

Review Topics & Formulas for Unit 5

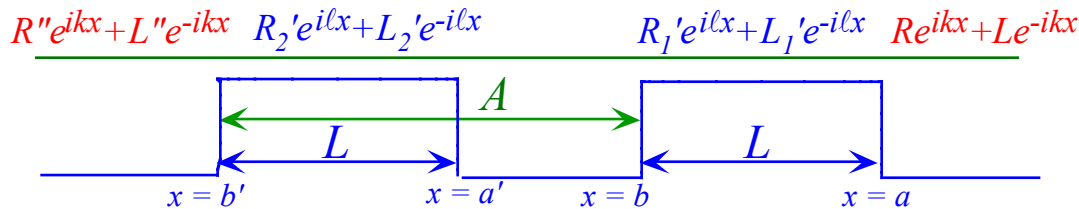


Fig. 14.1.5 C_2 -symmetric double barrier .

$$\begin{pmatrix} R'' \\ L'' \end{pmatrix} = \begin{pmatrix} e^{i2kL} \chi^* + e^{-i2kA} \xi^2 & -i\xi(e^{-i2kb} \chi^* + e^{-i2ka'} \chi) \\ i\xi(e^{i2kb} \chi + e^{i2ka'} \chi^*) & e^{-i2kL} \chi^2 + e^{i2kA} \xi^2 \end{pmatrix} \begin{pmatrix} R \\ L \end{pmatrix} \quad (14.1.6)$$

$$\chi = \cosh \kappa L - i \sinh 2\beta \sinh \kappa L, \text{ and: } \xi = \cosh 2\beta \sinh \kappa L, \quad (14.1.7)$$

$$\cosh 2\beta = \frac{1}{2} \left(\frac{\kappa}{k} + \frac{k}{\kappa} \right) = \frac{\kappa^2 + k^2}{2k\kappa}, \quad \sinh 2\beta = \frac{1}{2} \left(\frac{\kappa}{k} - \frac{k}{\kappa} \right) = \frac{\kappa^2 - k^2}{2k\kappa} \quad (14.1.8)$$

$$\text{Model Lorentz resonance function } \left| \frac{1}{C_{11}(\omega)} \right|^2 = \left| \frac{c_n}{\omega - \omega_n + i\Gamma_n} \right|^2 = \frac{|c_n|^2}{(\omega - \omega_n)^2 + \Gamma_n^2} \quad (14.1.10)$$

resonance frequency ω_n , resonance decay rate Γ_n , resonance peak strength $|c_n/\Gamma_n|^2$

Γ_n is the *Lorentzian Half-Width at Half-Maximum (HWHM)*.

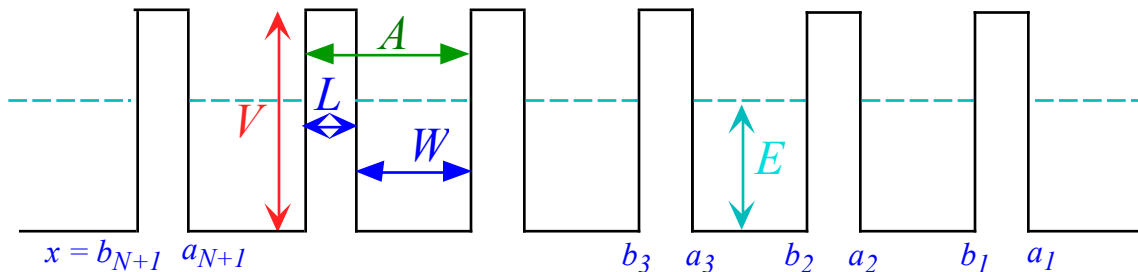


Fig. 14.1.18 $(N+1)$ -barrier (N) -well potential

$$C^{N+1 \text{ barrier}} = C^{[N+1]} \dots C' \cdot C =$$

$$\begin{pmatrix} e^{ikL} \chi^* & -ie^{-ik(a_{N+1}+b_{N+1})\xi} \\ ie^{ik(a_{N+1}+b_{N+1})\xi} & e^{-ikL} \chi \end{pmatrix} \dots \begin{pmatrix} e^{ikL} \chi^* & -ie^{-ik(a_2+b_2)\xi} \\ ie^{ik(a_2+b_2)\xi} & e^{-ikL} \chi \end{pmatrix} \begin{pmatrix} e^{ikL} \chi^* & -ie^{-ik(a_1+b_1)\xi} \\ ie^{ik(a_1+b_1)\xi} & e^{-ikL} \chi \end{pmatrix} \quad (14.1.17a)$$

For $(E < V)$ are $k = \sqrt{2E}$, $\kappa = \sqrt{2V-2E}$, and $\sinh 2\beta = (\kappa^2 - k^2)/(2k\kappa)$,

$$\chi = \cosh \kappa L - i \sinh 2\beta \sinh \kappa L, \text{ and: } \xi = \cosh 2\beta \sinh \kappa L, \quad (14.1.17a)$$

For $(E > V)$ they are $\ell = \sqrt{2E-2V}$, and $\cosh 2\alpha = (\ell^2 + k^2)/(2k\ell)$.

$$\chi = \cos \ell L + i \cosh 2\alpha \sin \ell L, \text{ and: } \xi = \sinh 2\alpha \sin \ell L. \quad (14.1.17b)$$

Pendulum model:
$$\mathbf{H}|\varepsilon_k\rangle = \begin{pmatrix} H & -S & 0 \\ -S & H & -S \\ 0 & -S & H \end{pmatrix} \begin{pmatrix} \langle 1|\Psi\rangle \\ \langle 2|\Psi\rangle \\ \langle 3|\Psi\rangle \end{pmatrix} = \varepsilon_k \begin{pmatrix} \langle 1|\Psi\rangle \\ \langle 2|\Psi\rangle \\ \langle 3|\Psi\rangle \end{pmatrix} = \varepsilon_k |\Psi\rangle \quad (14.1.18)$$

$$\varepsilon_m = H - 2S \cos(\pi m/4). \quad (14.1.21b)$$

$$\begin{aligned} \langle \varepsilon_1 | &= \left(1 \quad \sqrt{2} \quad 1 \right) / 2 & \varepsilon_1 &= H - \sqrt{2}S \\ \langle \varepsilon_2 | &= \left(1 \quad 0 \quad -1 \right) / \sqrt{2} & \varepsilon_2 &= H \\ \langle \varepsilon_3 | &= \left(1 \quad -\sqrt{2} \quad 1 \right) / 2 & \varepsilon_3 &= H + \sqrt{2}S \end{aligned} \quad (14.1.21c)$$

Kronig-Penney band conditions.

$$\left. \begin{aligned} (\text{for } E > V): \quad & \cos kW \cos \ell L - \frac{2E - V}{2\sqrt{E(E - V)}} \sin kW \sin \ell L \\ (\text{for } E < V): \quad & \cos kW \cosh \kappa L + \frac{V - 2E}{2\sqrt{E(V - E)}} \sin kW \sinh \kappa L \end{aligned} \right\} = \cos \phi \quad (14.2.5b)$$

where rational units are used for energy.

$$\phi = m \frac{2\pi}{N}, \quad k = \sqrt{2E}, \quad \ell = \sqrt{2(E - V)}, \quad \kappa = \sqrt{2(V - E)}. \quad (14.2.5c)$$

Bohr units
$$\varepsilon_1^{Bohr}(A) = \frac{\hbar^2 \pi^2}{2M A^2} = \frac{(1.05 \cdot 10^{-34} \pi \text{J} \cdot \text{s})^2}{(2 \cdot 9.109 \cdot 10^{-31} \text{kg})} \frac{10^3 \text{meV}}{1.602 \cdot 10^{-19} \text{J}} \frac{1}{(A \cdot 10^{-8} \text{m})^2} \quad (14.2.10a)$$

$$= \frac{3.76 \text{meV}}{A^2} \quad (A \text{ in units of } 100\text{\AA})$$

Our rational units:
$$\varepsilon_1^{Bohr}(A) = \frac{\pi^2 / 2}{A^2} = \frac{4.93}{A^2} = 1.23 \quad (\text{for } A=2 \text{ in } 100\text{\AA} \text{ units}) \quad (14.2.11)$$

$$\begin{array}{c|ccc}
 D_2 & \mathbf{1} & \mathbf{R}_z & \mathbf{R}_y & \mathbf{R}_x \\
 \hline
 A_1 & 1 & 1 & 1 & 1 \\
 B_1 & 1 & -1 & 1 & -1 \\
 \hline
 A_2 & 1 & 1 & -1 & -1 \\
 B_2 & 1 & -1 & -1 & 1
 \end{array} \quad (15.1.4)$$

$$\begin{array}{c|ccc}
 D_3 \text{ characters } \mathbf{g} = & \mathbf{1} & \{\mathbf{r}, \mathbf{r}^2\} & \{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\} \\
 \hline
 \text{Trace} D^{A_1}(\mathbf{g}) = \chi^{A_1}(\mathbf{g}) & 1 & 1 & 1 \\
 \text{Trace} D^{A_2}(\mathbf{g}) = \chi^{A_2}(\mathbf{g}) & 1 & 1 & -1 \\
 \text{Trace} D_{x_2 y_2}^{E_1}(\mathbf{g}) = \chi^{E_1}(\mathbf{g}) & 2 & -1 & 0
 \end{array} \quad (15.1.13)$$

$$\begin{array}{c|cccccc}
 \mathbf{g} = & \mathbf{1} & \mathbf{r} & \mathbf{r}^2 & \mathbf{i}_1 & \mathbf{i}_2 & \mathbf{i}_3 \\
 \hline
 D_{c_3 d_3}^{E_1}(\mathbf{g}) = & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} \varepsilon_- & 0 \\ 0 & \varepsilon_+ \end{pmatrix} & \begin{pmatrix} \varepsilon_+ & 0 \\ 0 & \varepsilon_- \end{pmatrix} & \begin{pmatrix} 0 & \varepsilon_+ \\ \varepsilon_- & 0 \end{pmatrix} & \begin{pmatrix} 0 & \varepsilon_- \\ \varepsilon_+ & 0 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
 \end{array} \quad (15.1.8)$$

$$\begin{array}{c|cccccc}
 \mathbf{g} = & \mathbf{1} & \mathbf{r} & \mathbf{r}^2 & \mathbf{i}_1 & \mathbf{i}_2 & \mathbf{i}_3 \\
 \hline
 D_{x_2 y_2}^{E_1}(\mathbf{g}) = & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} & \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix} & \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix} & \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
 \end{array}$$

Wigner-Weyl projection formula

$$\mathbf{g} = \sum_{\mu} \sum_m \sum_n D_{mn}^{\mu}(\mathbf{g}) \mathbf{P}_{mn}^{\mu} = D^{A_1}(\mathbf{g}) \mathbf{P}^{A_1} + D^{A_2}(\mathbf{g}) \mathbf{P}^{A_2} + D_{11}^{E_1}(\mathbf{g}) \mathbf{P}_{11}^{E_1} + D_{12}^{E_1}(\mathbf{g}) \mathbf{P}_{12}^{E_1} + D_{21}^{E_1}(\mathbf{g}) \mathbf{P}_{21}^{E_1} + D_{22}^{E_1}(\mathbf{g}) \mathbf{P}_{22}^{E_1} \quad (15.1.20a)$$

$$\mathbf{P}_{mn}^{\mu} = \frac{\ell^{\mu}}{o_G} \sum_{\mathbf{g}} D_{mn}^{\mu*}(\mathbf{g}) \mathbf{g} \quad (15.1.20d)$$

$$\mathbf{P}_{jk}^{\mu} \mathbf{P}_{mn}^{\nu} = \delta^{\mu\nu} \delta_{km} \mathbf{P}_{jn}^{\mu} \quad (15.1.20b)$$

$$\mathbf{g} \mathbf{P}_{mn}^{\mu} = \sum_{m'} D_{m'm}^{\mu}(\mathbf{g}) \mathbf{P}_{m'n}^{\mu} \quad (15.1.21a)$$

$$\mathbf{P}_{mn}^{\mu} \mathbf{g} = \sum_{n'} D_{nn'}^{\mu}(\mathbf{g}) \mathbf{P}_{mn'}^{\mu} \quad (15.1.21b)$$

grand D-orthonormality relations.

$$D_{mn}^{\mu}(\mathbf{P}_{m'n'}^{\mu'}) = \delta^{\mu\mu'} \delta_{mm'} \delta_{nn'} \quad \text{or:} \quad \sum_{\mathbf{g}} D_{mn}^{\mu}(\mathbf{g}) D_{m'n'}^{\mu'*}(\mathbf{g}) = \frac{o_G}{\ell^{\mu'}} \delta^{\mu\mu'} \delta_{mm'} \delta_{nn'} \quad (15.1.30)$$

$$\mathbb{P}^{\mu} = \sum_{m=1}^{\ell^{\mu}} \mathbf{P}_{mm}^{\mu} = \frac{\ell^{\mu}}{o_G} \sum_{\mathbf{g}} \sum_{m=1}^{\ell^{\mu}} D_{mm}^{\mu*}(\mathbf{g}) \mathbf{g} = \frac{\ell^{\mu}}{o_G} \sum_{\mathbf{g}} \chi^{\mu*}(\mathbf{g}) \mathbf{g} \quad \mathbf{c}_{\mathbf{g}} = \sum_{\text{ireps } \mu} \frac{o_G \chi_{\mathbf{g}}^{\mu}}{\ell^{\mu}} \mathbb{P}^{\mu} \quad (15.2.5b)$$

\mathbb{P}^{μ} is the (μ) -th *all-commuting idempotent* \mathbb{P}^{μ} or *class projector*.

$$\chi^{\mu}_I = \ell^{\mu} = \sqrt{o_G \frac{\ell^{\mu} \chi_1^{\mu*}}{o_G}} = \sqrt{o_G (\mathbf{c}_I \text{ coefficient in } \mathbf{P}^{\mu})} = \sqrt{(\ell^{\mu})^2} \quad (15.2.10g)$$

$$\text{Duality principle } \mathbf{g}|\mathbf{1}\rangle = |\mathbf{g}\rangle = \bar{\mathbf{g}}^{\dagger}|\mathbf{1}\rangle = \bar{\mathbf{g}}^{-1}|\mathbf{1}\rangle, \quad \text{or: } \mathbf{g}^{-1}|\mathbf{1}\rangle = \mathbf{g}^{\dagger}|\mathbf{1}\rangle = |\mathbf{g}^{-1}\rangle = \bar{\mathbf{g}}|\mathbf{1}\rangle = \bar{\mathbf{g}}|\mathbf{1}\rangle. \quad (15.3.8)$$

$$\text{Duality-relativity principle } \bar{\mathbf{g}}|\mathbf{t}\rangle = \mathbf{t} \cdot \mathbf{g}^{\dagger} \cdot \mathbf{t}^{-1}|\mathbf{t}\rangle = \mathbf{t} \cdot \mathbf{g}^{\dagger} \cdot \mathbf{t}^{\dagger}|\mathbf{t}\rangle. \quad (15.3.9)$$

$$\mathbf{g} \left| \begin{smallmatrix} \mu \\ mn \end{smallmatrix} \right\rangle = \sum_{m'=1}^{\ell^{\mu}} D_{m'm}^{\mu}(\mathbf{g}) \left| \begin{smallmatrix} \mu \\ m'n \end{smallmatrix} \right\rangle \quad \bar{\mathbf{g}} \left| \begin{smallmatrix} \mu \\ mn \end{smallmatrix} \right\rangle = \sum_{n'=1}^{\ell^{\mu}} D_{n'n}^{\mu*}(\mathbf{g}) \left| \begin{smallmatrix} \mu \\ mn' \end{smallmatrix} \right\rangle \quad (15.3.10)$$

Regular representation of operators \mathbf{g} and dual operators $\bar{\mathbf{g}}$.

$$R_{h,f}^G(\mathbf{g}) = \langle h | \mathbf{g} | f \rangle = \delta_{h=gf} = \begin{cases} 1 & \text{if: } \mathbf{h} = \mathbf{g} \cdot \mathbf{f} \\ 0 & \text{if: } \mathbf{h} \neq \mathbf{g} \cdot \mathbf{f} \end{cases} = \delta_{f^\dagger = h^\dagger g} \quad R_{h,f}^G(\bar{\mathbf{g}}) = \langle h | \bar{\mathbf{g}} | f \rangle = \langle 1 | \mathbf{h}^\dagger \mathbf{f} \cdot \mathbf{g}^\dagger | 1 \rangle = \delta_{f=hg} \quad (15.3.11)$$

Symmetry: $\mathbf{g} \mathbf{H} = \mathbf{H} \mathbf{g}$ of Hamiltonian $\mathbf{H} = H\bar{1} + R\bar{\mathbf{r}} + R^*\bar{\mathbf{r}}^2 + L\bar{\mathbf{i}}_1 + M\bar{\mathbf{i}}_2 + S\bar{\mathbf{i}}_3$ (15.4.2a)

Solution: $H_{ab}^\mu = \sum_{g=1}^{\circ G} \langle \mathbf{1} | \mathbf{H} | \mathbf{g} \rangle D_{ab}^{\mu*}(g)$ (15.4.5c)