しく振動

→ 積分は正負が打ち消し合いゼロに

→ 但し、停留点 ( $\frac{\delta}{\delta x} S = 0$ ) 近傍では打ち消し合いがおこらない

半古典近似:  $x(t) = x_{cl}(t) + \delta x(t)$  とおき  
 $\delta x$  の 2次まで考慮 (停留位相近似)

$$\downarrow$$

$$V(x) \sim V(x_{cl}) + \cancel{(\delta x) V'(x_{cl})} + \frac{(\delta x)^2}{2} V''(x_{cl}) + \dots$$

停留条件で零となる

(→ 半古典近似は 2次関数ポテンシャルに対しては exact)

$$K(x_i, x_f, T) \sim (\text{係数}) \times e^{iS_{cl}/\hbar}$$