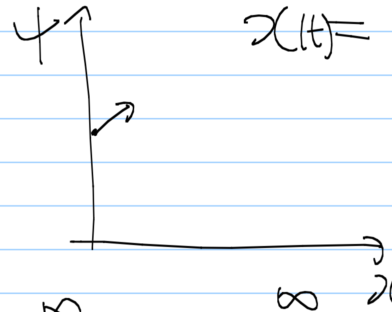
基礎物理化学A　2007年度 前期

ノートのタイトル　2007/05/09

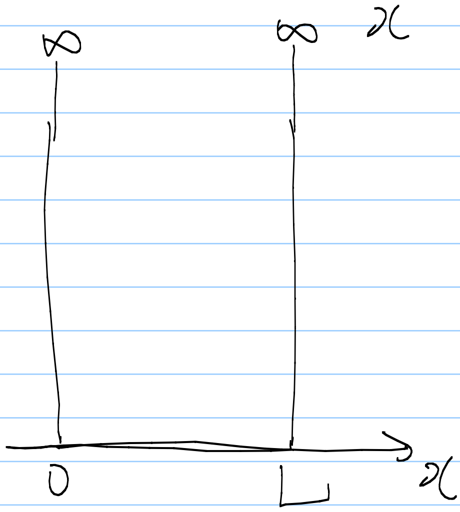


$$x(t) = x_0 + vt$$

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

$$\psi = \psi(0) + \psi' \Delta x$$

$$\psi' = \psi'(0) + \psi'' \Delta x$$



$$V(x) = \begin{cases} 0 & (0<x<L) \\ +\infty & (x \leq 0,\ x \geq L) \end{cases}$$

$0<x<L$ で

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

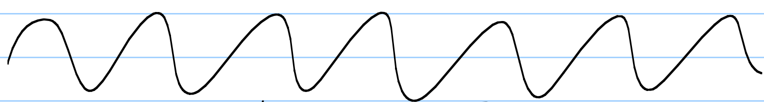
$$\psi'' = -\underbrace{\frac{2mE}{\hbar^2}}_{=k^2}\psi = -k^2\psi$$

$$\psi = \cancel{A} e^{ikx}, \quad \psi = e^{-ikx}$$

$$\psi' = ik\, e^{ikx}$$

$$\psi'' = \underbrace{(ik)^2}_{-k^2} e^{ikx}$$

$$\psi = Ae^{ikx} + Be^{-ikx}$$



自由粒子

境界条件 $\begin{cases} \psi(0)=0 & \cdots ① \\ \psi(L)=0 & \cdots ② \end{cases}$

さもないと、$V=+\infty$ の領域に粒子を見いだす確率 $\neq 0$　　$|\psi|^2$

① より　$A+B=0$　$(e^0=1)$

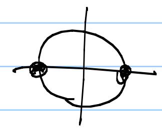
$$\psi(x)=A\left(e^{ikx}-e^{-ikx}\right)$$

$\cancel{\cos + i}$

$$= 2iA \sin kx$$

改めて A と書く

② より　$A\sin kL=0$



よって　$kL=\cancel{2}n\pi$　$(n=0,\pm1,\pm2\cdots)$

$$k=\frac{n\pi}{L}$$

波長 λ

$\sin\left(\frac{2\pi}{\lambda}x\right)$　　$k=\frac{2\pi}{\lambda}$ 波数

$$\frac{2mE}{\hbar^2}=k^2 \rightarrow E=\frac{\hbar^2k^2}{2m}$$

$$E=\frac{\hbar^2\pi^2}{2mL^2}n^2$$

$\frac{\hbar^2\pi^2}{2mL^2}=\varepsilon$

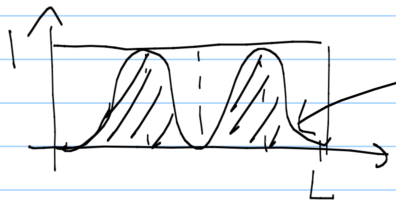
$$E=\varepsilon,\ 4\varepsilon,\ 9\varepsilon,\ 16\varepsilon\ \cdots$$

エネルギーの量子化

$$\psi(x) = A \sin\left(\frac{n\pi}{L}x\right)$$

規格化 $\int_0^L |\psi|^2 dx = 1$

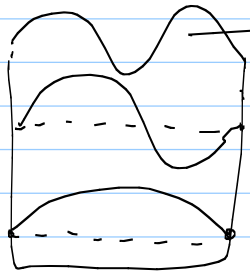
$\Longrightarrow$ A を決める.



$\sin^2 kx$

$$\int_0^L \sin^2 kx \, dx = \frac{L}{2}$$

$$A = \sqrt{\frac{2}{L}}$$



$$L = \frac{\lambda}{2} n = \frac{2\pi}{k} \cdot \frac{n}{2}$$

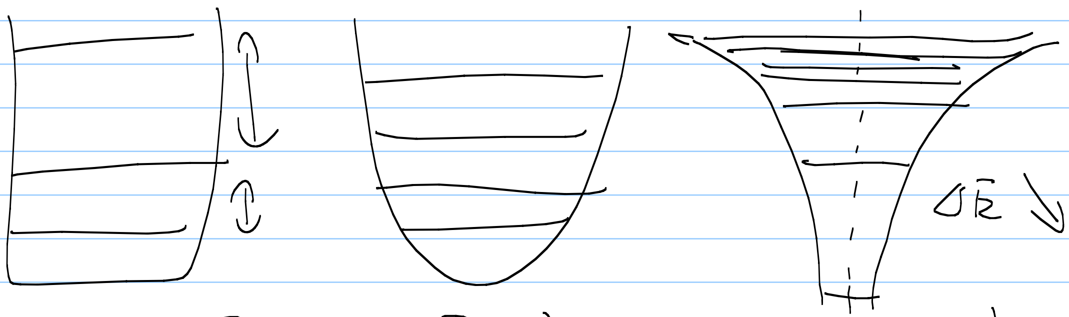
~~x2~~

$$k = \frac{n\pi}{L}$$

$$E \propto \frac{1}{mL^2}$$

軽い粒子、狭い領域

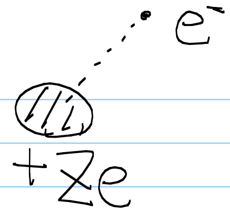
→ エネルギー量子 大



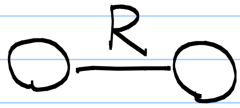
ΔE ↗ ΔE 一定 $V(r) \propto -\frac{1}{r}$

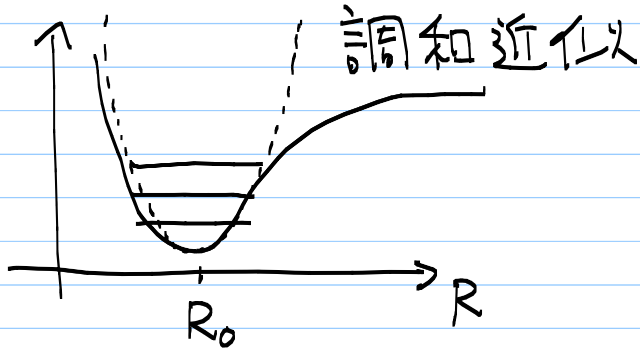
$E_n \propto n^2$ $E_n \propto n$ $E_n \propto \frac{1}{n^2}$

水素類似原子
(1電子)

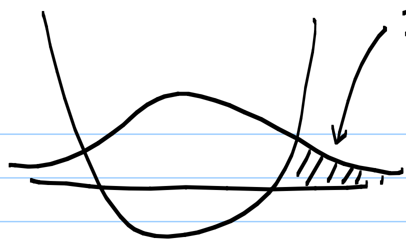


H, He^+, Li^{2+}, ……

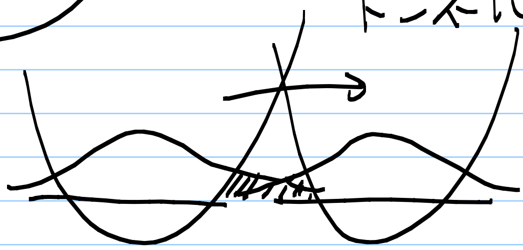




固体結晶　音波
→ phonon

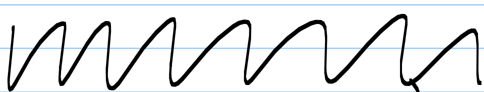


非古典的なしみ出し

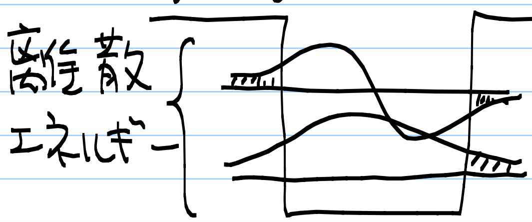


トンネル効果

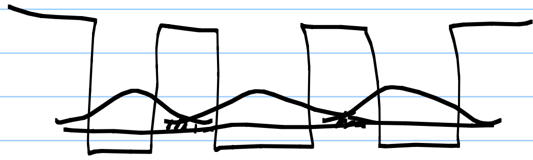
有限深さのポテンシャル

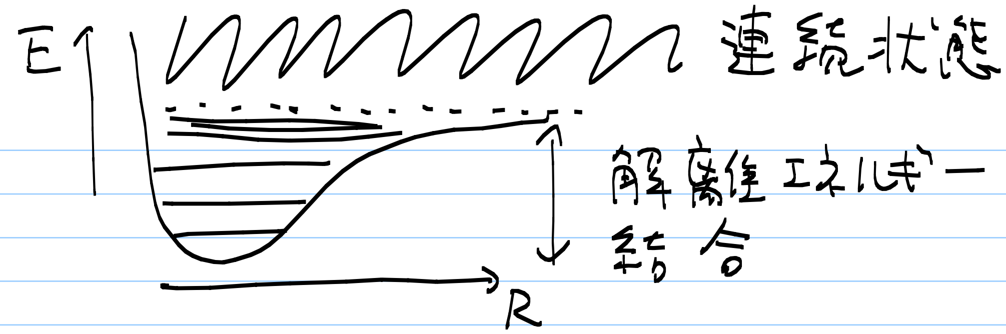


(井戸型ポテンシャル)

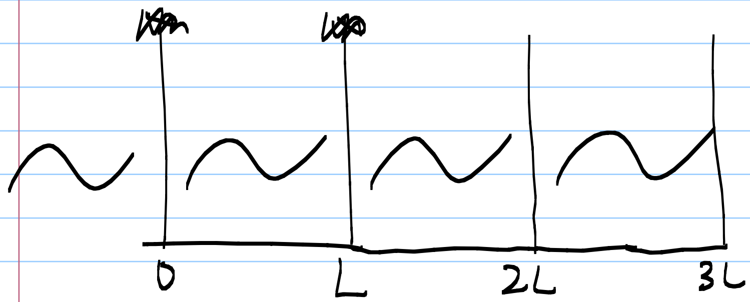


連続エネルギー





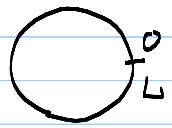
1次元の箱の中の粒子
周期的境界条件を適用する場合



$V(x) = 0$

$\psi(x+L) = \psi(x) \cdots ①$

(固体結晶内電子・原子核運動のモデル)



$$-\frac{\hbar^2}{2m}\psi'' = E\psi \rightarrow \psi \propto e^{\pm ikx}$$

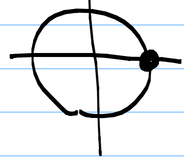
$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

$\psi(x) = Ae^{ikx}$ とおいて、① を適用

$$Ae^{ik(x+L)} = Ae^{ikx}$$

$$\rightarrow e^{ikL} = 1$$

$e^{ix} = \cos x + i\sin x$



$$kL = 2\pi n \quad (n = 0, \pm 1, \pm 2, \cdots) \quad ②$$

$$k = \frac{2\pi}{L}n \quad (\text{量子化された})$$

規格化 $\int_0^L |\psi(x)|^2 dx = 1$

$$\rightarrow |A|^2 \int_0^L 1\, dx = 1$$

$$\rightarrow |A|^2 L = 1 \rightarrow A = \sqrt{\frac{1}{L}}$$

とればよい

$$\psi(x) = \sqrt{\frac{1}{L}}\, e^{ikx}$$

（これの重ね合せ

$$\psi(x) = \sum_k A_k e^{ikx}$$

を取っても良い）

②で

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\cdot\frac{4\pi^2}{L^2} n^2$$

$$\left(\hbar = \frac{h}{2\pi}\right) \qquad = \frac{2\hbar^2\pi^2}{mL^2} n^2 = \frac{h^2}{2mL^2} n^2$$