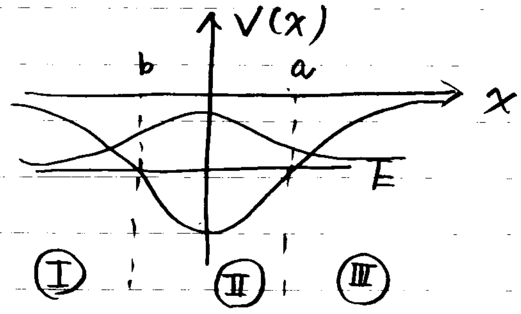
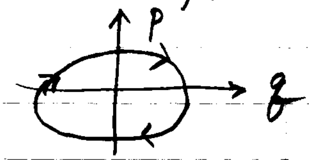
DEPARTMENT OF PHYSICS
GRADUATE SCHOOL OF SCIENCE
KYOTO UNIVERSITY

4.3. ボーア・ゾンマーフェルトの量子化条件



cf. ボーアの原子模型



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

領域 I $(x < b)$:

$$\psi_{\mathrm{I}}(x) = \frac{1}{\sqrt{\gamma(x)}} e^{-\int_x^b \gamma(x')dx'} \qquad (x<b)$$

→ 領域 II $(b \le x < a)$ に接続:

$$\psi_{\mathrm{II}}(x) = \frac{2}{\sqrt{k(x)}} \cos\Big(\underbrace{\int_b^x k(x')dx'}_{\int_b^a dx' - \int_x^a dx'} - \frac{\pi}{4} \Big) \qquad (b \le x < a)$$

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

$$+ \frac{2}{\sqrt{k(x)}} \sin\left(\qquad \right) \sin\left(\qquad \right)$$

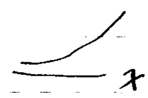
$$= -\frac{2}{\sqrt{k(x)}} \cos\left(\int_b^a dx' k(x')\right) \sin\left(\int_x^a dx' k(x') - \frac{\pi}{4}\right)$$

$$+ \frac{2}{\sqrt{k(x)}} \sin\left(\qquad \right) \cos\left(\qquad \right)$$

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

→ 領域 III $(x \geq a)$ へ

$$\psi_{III}(x) = \frac{2}{\sqrt{\gamma(x)}} \cos\left(\int_b^a dx' \, k(x') \right) e^{\int_a^x \gamma(x') dx'}$$



$$+ \frac{1}{\sqrt{\gamma(x)}} \sin\left(\int_b^a dx' \, k(x') \right) e^{-\int_a^x \gamma(x') dx'}$$

↓ 領域 III で解が exponential 的に小さくなるためには

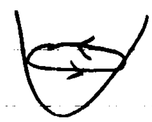
$$\cos\left(\int_b^a dx \, k(x) \right) = 0$$ が必要

↓

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

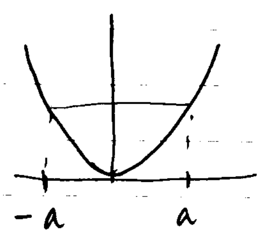
↓

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



↑ $p(x) = k(x)\hbar$ 　 $2\pi\hbar = h$

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



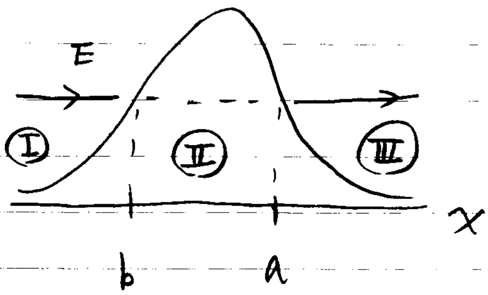
$$\int_{-a}^{a} dx \, k(x) = \cdots = \frac{\pi E}{\hbar\omega}$$

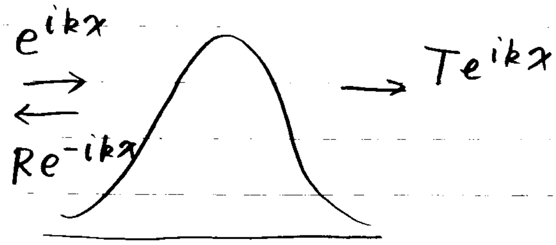
↓

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

4.4. トンネリング

$x \to \pm\infty$ で





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

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

$\longrightarrow$ 領域 II へ

$$\psi_{II}(x) = \frac{C}{\sqrt{\gamma(x)}}\, e^{\int_x^a \gamma(x')dx'} + \cancel{\frac{iC}{2}\frac{1}{\sqrt{\gamma(x)}}\, e^{-\int_x^a \gamma(x')dx'}} \sim 0$$

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

$\longrightarrow$ 領域 I へ

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

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

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

$\longrightarrow$ Eの関数として exp. 的，mが大きいほどP(E)は小，

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4.5. 経路積分と半古典近似

経路積分

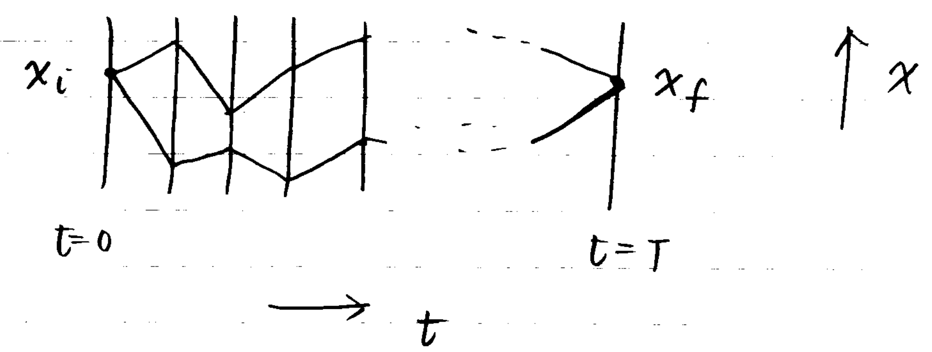
座標 $x_i \xrightarrow{\text{時間}T} x_f$ の遷移

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

時間インターバルを N 等分

$$e^{-i\hat{H}T/\hbar} = \underbrace{e^{-i\hat{H}\Delta t/\hbar}\, e^{-i\hat{H}\Delta t/\hbar} \cdots e^{-i\hat{H}\Delta t/\hbar}}_{N\text{コ}} \quad \left(\Delta t = \frac{T}{N}\right)$$

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



x_i と x_f を結ぶすべての経路を足し合わせる。

$$K(x_f, x_i; T) = \cdots = \lim_{N\to\infty} \sqrt{\frac{m}{2\pi\hbar \cdot i\Delta t}} \prod_{i=1}^{N-1} \int \left(\sqrt{\frac{m}{2\pi\hbar i\Delta t}}\, dx_i \right)$$

$$\times e^{\frac{i}{\hbar}\Delta t \left(\frac{m}{2} \left(\frac{x_i - x_{i-1}}{\Delta t}\right)^2 - V\left(\frac{x_i + x_{i+1}}{2}\right)\right)}$$

$$= \int_{\substack{x(0)=x_i \\ x(T)=x_f}} d\mathcal{l}[x(t)]\, e^{\frac{i}{\hbar}S(x,T)}$$ （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

$\hbar \to 0$ では $e^{iS/\hbar}$ 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 $\left(\frac{\delta}{\delta x} S = 0\right)$ 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
δx の2次まで考慮．（停留位相近似）

$$V(x) \sim V(x_{cl}) + \underbrace{\cancel{(\delta x) V'(x_{cl})}}_{\text{停留条件で寄与なし}} + \frac{(\delta x)^2}{2} V''(x_{cl}) + \cdots$$

(→ 半古典近似は2次関数ポテンシャルに対しては exact).

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