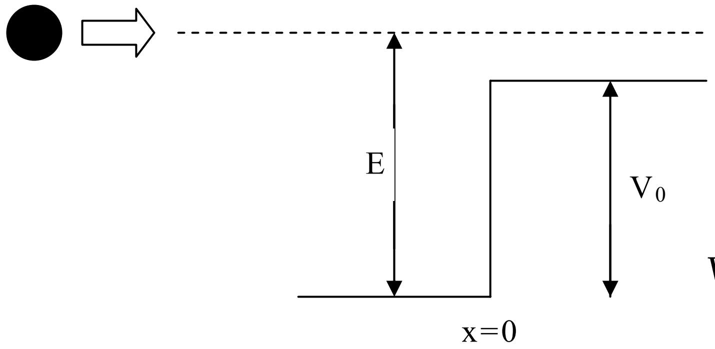
POSTECH 이성익 교수의
양자 세계에 관한 강연
- 4장 -

편집 도우미: POSTECH 학부생 정윤영

Chapter 4

One-Dimensional Potentials



$$V(x)=\begin{cases}0 & ,x<0\\ V_0 & ,x>0\end{cases}$$

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}+V(x)\cdot u(x)=E\cdot u(x)$$

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

x<0,

$$\frac{d^2u(x)}{dx^2}=-\frac{2mE}{\hbar^2}u(x)=-k^2\cdot u(x) \qquad k=\frac{\sqrt{2mE}}{\hbar}$$

$$\therefore u(x)=e^{ikx}+R\cdot e^{-ikx}$$

x>0,

$$\frac{d^2u(x)}{dx^2}=-\frac{2m(E-V_0)}{\hbar^2}\cdot u(x)=-q^2\cdot u(x)$$

$$q=\frac{\sqrt{2m(E-V_0)}}{\hbar}$$

$$\therefore u(x)=T\cdot e^{iqx}$$

$$j=\frac{\hbar}{2im}\left(\psi^{*}\frac{d\psi}{dx}-\frac{d\psi^{*}}{dx}\psi\right)$$: Continuity equation

x<0,

$$j=\frac{\hbar}{2im}\left(\left(e^{-ikx}+R^{*}e^{ikx}\right)\left(ike^{ikx}-Rike^{-ikx}\right)-\left(-ike^{-ikx}+R^{*}ike^{ikx}\right)\left(e^{ikx}+Re^{-ikx}\right)\right)$$

$$=\frac{\hbar k}{m}\left(1-|R|^{2}\right)$$

x>0,

$$j=\frac{\hbar q}{m}|T|^{2}$$

$$\therefore k\left(1-|R|^{2}\right)=q|T|^{2}$$

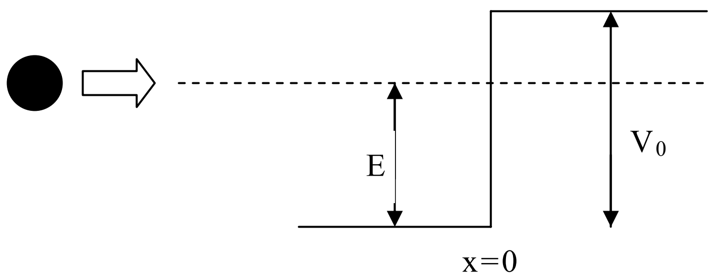
x=0에서의 boundary condition을 적용하면,

$$1+R=T \qquad \left(\because \psi\left(\varepsilon^{-}\right)=\psi\left(\varepsilon^{+}\right)\right)$$

$$k(1-R)=T\cdot q \qquad \left(\because \psi'\left(\varepsilon^{-}\right)=\psi'\left(\varepsilon^{+}\right)\right)$$

$$\therefore T=\frac{2k}{k+q} \qquad R=\frac{k-q}{k+q}$$

$$\therefore k\left(1-|R|^{2}\right)=k\left(1-\frac{(k-q)^{2}}{(k+q)^{2}}\right)=\frac{4k^{2}q}{(k+q)^{2}}=q|T|^{2}$$



$$V(x)=\begin{cases}0 & ,x<0\\ V_0 & ,x>0\end{cases}$$

x<0,

$$u(x)=e^{ikx}+R\cdot e^{-ikx}\quad k=\frac{\sqrt{2mE}}{\hbar}$$

x>0,

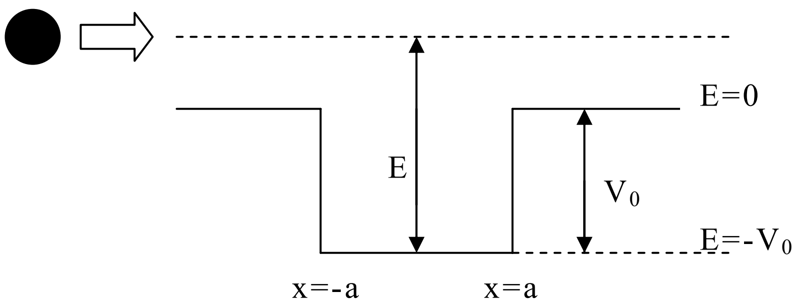
$$u(x)=T\cdot e^{-Qx}\qquad\qquad Q=\sqrt{\frac{2m}{\hbar^2}(V_0-E)}$$

$$\therefore 1+R=T$$

$$ik(1-R)=-Q\cdot T$$

$$\therefore T=\frac{2}{1+\frac{iQ}{k}}\qquad\qquad R=\frac{1-\frac{iQ}{k}}{1+\frac{iQ}{k}}$$

Potential Well



$$V(x)=\begin{cases}-V_0 & ,-a<x<a\\ 0 & ,otherwise\end{cases}$$

x<-a, $u(x)=e^{ikx}+R\cdot e^{-ikx}$

-a<x<a, $u(x)=A\cdot e^{iqx}+B\cdot e^{-iqx}$

x>a, $u(x)=T\cdot e^{ikx}$

$$k=\frac{\sqrt{2mE}}{\hbar} \qquad q=\frac{\sqrt{2m(E+V_0)}}{\hbar}$$

$$\therefore \frac{\hbar k}{m}\left(1-|R|^2\right)=\frac{\hbar q}{m}\left(|A|^2-|B|^2\right)=\frac{\hbar k}{m}|T|^2$$ (by the continuity equation)

x=-a & x=a에서의 boundary condition을 적용하면,

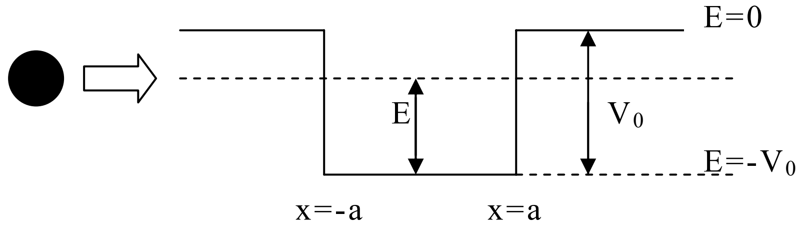
$$e^{-ika}+R\cdot e^{ika}=A\cdot e^{-iqa}+B\cdot e^{iqa}$$
$$ike^{-ika}-R\cdot ike^{ika}=A\cdot iqe^{-iqa}-B\cdot iqe^{iqa}$$
$$A\cdot e^{iqa}+B\cdot e^{-iqa}=T\cdot e^{ika}$$
$$iq\left(A\cdot e^{iqa}-B\cdot e^{-iqa}\right)=ikT\cdot e^{ika}$$

$$\therefore R=\frac{\left(q^2-k^2\right)e^{-2ika}\sin 2qa}{\sin 2qa\left(q^2+k^2\right)-2iqk\cos 2qa}$$

$$T=e^{-2ika}\frac{2kq}{2kq\cos 2qa-i\left(q^2+k^2\right)\sin 2qa}$$

1. E→0이면, k→0, T→0, & R→1이다. 하지만 고전역학적으로 생각해 보면 E→0인 조건에서 T→0이 될 수 없다.

2. $\sin 2qa=0$ 이면, R=0 & $|T|^2=1$.



$$V(x) = \begin{cases} -V_0 & ,-a < x < a \\ 0 & ,otherwise \end{cases}$$

$$u(x) = \begin{cases} C_1 \cdot e^{kx} & , \quad x < -a \\ C_2 \cdot e^{-kx} & , \quad x > a \\ A \cdot \cos qx + B \cdot \sin qx & , \quad -a \le x \le a \end{cases}$$

$$q = \frac{\sqrt{2m(V_0 + E)}}{\hbar} \qquad k = \frac{\sqrt{-2mE}}{\hbar^2}$$

x=-a & x=a에서의 boundary condition을 적용하면,

$$C_1 \cdot e^{-ka} = A \cdot \cos qa - B \cdot \sin qa$$
$$kC_1 \cdot e^{-ka} = qA \cdot \sin qa + qB \cdot \cos qa$$
$$C_2 \cdot e^{-ka} = A \cdot \cos qa + B \cdot \sin qa$$
$$-kC_2 \cdot e^{-ka} = -qA \cdot \sin qa + qB \cdot \cos qa$$

⋮

⋮

∴ A or B = 0

Even parity,

$$u(x) = \begin{cases} e^{kx} & , \quad x < -a \\ e^{-kx} & , \quad x > a \\ A \cdot \cos qx & , \quad -a \le x \le a \end{cases}$$

x=0에서 symmetric하므로, x=a에서 boundary condition을 만족하면 x=-a에서도 만족할 것이다. 즉, x=a에서의 boundary condition만 따져주면 된다.

$$e^{-ka} = A \cdot \cos qa$$

$$-ke^{-ka} = -qA \cdot \sin qa$$

$$\therefore k = q\frac{\sin qa}{\cos qa} = q\tan qa$$

$$\therefore \sqrt{\frac{-2mE}{\hbar^2}} = \sqrt{\frac{2m\left(E+V_0\right)}{\hbar^2}}\tan qa$$

$$\therefore \sqrt{-\frac{E}{E+V_0}} = \tan qa = \tan\sqrt{\frac{2m\left(E+V_0\right)}{\hbar^2}}a$$

$\lambda \equiv \dfrac{2mV_0a^2}{\hbar^2}$ 로 정의하면,

$$\therefore \frac{E}{E+V_0} = \frac{\frac{2m}{\hbar^2}Ea^2}{\frac{2m}{\hbar^2}\left(E+V_0\right)a^2} = \frac{\frac{2m}{\hbar^2}\left(E+V_0\right)a^2 - \frac{2m}{\hbar^2}V_0a^2}{\frac{2m}{\hbar^2}\left(E+V_0\right)a^2}$$

$$= \frac{q^2a^2-\lambda}{q^2a^2} = \frac{y^2-\lambda}{y^2}$$

$$\therefore \tan y = \frac{\sqrt{\lambda - y^2}}{y}$$

$$\begin{cases} \sqrt{\lambda} < \pi & , \text{ 한개} \\ \pi < \sqrt{\lambda} < 2\pi & , \text{ 두개} \\ \vdots & , \end{cases}$$

Potential이 아무리 얇아도 최소한 1개의 energy state가 존재한다.

Odd parity,

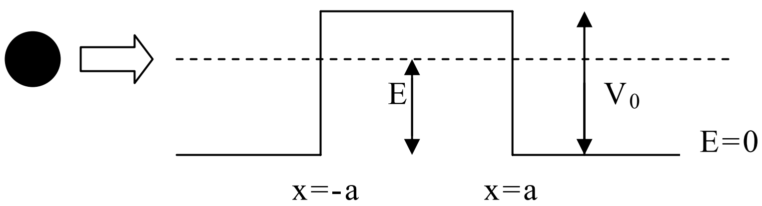
$$\sqrt{\frac{-2mE}{\hbar^2}} = -q\cot qa$$

$$\cot qa = -\frac{\sqrt{\lambda - y^2}}{y}$$

$$\therefore \frac{\sqrt{\lambda - y^2}}{y} = -\cot qa$$

$\sqrt{\lambda} < \dfrac{\pi}{2}$ 이면, 해가 존재하지 않는다.

Potential Barrier



$$V(x) = \begin{cases} V_0 & ,-a < x < a \\ 0 & ,otherwise \end{cases}$$

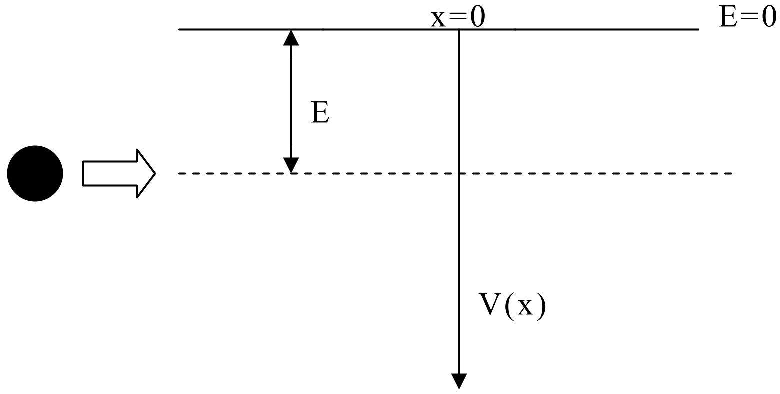
$$|T|^2 = \frac{(2\kappa k)^2}{(2\kappa k)^2 + (\kappa^2 + k^2)\sinh^2 2\kappa a}$$

$\kappa a >> 1$,

$$\sinh 2\kappa a = \frac{1}{2}\left(e^{2\kappa a} - e^{-2\kappa a}\right) \simeq \frac{1}{2}e^{2\kappa a}$$

$$\therefore |T|^2 \simeq \frac{16k^2}{\kappa^2}e^{-4\kappa a}$$

Single Delta-Potential Well



$$V(x) = -\frac{\hbar^2 \lambda}{2ma}\delta(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + V(x).u(x) = E\cdot u(x)$$

$$\int_{\varepsilon^-}^{\varepsilon^+} -\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} - \frac{\hbar^2\lambda}{2ma}\delta(x).u(x)dx = \int_{\varepsilon^-}^{\varepsilon^+} E\cdot u(x)$$

$$(\text{우변}) = 0$$

$$(\text{좌변}) = \int_{\varepsilon^-}^{\varepsilon^+} -\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} - \frac{\hbar^2\lambda}{2ma}\delta(x)\cdot u(x)dx$$

$$= -\frac{\hbar^2}{2m}\left(u'\left(\varepsilon^+\right) - u'\left(\varepsilon^-\right)\right) - \frac{\hbar^2\lambda}{2ma}u(0)$$

$$\therefore u'\left(\varepsilon^+\right) - u'\left(\varepsilon^-\right) = -\frac{\lambda}{a}u(0)$$

$$\frac{d^2u(x)}{dx^2} - \kappa^2\cdot u(x) = 0 \qquad \kappa = \frac{\sqrt{-2mE}}{\hbar}$$

x<0,

$$u(x) = e^{\kappa x}$$

x>0,

$$u(x) = e^{-\kappa x}$$

$$\therefore -\kappa e^{-\kappa\cdot 0} - \kappa e^{\kappa\cdot 0} = -\frac{\lambda}{a}$$

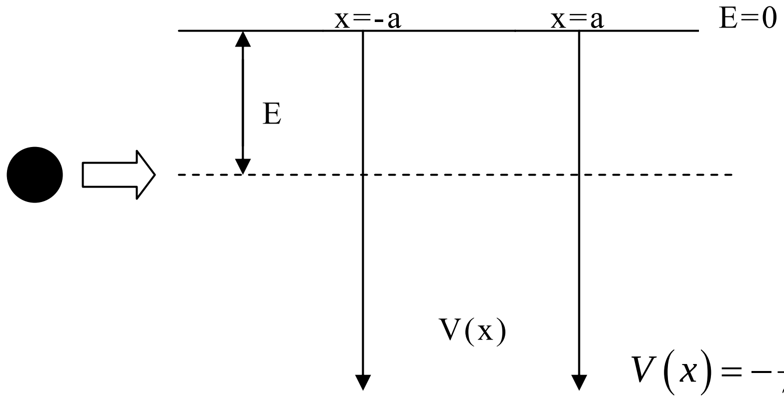
$$\therefore \kappa = \frac{\lambda}{2a}$$

There exists only one even solution.
There exists no odd solution.

Solution이 존재할 조건.

1. u(0)에서 연속.
2. u'(0)에서 boundary condition 만족.
3. u(x)가 "well define"된다. (적분 값이 유한하다.)

Double Delta-Potential Well



$$V(x) = -\frac{\hbar^2\lambda}{2ma}\left(\delta(x-a)+\delta(x+a)\right)$$

Even solution,

$$u(x) = \begin{cases} e^{\kappa x} & , \quad x < -a \\ A\cdot\cosh\kappa x & , \quad -a \le x \le a \\ e^{-\kappa x} & , \quad x > a \end{cases} \qquad E = -\frac{\hbar^2\kappa^2}{2m}$$

x=a에서 boundary condition을 적용,

$$e^{-\kappa a} = A\cdot\cosh\kappa a$$

$$-\kappa e^{-\kappa a} - A\kappa\cdot\sinh\kappa a = -\frac{\lambda}{a}e^{-\kappa a}$$

$$\therefore \tanh \kappa a = \frac{\lambda}{\kappa a} - 1$$

$$\therefore 0 < \frac{\lambda}{\kappa a} - 1 < 1$$

$$\therefore \frac{\lambda}{\kappa a} < 2$$

$$\therefore \kappa > \frac{\lambda}{2a}$$

There always exists even solution.

(Single Delta-Potential Well에서는 $\kappa = \frac{\lambda}{2a}$)

Odd solution,

$$u(x) = \begin{cases} e^{\kappa x} & , \quad x < -a \\ A \cdot \sinh \kappa x & , \quad -a \le x \le a \\ e^{-\kappa x} & , \quad x > a \end{cases}$$

$$\therefore \tanh a\kappa = \frac{a\kappa}{\lambda - a\kappa}$$

There may or may not exists odd solution.

Harmonic Oscillator

$$V(x) = \frac{1}{2}kx^2 \qquad k = mw^2$$

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

$$\therefore -\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + \frac{1}{2}kx^2 \cdot u(x) = E \cdot u(x)$$

식을 간단하게 하기 위해 α를 다음과 같이 정의한다.

$$\alpha = \sqrt{\frac{\hbar}{mw}} \qquad\qquad x \equiv \alpha y$$

$$\therefore -\frac{d^2u(y)}{dy^2} + \frac{mk\alpha^4}{\hbar^2} y^2 \cdot u(y) = \frac{2mE\alpha^2}{\hbar^2} \cdot u(y)$$

$$\varepsilon = \frac{2m\alpha^2 E}{\hbar^2} = \frac{2E}{\hbar w}$$

$$\therefore \frac{d^2u(y)}{dy^2} + (\varepsilon - y^2) \cdot u(y) = 0$$

$y \to \pm\infty$ 일 때, $u \to 0$

$$\therefore \frac{d^2u(y)}{dy^2} - y^2 \cdot u(y) = 0$$

$\therefore u(y) = h(y) \cdot e^{-\frac{y^2}{2}}$ 라고 가정하고 h(y)를 구한다.

$$\therefore \frac{d^2u}{dy^2} = \frac{d^2h}{dy^2} e^{-\frac{y^2}{2}} - 2y\frac{dh}{dy} e^{-\frac{y^2}{2}} - he^{-\frac{y^2}{2}} + y^2 he^{-\frac{y^2}{2}}$$

$$\therefore 0 = \frac{d^2h}{dy^2} - 2y\frac{dh}{dy} + (\varepsilon - 1)h$$

$\therefore h(y) = \sum_{m=0}^{\infty} a_m \cdot y^m$ 라고 가정하고 partial differential equation을 푼다.

$$\therefore 0 = \sum_{m=2}^{\infty} a_m m(m-1) y^{m-2} - 2\sum_{m=1}^{\infty} a_m m \cdot y^m + (\varepsilon - 1)\sum_{m=0}^{\infty} a_m \cdot y^m$$

$$= \sum_{m=0}^{\infty} a_{m+2} (m+2)(m+1) y^m - 2\sum_{m=1}^{\infty} a_m m \cdot y^m + (\varepsilon - 1)\sum_{m=0}^{\infty} a_m \cdot y^m$$

m=0, $2\cdot a_2+(\varepsilon-1)a_0=0$

m≠0, $(m+2)(m+1)a_{m+2}=(2m-\varepsilon+1)a_m$

$$\therefore a_{m+2}=\frac{(2m-\varepsilon+1)}{(m+2)(m+1)}a_m$$

$m\to\infty$일 때, $a_{m+2}\sim\frac{2}{m}a_m$

$$\therefore h(y)=a_0y+a_2y^2+a_4y^4+a_6y^6+\cdots\sim e^{y^2}$$

$$\therefore u(y)=h(y)\cdot e^{-\frac{y^2}{2}}\sim e^{y^2}\cdot e^{-\frac{y^2}{2}}=e^{\frac{y^2}{2}}$$

This u(y) is not integrable..

$\rightarrow contradiction!$

위의 문제를 해결하기 위해서 특정 m 값 이상에서는 a_m이 0이 되도록 하여 h(y)가 exponential함수가 되지 않도록 한다.

$$\therefore \varepsilon=2N+1$$

$\varepsilon=\frac{2m\alpha^2E}{\hbar^2}=\frac{2E}{\hbar w}$(위의 계산과정에서 ε을 이와 같이 정의)

$$\therefore E=\left(N+\frac{1}{2}\right)\cdot\hbar w \qquad N=0,1,2,3,4,\cdots$$

h(y)는 Hermite Polynomial로 해가 다음과 같이 구해져 있다.

$$H_{N=0}(y)=1$$
$$H_{N=1}(y)=2y$$
$$H_{N=2}(y)=4y^2-2$$
$$H_{N=3}(y)=8y^3-12y$$
$$H_{N=4}(y)=16y^4-48y^2+12$$
$$\vdots$$