H.W. #2.

2. kronig-penney model (fig. 4.9)

at region I : $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$ $(V_0 = 0)$

region II : $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0$

$$\Rightarrow \psi_I = A \cdot e^{i\alpha x} + B \cdot e^{-i\alpha x} \quad \left(\alpha = \sqrt{\frac{2mE}{\hbar^2}}\right)$$

$$\psi_{II} = C \cdot e^{-\gamma x} + D \cdot e^{\gamma x} \quad \left(\gamma = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}\right)$$

Boundary condition에 의하여,

$$\psi_I(x=0) = \psi_{II}(x=0), \quad \frac{d\psi_I(x=0)}{dx} = \frac{d\psi_{II}(x=0)}{dx}$$

$$\psi_I(x=a) = \psi_{II}(x=-b), \quad \frac{d\psi_I(x=a)}{dx} = \frac{d\psi_{II}(x=-b)}{dx}$$

$$\Rightarrow \begin{pmatrix} 1 & 1 & -1 & -1 \\ i\alpha & -i\alpha & \gamma & -\gamma \\ e^{i\alpha a} & e^{-i\alpha a} & -e^{\gamma b} & -e^{-\gamma b} \\ i\alpha e^{i\alpha a} & -i\alpha e^{-i\alpha a} & \gamma \cdot e^{\gamma b} & -\gamma e^{-\gamma b} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

A=B=C=D=0 이외의 해가 존재하기 위해선 위 행렬식이 0 이어야 한다.

$$\det X = -i\alpha \cdot 2\gamma + \gamma \cdot e^{\gamma b - i\alpha a}(\gamma + i\alpha) - \gamma \cdot e^{\gamma b - i\alpha a}(\gamma - i\alpha) - i\alpha \cdot 2\gamma + \gamma \cdot e^{-\gamma b + i\alpha a}(-\gamma + i\alpha)$$
$$+ \gamma \cdot e^{\gamma b + i\alpha a}(\gamma + i\alpha) + i\alpha e^{-\gamma b - i\alpha a}(\gamma + i\alpha) - i\alpha \cdot e^{-\gamma b + i\alpha a}(-\gamma + i\alpha) + \gamma \cdot (-2i\alpha)$$
$$+ i\alpha \cdot e^{\gamma b - i\alpha a}(\gamma - i\alpha) + i\alpha \cdot e^{\gamma b + i\alpha a}(\gamma + i\alpha) + \gamma \cdot (-2i\alpha)$$
$$= -4i\alpha\gamma + e^{-\gamma b - i\alpha a}(\gamma + i\alpha)^2 - e^{\gamma b - i\alpha a}(\gamma - i\alpha)^2 - e^{-\gamma b + i\alpha a}(-\gamma + i\alpha)^2 +$$
$$e^{\gamma b + i\alpha a}(\gamma + i\alpha)^2 - 4i\alpha\gamma$$
$$= -8i\alpha\gamma + (\gamma + i\alpha)^2 \cdot (e^{\gamma b + i\alpha a} + e^{-\gamma b - i\alpha a}) - (\gamma - i\alpha)^2 \cdot (e^{\gamma b - i\alpha a} + e^{-\gamma b + i\alpha a})$$
$$= -8i\alpha\gamma + (\gamma^2 - \alpha^2) \cdot (e^{\gamma b + i\alpha a} + e^{-\gamma b - i\alpha a} - e^{\gamma b - i\alpha a} - e^{-\gamma b + i\alpha a}) + 2i\alpha\gamma \cdot (e^{\gamma b + i\alpha a}$$
$$+ e^{-\gamma b - i\alpha a} + e^{\gamma b - i\alpha a} + e^{-\gamma b - i\alpha a})$$

$$= -8i\alpha\gamma + (\gamma^2-\alpha^2)\cdot(e^{\gamma b}\cdot(e^{i\alpha a}-e^{-i\alpha a}) + e^{-\gamma b}\cdot(e^{-i\alpha a}-e^{i\alpha a}))$$

$$+2i\alpha\gamma\cdot(e^{\gamma b}\cdot(e^{i\alpha a}+e^{-i\alpha a}) + e^{-\gamma b}\cdot(e^{i\alpha a}+e^{-i\alpha a}))$$

$$= -8i\alpha\gamma + (\gamma^2-\alpha^2)\cdot(e^{\gamma b}-e^{-\gamma b})\cdot(e^{i\alpha a}-e^{-i\alpha a}) + 2i\alpha\gamma\cdot(e^{\gamma b}+e^{-\gamma b})\cdot$$

$$(e^{i\alpha a}+e^{-i\alpha a})$$

$$= -8i\alpha\gamma + (\gamma^2-\alpha^2)\cdot 2\cdot\sinh(\gamma b)\cdot 2i\sin(\alpha a) + 2i\alpha\gamma\cdot 2\cdot\cosh(\gamma b)\cdot 2\cos(\alpha a)$$

$$= 0$$

$$(\gamma^2-\alpha^2)\cdot\sinh(\gamma b)\cdot\sin(\alpha a) + 2\alpha\gamma\cosh(\gamma b)\cdot\cos(\alpha a) = 2\alpha\gamma$$

$$\therefore \frac{(\gamma^2-\alpha^2)}{2\alpha\gamma}\cdot\sinh(\gamma b)\cdot\sin(\alpha a) + \cosh(\gamma b)\cos(\alpha a) = 1$$ 이다.

우변이 1로 바뀜. 따라서, 에너지는 특정 범위가 아닌 특정값만을 가지게 된다.

3. boundary condition에 의해 구해진 (4.57) ~ (4.60) 식을 행렬로 나타내면

$$\begin{pmatrix} 1 & 1 & -1 & -1 \\ i\alpha-ik & -i\alpha-ik & \gamma+ik & -\gamma+ik \\ e^{(i\alpha-ik)a} & e^{(-i\alpha-ik)a} & -e^{(ik+\gamma)b} & -e^{(ik-\gamma)b} \\ i(\alpha-k)e^{ia(\alpha-k)} & -i(\alpha+k)e^{-ia(\alpha+k)} & (\gamma+ik)e^{(ik+\gamma)b} & -(\gamma-ik)e^{(ik-\gamma)b} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$A=B=C=D=0$ 이외의 해가 존재하기 위해선 위 행렬식이 0이어야 한다.

$$\begin{aligned}
\det.X = {} & (-i\alpha-ik)\cdot\{(\gamma-ik)e^{(ik+\gamma)b+(ik-\gamma)b}+(\gamma+ik)e^{(ik+\gamma)b+(ik-\gamma)b}\} \\
& -(\gamma+ik)\cdot\{-(\gamma-ik)e^{(-i\alpha-ik)a+(ik-\gamma)b}-i(\alpha+k)e^{(ik-\gamma)b-ia(\alpha+k)}\} \\
& +(-\gamma+ik)\cdot\{(\gamma+ik)e^{(ik+\gamma)b+(i\alpha-ik)a}-i(\alpha+k)e^{(ik+\gamma)b-ia(\alpha+k)}\} \\
& -(i\alpha-ik)\cdot\{(\gamma-ik)\cdot e^{(ik-\gamma)b+(ik+\gamma)b}+(\gamma+ik)e^{(ik-\gamma)b+(ik+\gamma)b}\} \\
& +(\gamma+ik)\cdot\{-(\gamma-ik)e^{(i\alpha-ik)a+(ik-\gamma)b}+i(\alpha-k)e^{(ik-\gamma)b+ia(\alpha-k)}\} \\
& -(-\gamma+ik)\cdot\{(\gamma+ik)e^{(ik+\gamma)b+(i\alpha-ik)a}+i(\alpha-k)e^{(ik+\gamma)b+ia(\alpha-k)}\} \\
& -(i\alpha-ik)\cdot\{-(\gamma-ik)e^{(-i\alpha-ik)a+(ik-\gamma)b}-i(\alpha+k)e^{-ia(\alpha+k)+(ik-\gamma)b}\} \\
& +(-i\alpha-ik)\cdot\{-(\gamma-ik)e^{(ik-\gamma)b+(i\alpha-ik)a}+i(\alpha-k)e^{ia(\alpha-k)+(ik-\gamma)b}\} \\
& -(-\gamma+ik)\cdot\{-i(\alpha+k)e^{-ia(\alpha+k)+(i\alpha-ik)a}-i(\alpha-k)e^{ia(\alpha-k)+(-i\alpha-ik)a}\} \\
& +(i\alpha-ik)\cdot\{(\gamma+ik)e^{(ik+\gamma)b+(i\alpha-ik)a}-i(\alpha+k)e^{-ia(\alpha+k)+(ik+\gamma)b}\} \\
& -(-i\alpha-ik)\cdot\{(\gamma+ik)e^{(ik+\gamma)b+(i\alpha-ik)a}+i(\alpha-k)e^{ia(\alpha-k)+(ik+\gamma)b}\} \\
& +(\gamma+ik)\cdot\{-i(\alpha+k)e^{-ia(\alpha+k)+(i\alpha-ik)a}-i(\alpha-k)e^{ia(\alpha-k)+(-i\alpha-ik)a}\} \\
= {} & (-i\alpha-ik)\cdot e^{(ik+\gamma)b+(ik-\gamma)b}\cdot 2\gamma-(\gamma+ik)e^{(ik-\gamma)b-ia(\alpha+k)}\cdot(-\gamma-i\alpha) \\
& +(-\gamma+ik)e^{(ik+\gamma)b-ia(\alpha+k)}(\gamma-i\alpha)-(i\alpha-ik)e^{(ik-\gamma)b+(ik+\gamma)b}\cdot 2\gamma \\
& +(\gamma+ik)e^{(ik-\gamma)b+ia(\alpha-k)}\cdot(-\gamma+i\alpha)-(-\gamma+ik)e^{(ik+\gamma)b+ia(\alpha-k)}\cdot(\gamma+i\alpha) \\
& -(i\alpha-ik)e^{(ik-\gamma)b-ia(\alpha+k)}\cdot(-\gamma-i\alpha)+(-i\alpha-ik)e^{(ik-\gamma)b+ia(\alpha-k)}\cdot(-\gamma+i\alpha) \\
& -(-\gamma+ik)e^{-ia(\alpha+k)+ia(\alpha-k)}\cdot(-2i\alpha)+(i\alpha-ik)e^{(ik+\gamma)b-ia(\alpha+k)}\cdot(\gamma-i\alpha) \\
& -(-i\alpha-ik)e^{(ik+\gamma)b+ia(\alpha-k)}\cdot(\gamma+i\alpha)+(\gamma+ik)e^{ia(\alpha-k)-ia(\alpha+k)}\cdot(-2i\alpha)
\end{aligned}$$

$$= e^{2ikb}\cdot 2\gamma\cdot(-2i\alpha) + e^{(ik-\gamma)b-ia(\alpha+k)}(-\gamma-i\alpha)\cdot(-\gamma-i\alpha)$$

$$+ e^{(ik+\gamma)b-ia(\alpha+k)}\cdot(\gamma-i\alpha)(-\gamma+i\alpha) + e^{(ik-\gamma)b+ia(\alpha-k)}(-\gamma+i\alpha)(\gamma-i\alpha)$$

$$+ e^{(ik+\gamma)b+ia(\alpha-k)}\cdot(\gamma+i\alpha)(\gamma+i\alpha) + e^{-2iak}\cdot(-2i\alpha)\cdot(2\gamma)$$

$$= 2\gamma\cdot(-2i\alpha)(e^{2ikb}+e^{-2iak}) + (\gamma+i\alpha)^2\cdot(e^{ik-\gamma)b-ia(\alpha+k)} + e^{(ik+\gamma)b+ia(\alpha-k)})$$

$$(\gamma-i\alpha)(-\gamma+i\alpha)(e^{(ik+\gamma)b-ia(\alpha+k)} + e^{(ik-\gamma)b+ia(\alpha-k)})$$

$$= -4i\alpha\gamma(e^{2ikb}+e^{-2ika}) + (\gamma^2+2i\alpha\gamma-\alpha^2)e^{ikb-ika}(e^{\gamma b+i\alpha a}+e^{-\gamma b-i\alpha a})$$

$$-(\gamma^2-2i\alpha\gamma-\alpha^2)e^{ikb-ika}(e^{\gamma b-i\alpha a}+e^{-\gamma b+i\alpha a})$$

$$= (\gamma^2-\alpha^2)e^{ikb-ika}(e^{\gamma b+i\alpha a}+e^{-\gamma b-i\alpha a}-e^{\gamma b-i\alpha a}-e^{-\gamma b+i\alpha a})$$

$$+2i\alpha\gamma e^{ikb-ika}\cdot(e^{\gamma b+i\alpha a}+e^{-\gamma b-i\alpha a}+e^{\gamma b-i\alpha a}+e^{-\gamma b+i\alpha a}) - 4i\alpha\gamma(e^{2ikb}+e^{-2ika})$$

$$= (\gamma^2-\alpha^2)e^{ikb-ika}(e^{\gamma b}(e^{i\alpha a}-e^{-i\alpha a}) - e^{-\gamma b}(e^{i\alpha a}-e^{-i\alpha a}))$$

$$+2i\alpha\gamma e^{ikb-ika}(e^{\gamma b}(e^{i\alpha a}+e^{-i\alpha a}) + e^{-\gamma b}(e^{i\alpha a}+e^{-i\alpha a}))$$

$$-4i\alpha\gamma(e^{2ikb}+e^{-2ika})$$

$$= (\gamma^2-\alpha^2)e^{ikb-ika}\cdot 4i\cdot\sinh(\gamma b)\cdot\sin(\alpha a) + 2i\alpha\gamma e^{ikb-ika}\cdot 4\cdot\cosh(\gamma b)\cos(\alpha a)$$

$$-4i\alpha\gamma(e^{2ikb}+e^{-2ika})$$

$$= 0$$

$$\frac{(\gamma^2-\alpha^2)}{2\alpha\gamma}\sinh(\gamma b)\sin(\alpha a) + \cosh(\gamma b)\cos(\alpha a) = \frac{e^{2ikb}+e^{-2ika}}{2e^{ikb-ika}}$$

$$= \frac{1}{2}(e^{i(kb+ka)}+e^{-i(kb+ka)})$$

$$= \cos(ka+kb)$$

$$= \cos k(a+b)$$

$$\therefore \frac{(\gamma^2-\alpha^2)}{2\alpha\gamma}\sinh(\gamma b)\cdot\sin(\alpha a) + \cosh(\gamma b)\cos(\alpha a) = \cos k(a+b).$$

6. Potential well에 갇힌 전자가 가질 수 있는 에너지는

$$E_n = \frac{\hbar^2 \pi^2}{2ma^2} \cdot n^2 \qquad (n=1, 2, 3, \cdots) \qquad (4.18)$$

$$= 1.505 \times 10^{-18} \times n^2 \,[\text{Joule}] = 9.392 \times n^2 \,[\text{eV}]$$

n	E (J)	E (eV)
1	1.505×10^{-18}	9.392
2	6.020×10^{-18}	37.568
3	1.355×10^{-17}	84.528
4	2.408×10^{-17}	150.272

→ zero-point Energy.

7. 3-D infinite potential well

$$V = \begin{cases} 0 & (r \le a) \\ \infty & (r > a) \end{cases} \qquad \nabla^2\psi + \frac{2m}{\hbar^2}E\psi = 0$$

$$\nabla^2 = \frac{d^2}{dr^2} + \left(\frac{2}{r}\right)\frac{d}{dr}$$

(a) show that $\psi = \frac{1}{r}(Ae^{ikr} + Be^{-ikr})$

$$\left[\frac{d^2}{dr^2} + \left(\frac{2}{r}\right)\frac{d}{dr}\right]\psi + \frac{2m}{\hbar^2}E\psi = 0 \quad — ①$$

let $\psi = \frac{u}{r}$

$$\frac{d\psi}{dr} = \frac{1}{r}\frac{du}{dr} - \frac{u}{r^2} \quad — ②$$

$$\frac{d^2\psi}{dr^2} = \frac{1}{r}\frac{d^2u}{dr^2} - \frac{1}{r^2}\frac{du}{dr} - \frac{1}{r^2}\frac{du}{dr} + \frac{2u}{r^3}$$

$$= \frac{1}{r}\frac{d^2u}{dr^2} - \frac{2}{r^2}\frac{du}{dr} + \frac{2u}{r^3} \quad — ③$$

② & ③을 ①에 대입하면 ;

$$\frac{1}{r}\frac{d^2u}{dr^2} - \frac{2}{r^2}\frac{du}{dr} + \frac{2u}{r^3} + \frac{2}{r^2}\frac{du}{dr} - \frac{2u}{r^3} + \frac{2m}{\hbar^2}E\frac{u}{r} = 0$$

$$\frac{d^2u}{dr^2} + \frac{2m}{\hbar^2}Eu = 0$$

$$\therefore \quad u = A\exp(ikr) + B\exp(-ikr) \qquad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\therefore \quad u = \frac{u}{r} = \frac{1}{r}A\exp(ikr) + \frac{1}{r}B\exp(-ikr)$$

(b) $\lim_{r\to 0} \psi(r) = \lim_{r \to 0} \dfrac{Ae^{ikr} + Be^{-ikr}}{r}$

분모 $\to 0$ 이므로, 분자 $\to 0$ 이어야 극값 존재.

$\therefore A+B=0$, $A=-B$

$$\psi = \frac{A}{r}\left(e^{ikr} - e^{-ikr}\right) = \frac{2iA\sin kr}{r}$$

(c) $\psi(r=a) = 0$

$$\therefore \frac{2iA\cdot\sin(ka)}{r} = 0$$

$$\Rightarrow ka = n\pi , \quad k = \frac{n\pi}{a}$$

$$\Rightarrow E = \frac{\hbar^2 k^2}{2m} = \frac{\pi^2\hbar^2}{2ma^2}\cdot n^2$$

(d) 1-D 와 같은 결과.

8. (a) $\frac{\hbar^2}{2m}\cdot\frac{d^2\psi}{dx^2} + E\psi = 0$ ($\because x<0$ 에서 $V_0 = 0$)

$\psi_I = a\cdot e^{ibx}$ 대입 $\longrightarrow$ $b^2 = \frac{2mE}{\hbar^2} = k_1^2$ $\therefore k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

(b) $\frac{\hbar^2}{2m}\cdot\frac{d^2\psi}{dx^2} + (E-V_0)\psi = 0$

$E > V_0$; $\psi_{II} = C\cdot e^{ik_2x} \longrightarrow k_2^2 = \frac{2m(E-V_0)}{\hbar^2}$ $\therefore k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

$E < V_0$; $\psi_{II} = D\cdot e^{-\alpha x} \longrightarrow \alpha^2 = \frac{2m(V_0-E)}{\hbar^2}$ $\therefore \alpha = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$

(c) i) $E > V_0$

$\psi_I = \psi_{II}$ $(x=0)$, $\frac{d\psi_I}{dx} = \frac{d\psi_{II}}{dx}$ $(x=0)$

$A+B = C$, $ik_1A - ik_1B = ik_2C$

$\Rightarrow C = \frac{2k_1}{k_1+k_2}A$, $B = \frac{k_1-k_2}{k_1+k_2}A$

ii) $E < V_0$

$\psi_I = \psi_{II}$ $(x=0)$, $\frac{d\psi_I}{dx} = \frac{d\psi_{II}}{dx}$ $(x=0)$

$A+B = D$, $ik_1A - ik_1B = -\alpha D$

$\Rightarrow D = \frac{2ik_1}{ik_1-\alpha}A$, $B = \frac{ik_1+\alpha}{ik_1-\alpha}A$

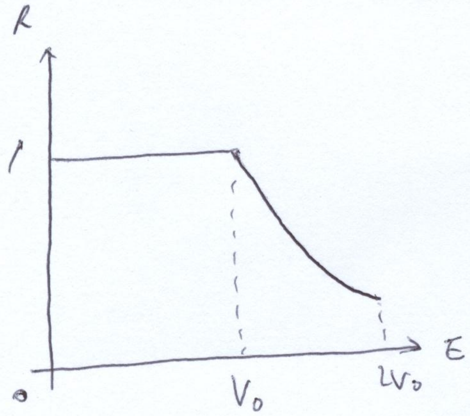
(d) i) $E > V_0$

$R = \left|\frac{B}{A}\right|^2 = \frac{(k_1-k_2)^2}{(k_1+k_2)^2} = \frac{2E - V_0 - 2\sqrt{E(E-V_0)}}{2E - V_0 + 2\sqrt{E(E-V_0)}}$

ii) $E < V_0$

$R = \left|\frac{B}{A}\right|^2 = \left|\frac{ik_1-\alpha}{ik_1+\alpha}\right|^2 = 1$

(e)



(f) $T = \dfrac{k_2}{k_1}\left|\dfrac{C}{A}\right|^2 = \dfrac{k_2}{k_1}\left(\dfrac{2k_1}{k_1+k_2}\right)^2$

$$T+R = \frac{4k_1k_2+(k_1-k_2)^2}{(k_1+k_2)^2} = \frac{(k_1+k_2)^2}{(k_1+k_2)^2} = 1$$

($E<V_0$ 경우에는 $C=0$; $T=0$ 이고 $R=1$ $\therefore T+R=1$)