

Group Theory in Quantum Mechanics

Lecture 14.5 (3.07.17)

C_N symmetry systems coupled, uncoupled, and re-coupled

(Quantum Theory for the Computer Age - Unit 3-5)

(Principles of Symmetry, Dynamics, and Spectroscopy - Sec. 1-12 of Ch. 2)

Breaking C_N cyclic coupling into linear chains

Review of 1D-Bohr-ring related to infinite square well

Breaking C_{2N+2} to approximate linear N -chain (Examples $C_2 \leftrightarrow C_6 \leftrightarrow C_{14}$)

Band-It simulation: Intro to scattering approach to quantum symmetry

How **Band-It** works: Match each Ψ and $D\Psi$, Let $L=0$ at Right end

Breaking C_{2N} cyclic coupling down to C_N symmetry

Acoustical modes vs. Optical modes

Intro to other examples of band theory

Avoided crossing view of band-gaps

Finally! Symmetry groups that are not just C_N

The "4-Group(s)" D_2 and C_{2v}

Spectral decomposition of D_2

Some D_2 modes

Outer product properties and the Crystal-Point Symmetry Group Zoo

Polygonal geometry of $U(2) \supset C_N$ character spectral function. $\chi^j(2\pi/n) = \frac{\sin(\pi(2j+1)/n)}{\sin(\pi/n)}$

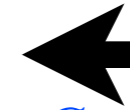
Algebra

Geometry

The **CPT** subgroup of Lorentz Group

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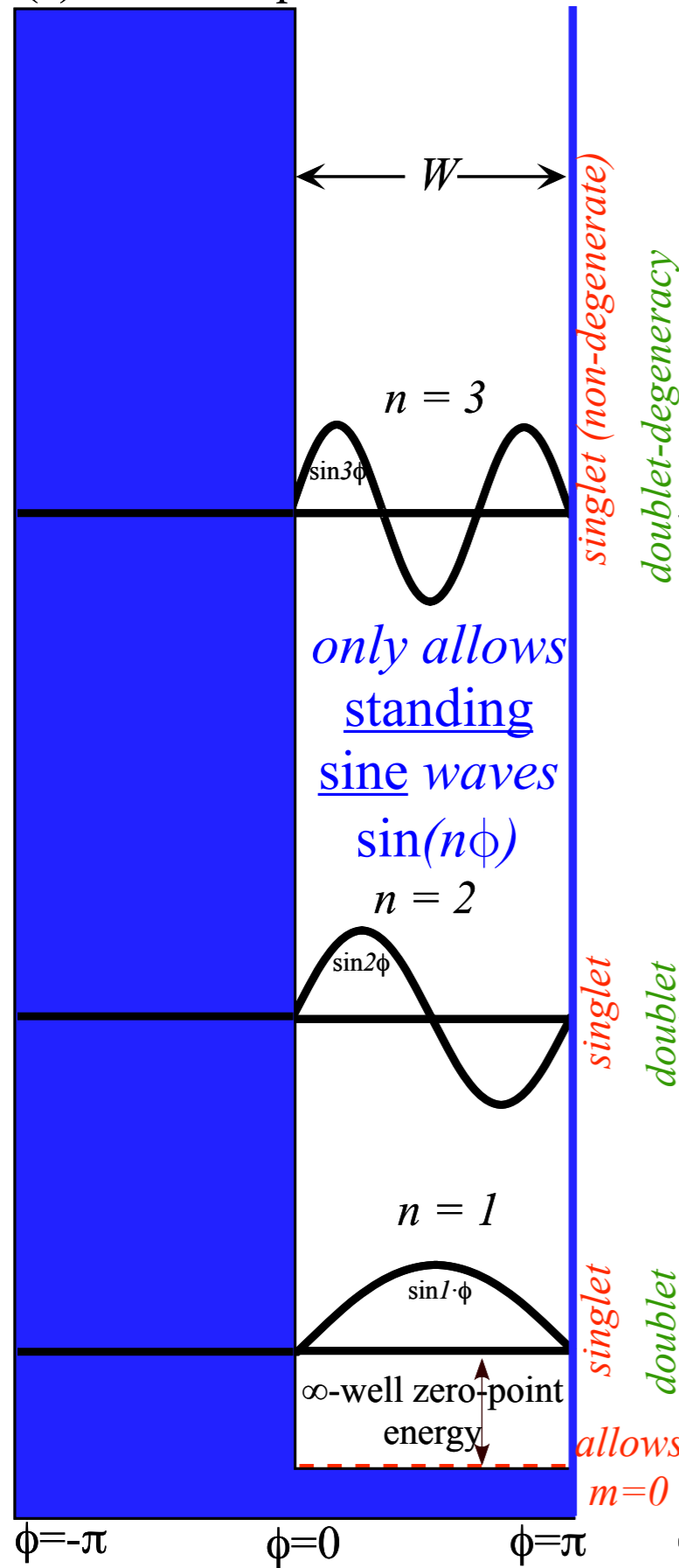
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∞ -Square well PE versus Bohr rotor

(a) Infinite Square Well



(b) Bohr Rotor

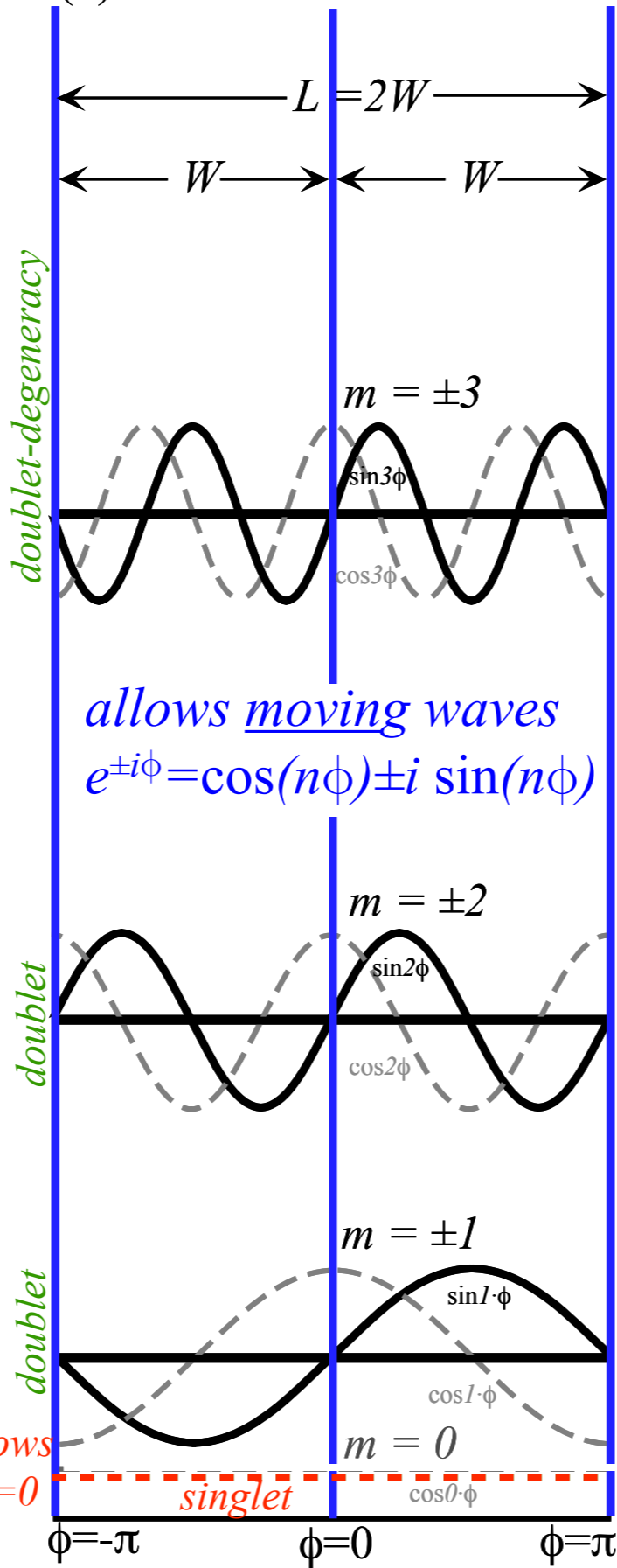
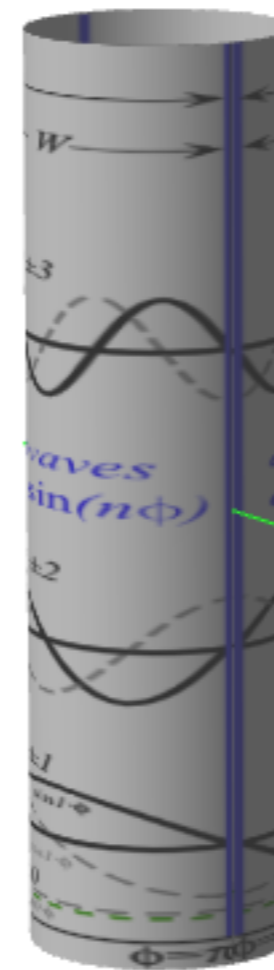
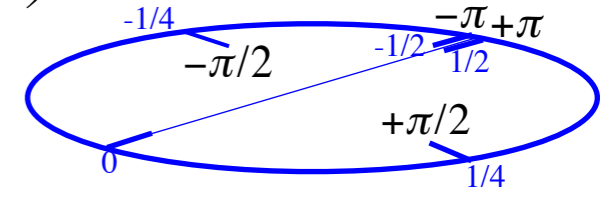


Fig. 12.2.6 Comparison of eigensolutions for

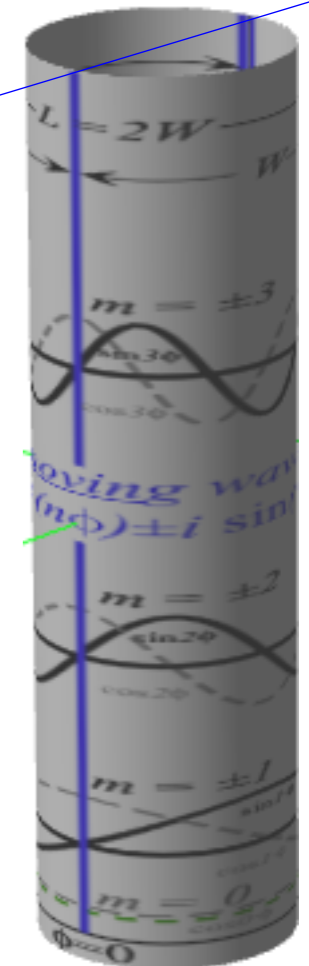
(a) Infinite square well, and (b) Bohr rotor.

From QTCA Unit 5 Ch. 12

$m = 0, \pm 1, \pm 2, \pm 3, \dots$ are momentum quanta in wavevector formula: $k_m = 2\pi m / L$
($k_m = m$ if: $L = 2\pi$)



Imagining "wrap-around" ϕ -coordinate



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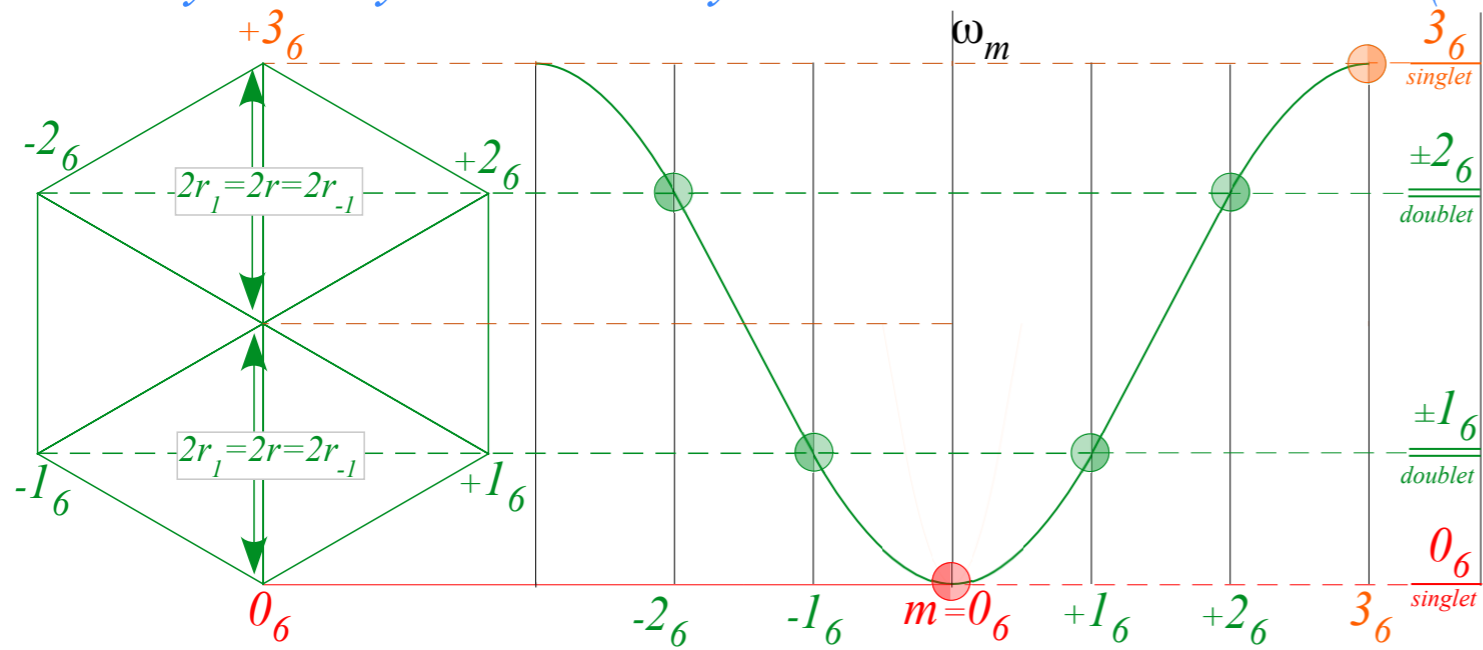
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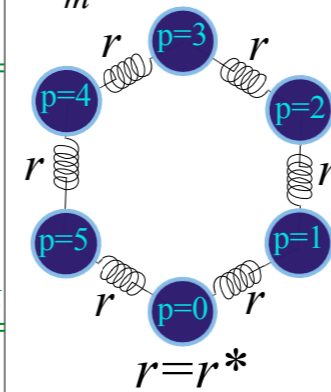
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C_6 symmetry: Elementary Bloch Hamiltonian $\mathbf{H}^{1B(6)}$ (1st neighbor coupling)

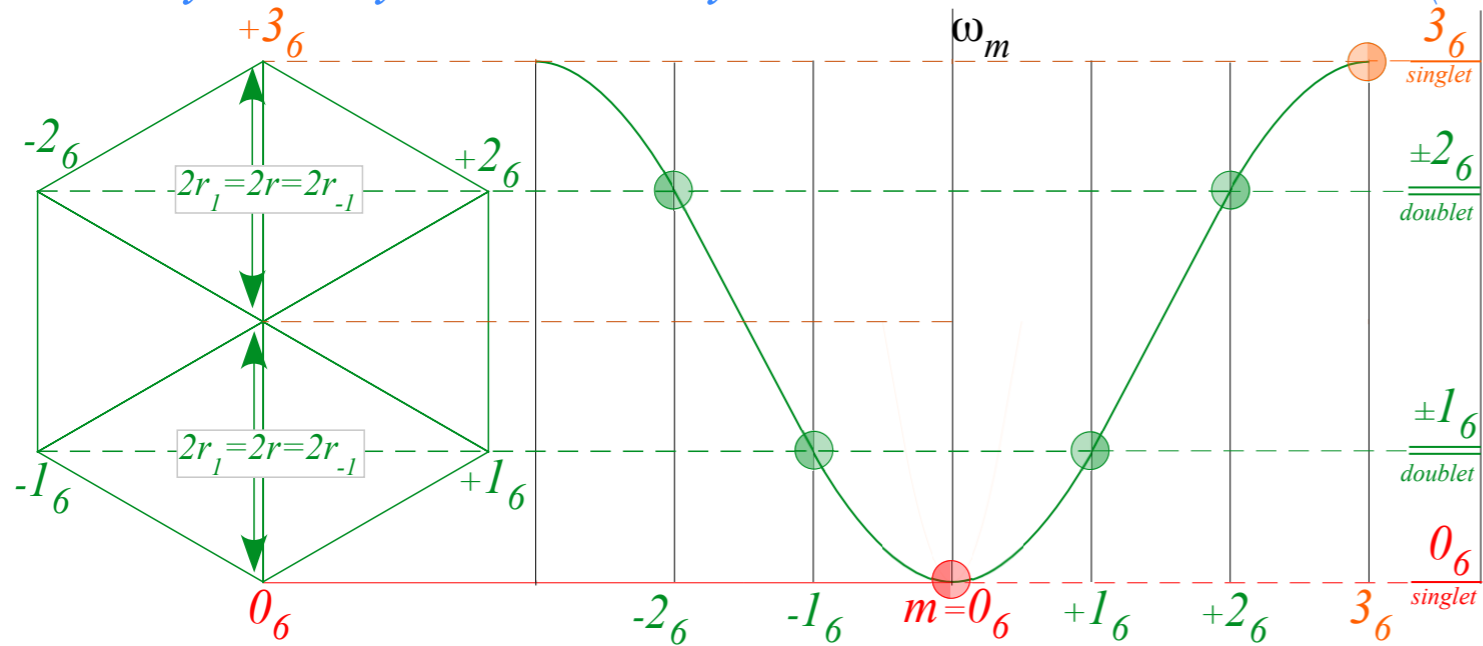


$\mathbf{H}^{1B(6)}$ eigenvalues

ω_m level spectrum

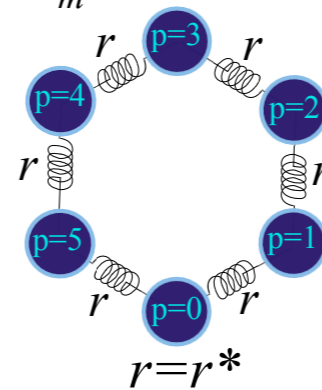


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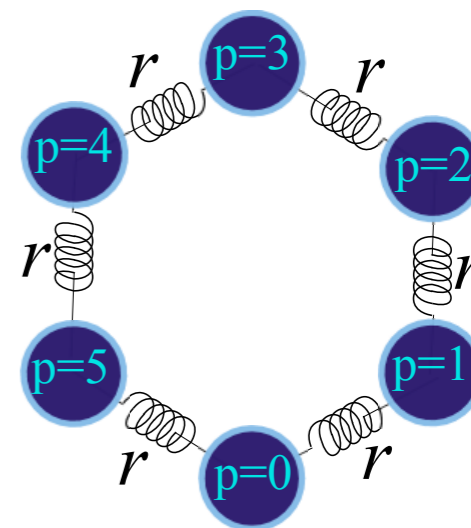


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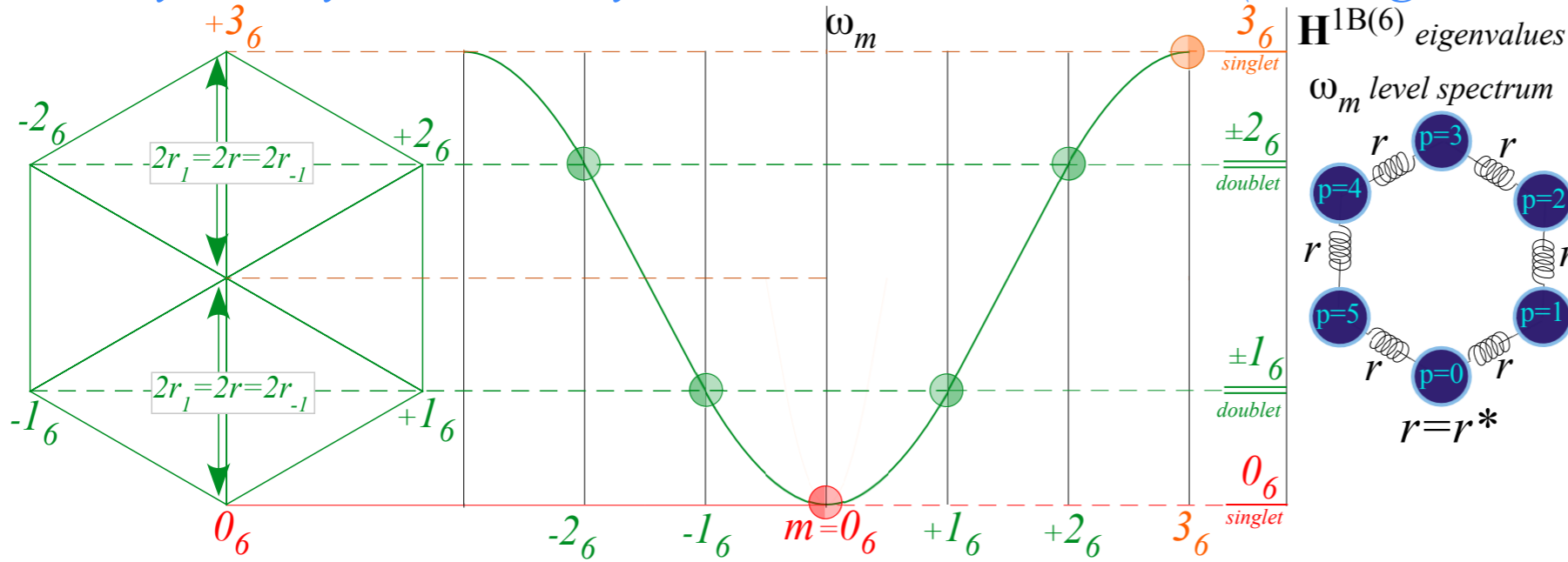
ω_m level spectrum



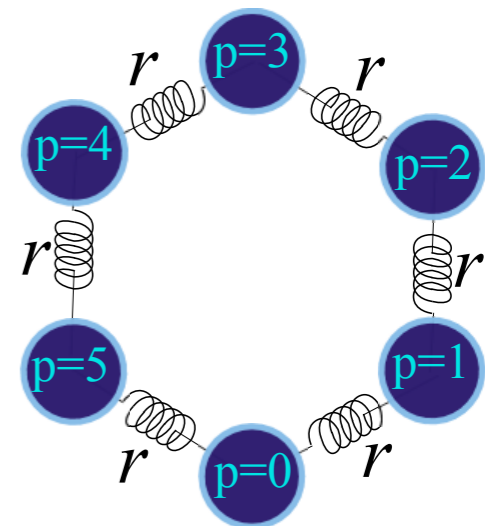
$$\mathbf{H}^{1B(6)} \begin{pmatrix} \psi^m_0 \\ \psi^m_1 \\ \psi^m_2 \\ \psi^m_3 \\ \psi^m_4 \\ \psi^m_5 \end{pmatrix} = \begin{pmatrix} p=0 & 1 & 2 & 3 & 4 & 5 \\ 2r & -r & \cdot & \cdot & \cdot & -r \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ -r & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix} \begin{pmatrix} \psi^m_0 \\ \psi^m_1 \\ \psi^m_2 \\ \psi^m_3 \\ \psi^m_4 \\ \psi^m_5 \end{pmatrix} = 2r(1 - \cos \frac{2\pi m}{6}) \begin{pmatrix} \psi^m_0 \\ \psi^m_1 \\ \psi^m_2 \\ \psi^m_3 \\ \psi^m_4 \\ \psi^m_5 \end{pmatrix}$$



C_6 symmetry: Elementary Bloch Hamiltonian $\mathbf{H}^{1B(6)}$ (1st neighbor coupling)



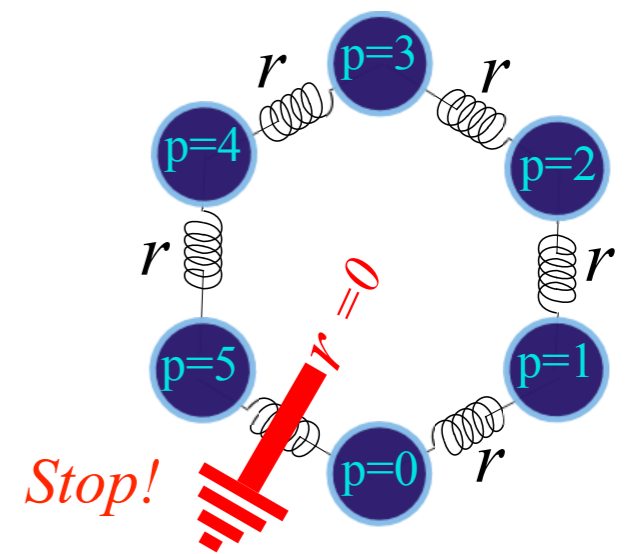
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$\mathbf{H}^{1B(6)}$ eigensolutions are very sensitive to zeroing or constraining a coupling!

$$\mathbf{H}^{1B(6)} \begin{pmatrix} \psi^m_0 \\ \psi^m_1 \\ \psi^m_2 \\ \psi^m_3 \\ \psi^m_4 \\ \psi^m_5 \end{pmatrix} = \begin{pmatrix} p=0 & 1 & 2 & 3 & 4 & 5 \\ 2r & -r & \cdot & \cdot & \cdot & 0 \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ 0 & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix} \begin{pmatrix} \psi^m_0 \\ \psi^m_1 \\ \psi^m_2 \\ \psi^m_3 \\ \psi^m_4 \\ \psi^m_5 \end{pmatrix} = ? \begin{pmatrix} ? \\ ? \\ ? \\ ? \\ ? \\ ? \end{pmatrix}$$

(Not eigenvectors)



Consider sine and cosine eigenvectors of a 14-by-14 elementary Bloch matrix $\mathbf{H}^{\text{EB}(14)}$

$$\langle \cos^m | = \left(\begin{array}{c|cccccc|c|cccccc} c_0^m=1 & c_1^m & c_2^m & c_3^m & c_4^m & c_5^m & c_6^m & c_7^m=1 & c_{-6}^m & c_{-5}^m & c_{-4}^m & c_{-3}^m & c_{-2}^m & c_{-1}^m \end{array} \right) \quad c_p^m = \cos\left(m \cdot p \frac{\pi}{7}\right) = c_{-p}^m$$

$$\langle \sin^m | = \left(\begin{array}{c|cccccc|c|cccccc} s_0^m=0 & s_1^m & s_2^m & s_3^m & s_4^m & s_5^m & s_6^m & s_7^m=0 & s_{-6}^m & s_{-5}^m & s_{-4}^m & s_{-3}^m & s_{-2}^m & s_{-1}^m \end{array} \right) \quad s_p^m = \sin\left(m \cdot p \frac{\pi}{7}\right) = -s_{-p}^m$$

$$\mathbf{H}^{\text{EB}(14)} | \sin^m \rangle = \omega^{m(14)} | \sin^m \rangle$$

p/p'	0	1	2	3	4	5	6	7	-6	-5	-4	-3	-2	-1			
0	2r	-r	-r	0	0
1	-r	2r	-r									s_1^m	s_1^m
2	.	-r	2r	-r	.	.	.									s_2^m	s_2^m
3	.	.	-r	2r	-r	.	.									s_3^m	s_3^m
4	.	.	.	-r	2r	-r	.									s_4^m	s_4^m
5	-r	2r	-r									s_5^m	s_5^m
6	-r	2r	-r								s_6^m	s_6^m
7	.						-r	2r	-r							0	0
-6	.							-r	2r	-r		s_{-6}^m	s_{-6}^m
-5	.								-r	2r	-r	.	.	.		s_{-5}^m	s_{-5}^m
-4	.								.	-r	2r	-r	.	.		s_{-4}^m	s_{-4}^m
-3	.								.	.	-r	2r	-r	.		s_{-3}^m	s_{-3}^m
-2	-r	2r	-r		s_{-2}^m	s_{-2}^m
-1	-r								-r	2r		s_{-1}^m	s_{-1}^m

where:

$$\omega^{m(14)} = 2r(1 - \cos\frac{2\pi m}{14})$$

Consider sine and cosine eigenvectors of a *14-by-14* elementary Bloch matrix $\mathbf{H}^{\text{EB}(14)}$

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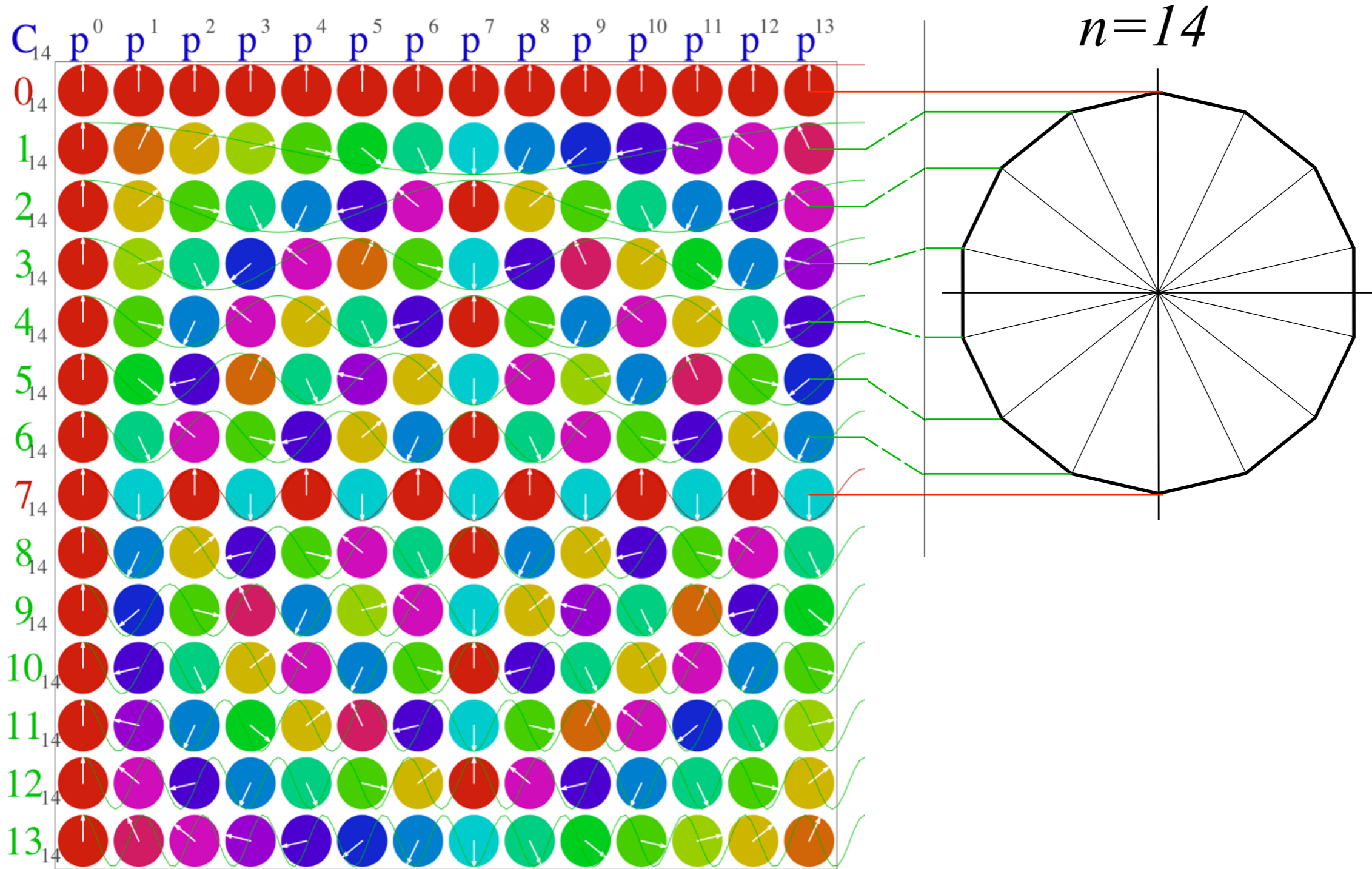
$\mathbf{H}^{\text{EB}(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{\text{CM}(6)}$

p'																																																								
0	2r							r						...						0	0																																			
1	-r	2r							-r						...						s_1^m	s_1^m																																		
2	.	-r							2r						-r						s_2^m	s_2^m																																		
3	.	.							-r						2r						s_3^m	s_3^m																																		
4	.	.							.						-r						2r						s_4^m	s_4^m																												
5						-r						2r						s_5^m	s_5^m																						
6	.	.							0						.						-r						2r						s_6^m	s_6^m																						
7	.							-r						2r						-r						0	0																													
-6	.							-r						2r						-r						s_{-6}^m	s_{-6}^m																													
-5	.							.						-r						2r						-r						s_{-5}^m	s_{-5}^m																							
-4	.							.						.						-r						2r						-r						s_{-4}^m	s_{-4}^m																	
-3						-r						2r						-r						s_{-3}^m	s_{-3}^m											
-2						-r						2r						-r						s_{-2}^m	s_{-2}^m					
-1	-r												-r						2r						s_{-1}^m	s_{-1}^m											

where:

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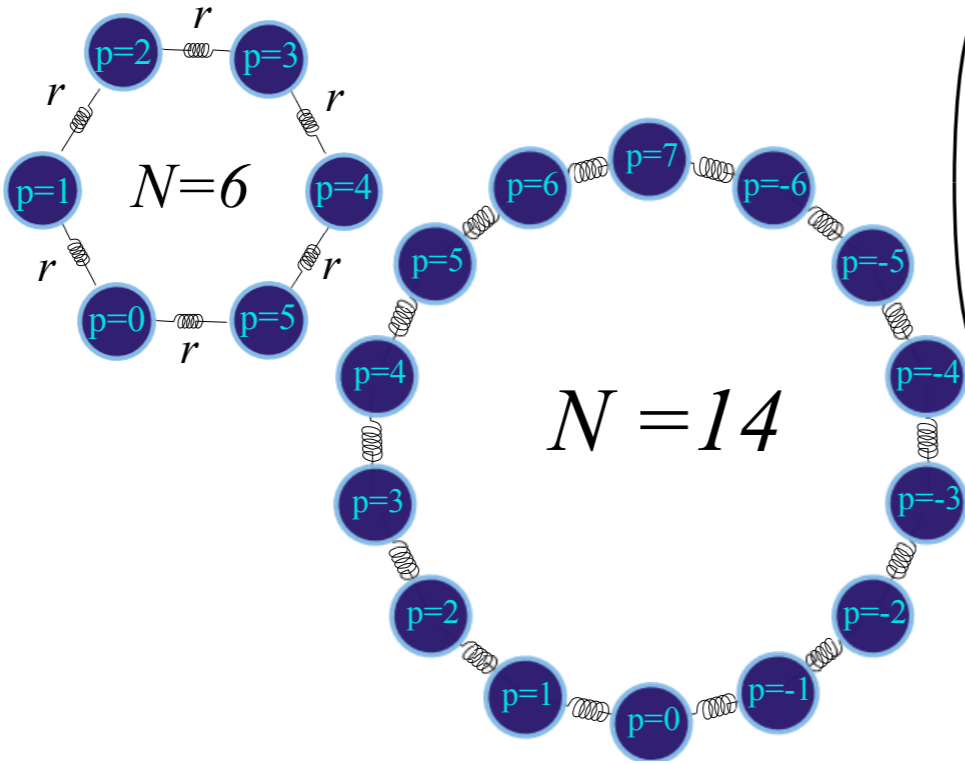
$\mathbf{H}^{\text{EB}(14)}$ gives eigensolution of a 6-by-6 constrained Bloch matrix $\mathbf{H}^{\text{CM}(6)}$ using its sine-waves only



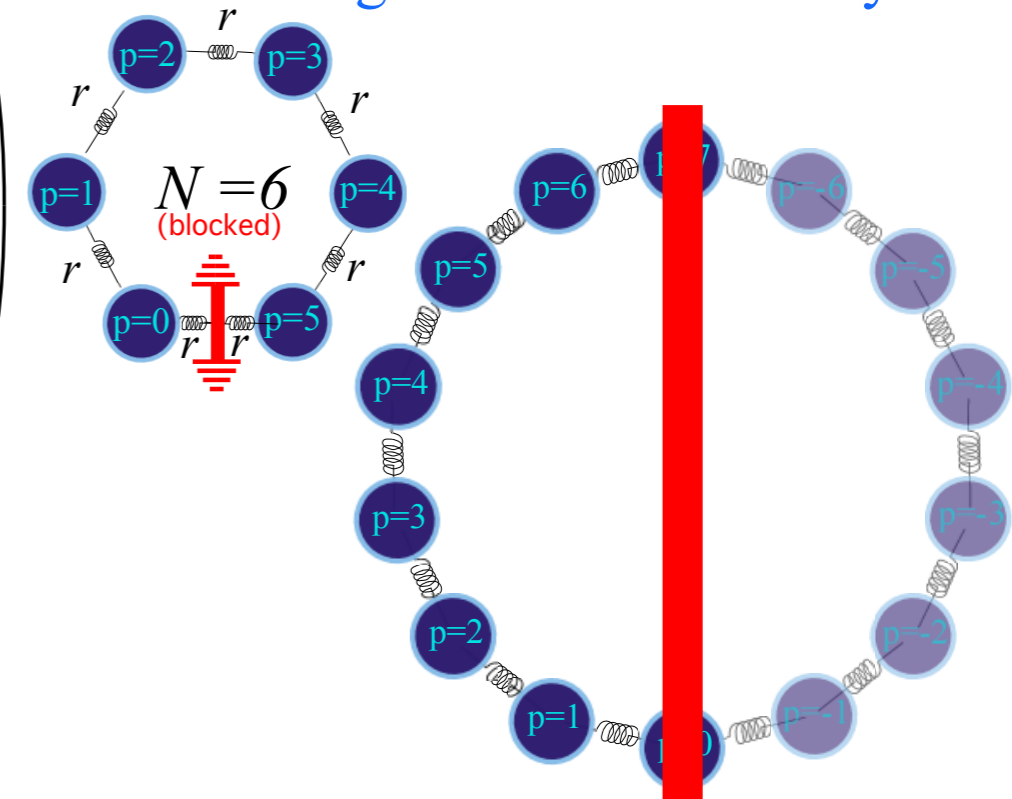
[WaveIt Web Simulation](#)
[C₁₄ Character Phasors](#)

$\mathbf{H}^{\text{EB}(14)}$ gives eigensolution of a 6-by-6 constrained Bloch matrix $\mathbf{H}^{\text{CM}(6)}$ using its sine-waves only

$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & -r \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ -r & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$

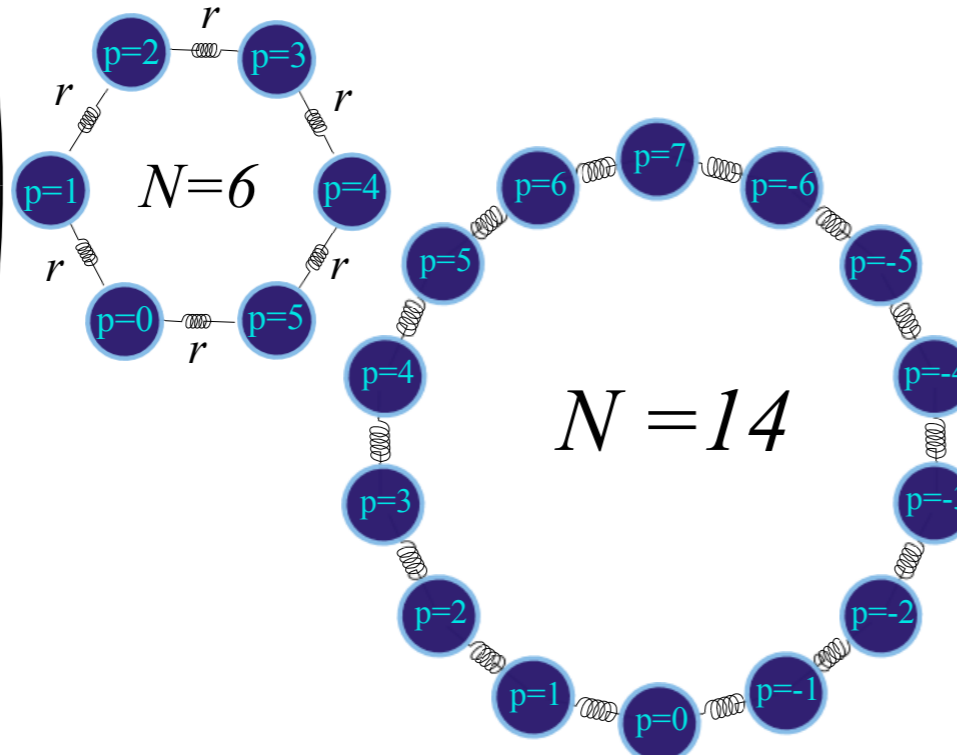


$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & 0 \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ 0 & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$

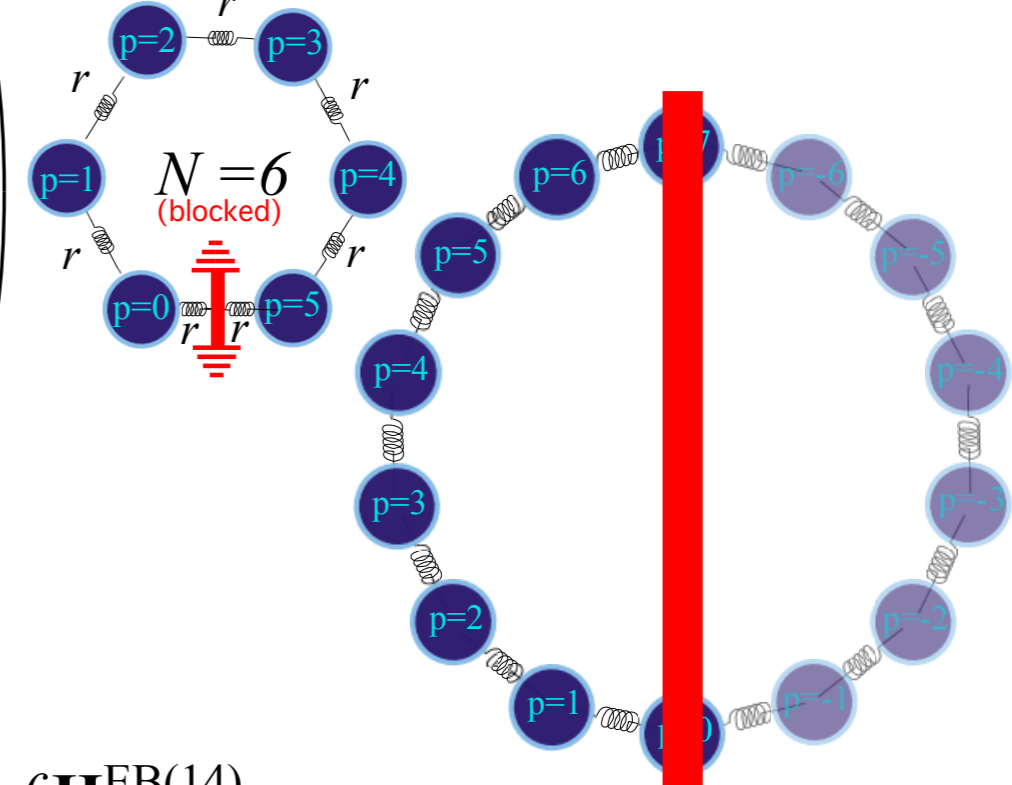


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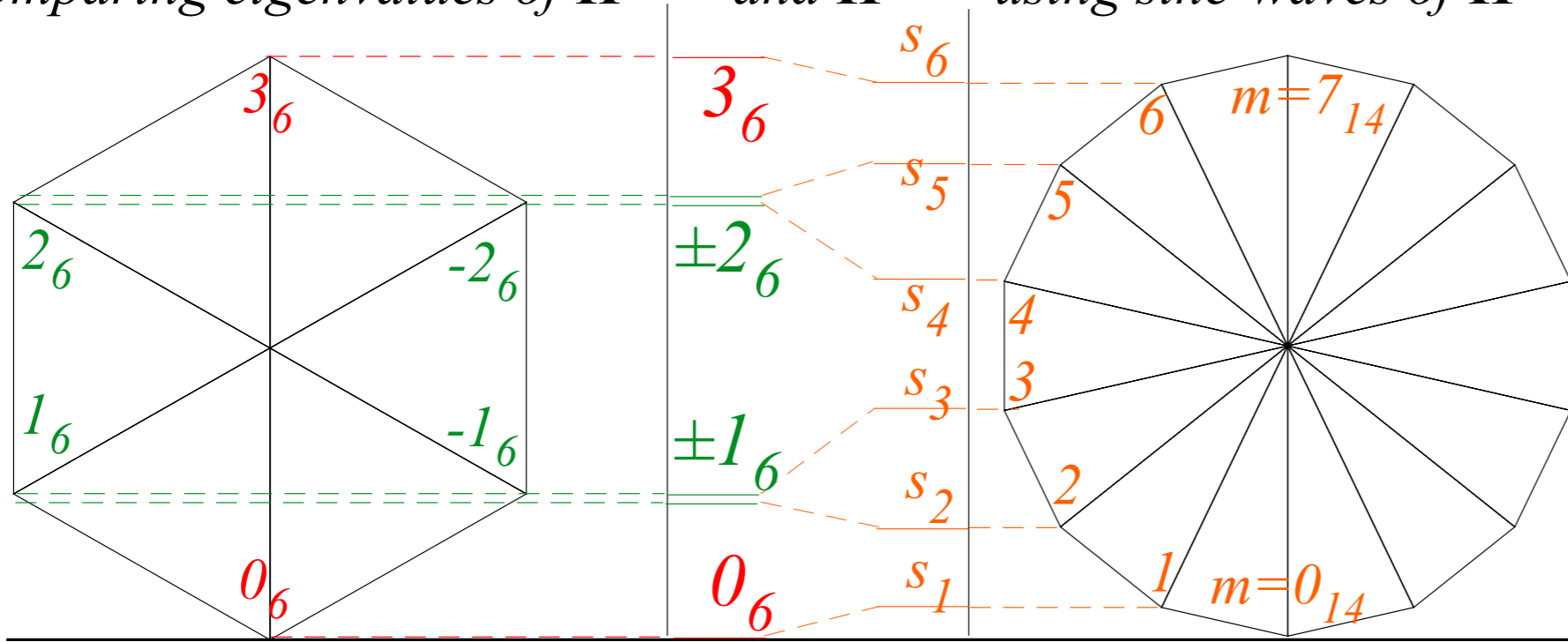
$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & -r \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ -r & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$



$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & 0 \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ 0 & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$

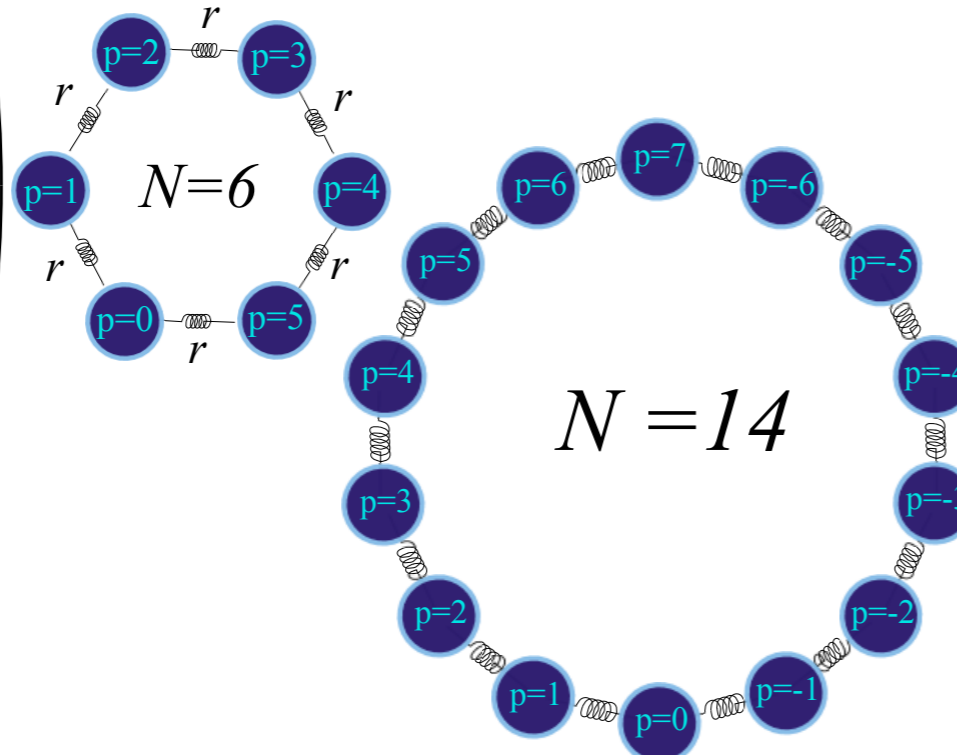


Comparing eigenvalues of $\mathbf{H}^{\text{EB}(6)}$ and $\mathbf{H}^{\text{CM}(6)}$ using sine-waves of $\mathbf{H}^{\text{EB}(14)}$

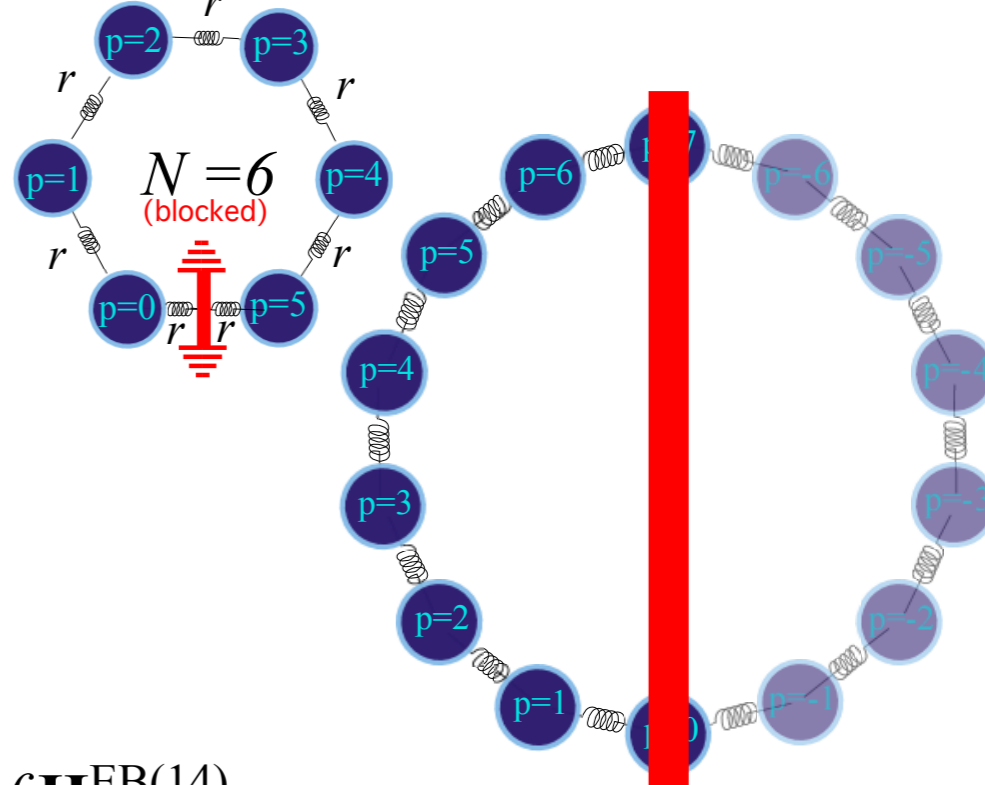


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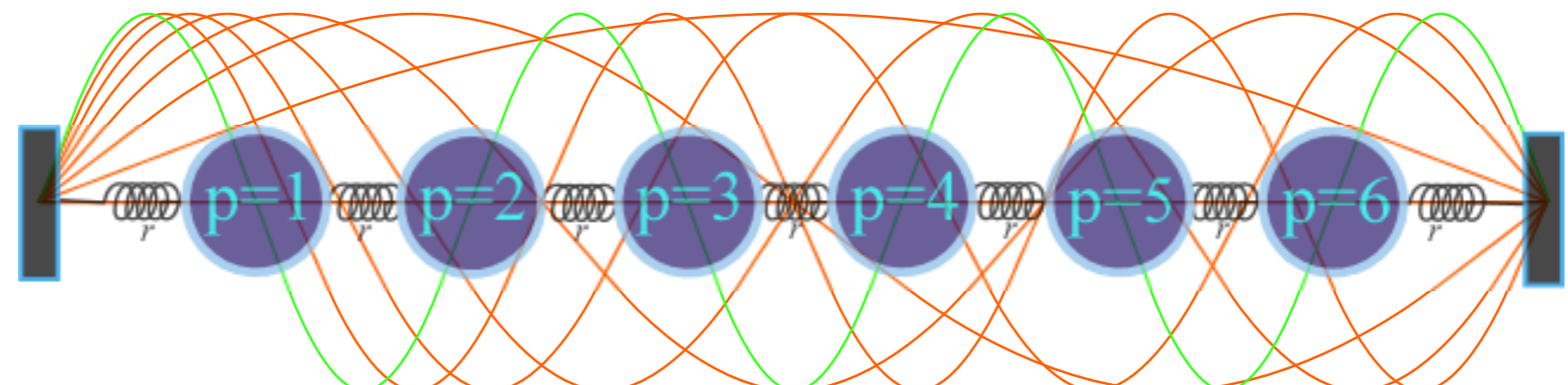
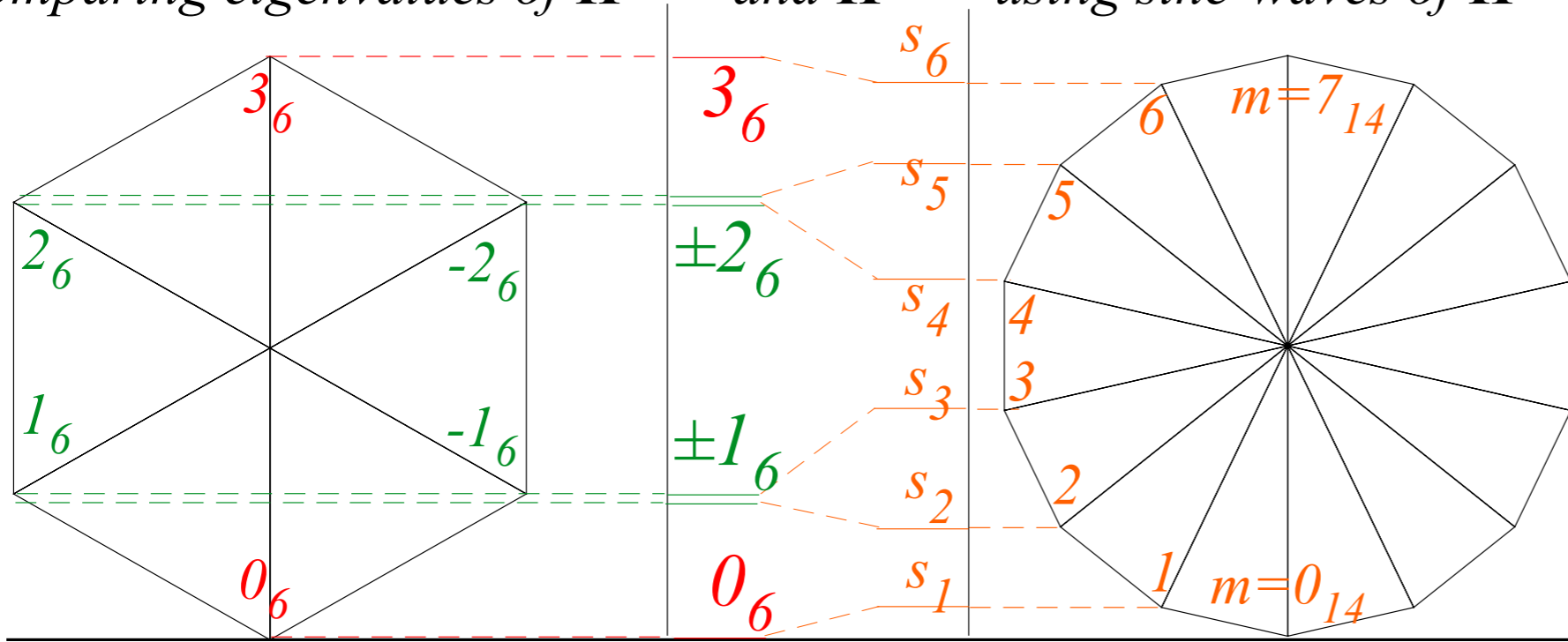
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$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & 0 \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ 0 & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$



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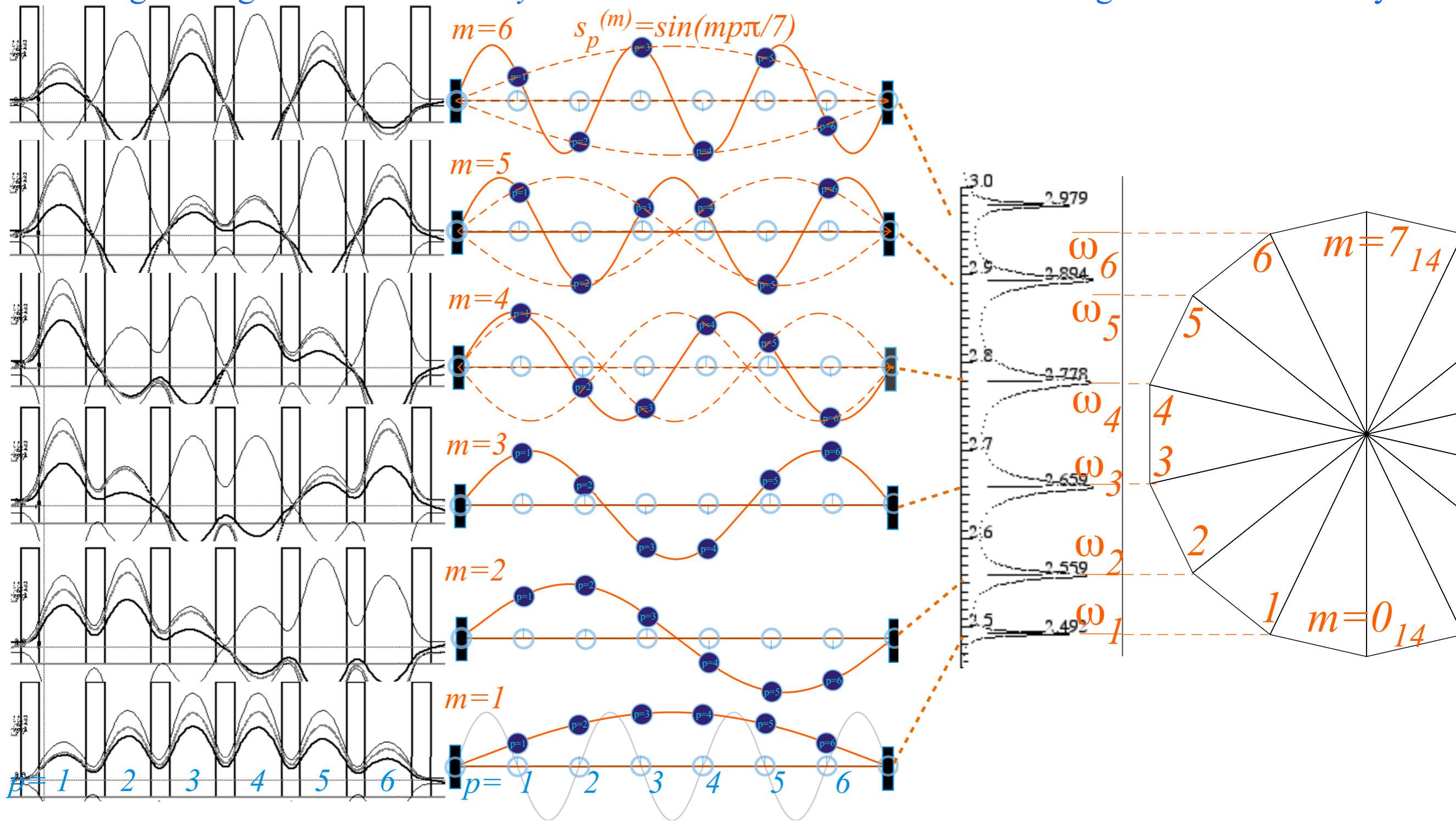
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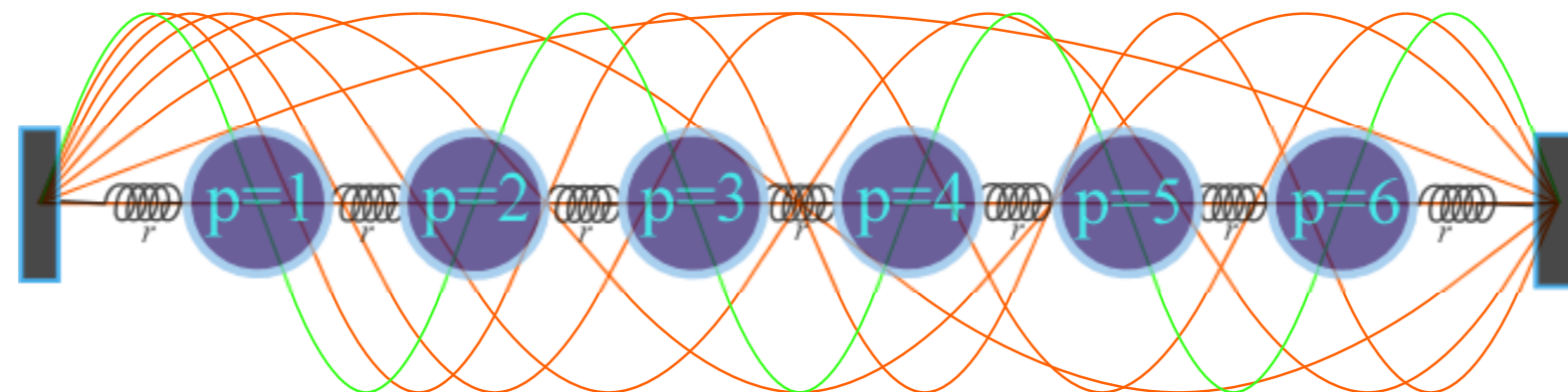
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*Band-It simulation is
Mac OS 9 application
not yet converted to web*

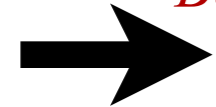


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How Band-It simulation works (from QTfCA Unit 4 Chapter 13)

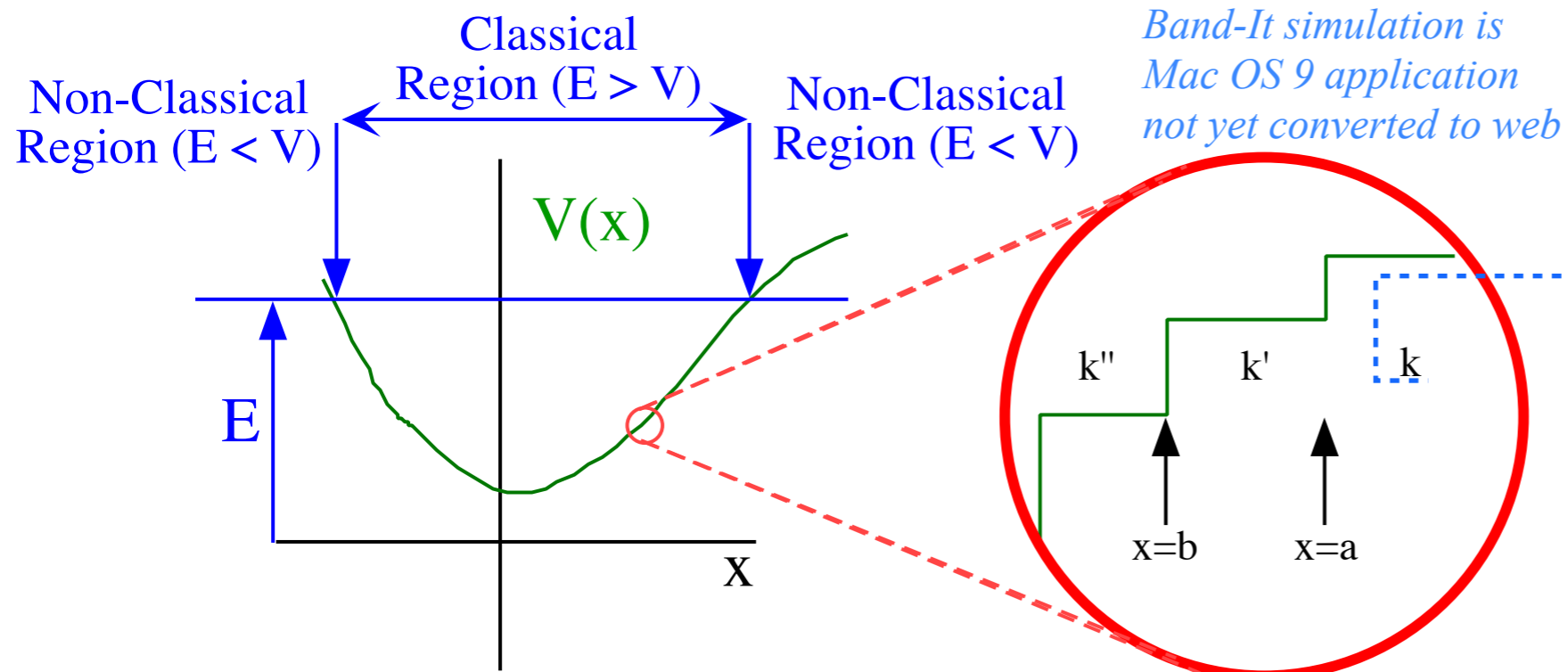


Fig. 13.1.1 Non-constant potential $V(x)$ approximated by a series of small constant- V steps.

Between each step potential, kinetic energy, and k are assumed constant.

$$\Psi_E(x, 0) = R e^{ikx} + L e^{-ikx}$$

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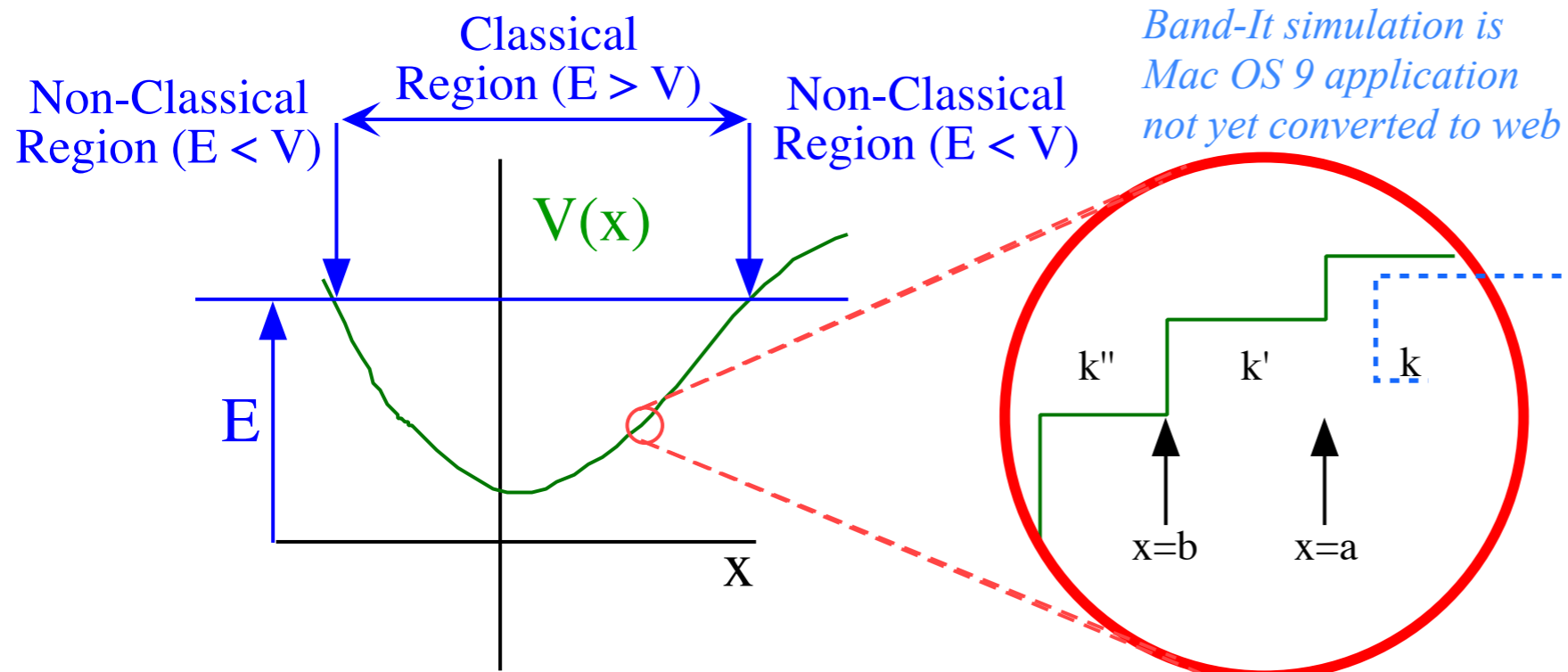


Fig. 13.1.1 Non-constant potential $V(x)$ approximated by a series of small constant- V steps.

Between each step potential, kinetic energy, and k are assumed constant. x -derivative is denoted by $D\Psi$

$$\Psi_E(x,0) = R e^{ikx} + L e^{-ikx} \quad \frac{\partial}{\partial x} \Psi_E(x,0) = ik R e^{ikx} - ik L e^{-ikx} \equiv D\Psi_E(x,0)$$

How Band-It simulation works (from QTfCA Unit 4 Chapter 13)

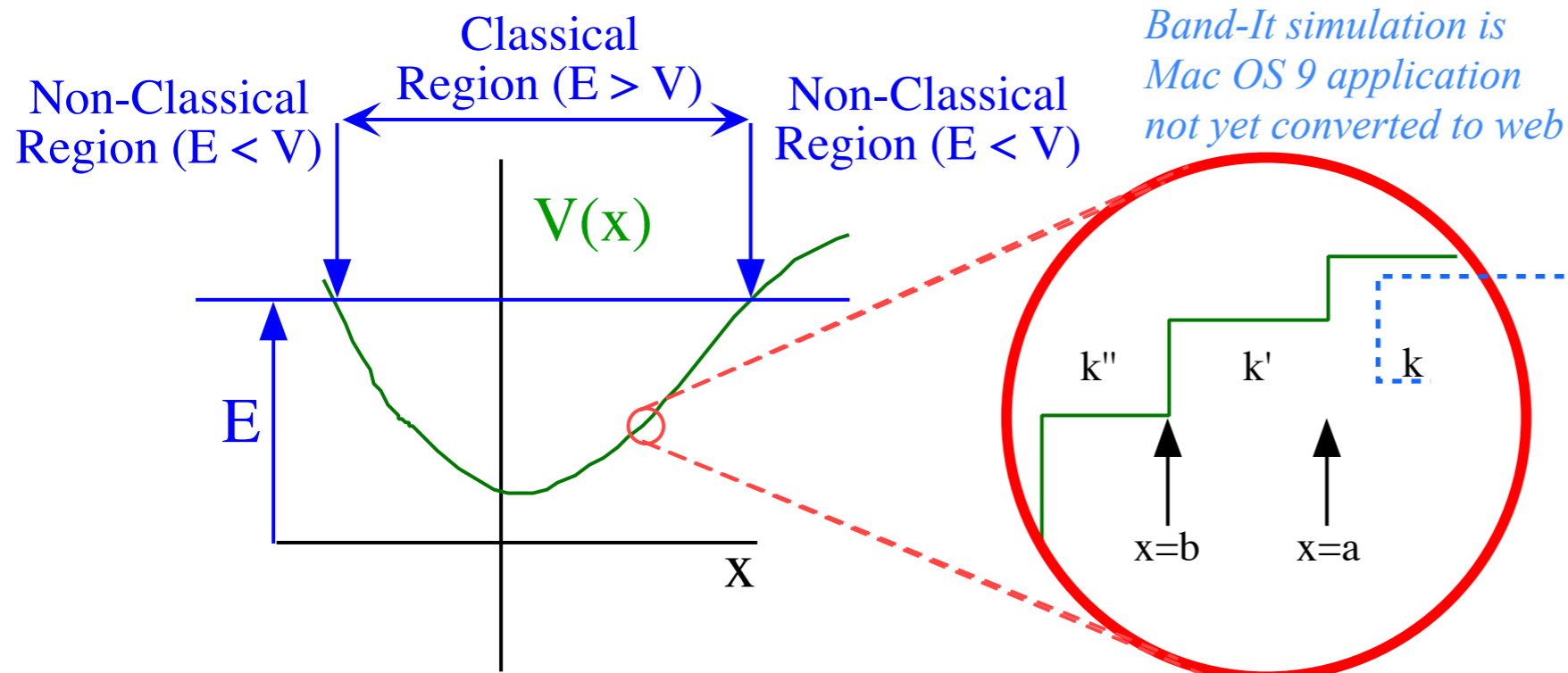


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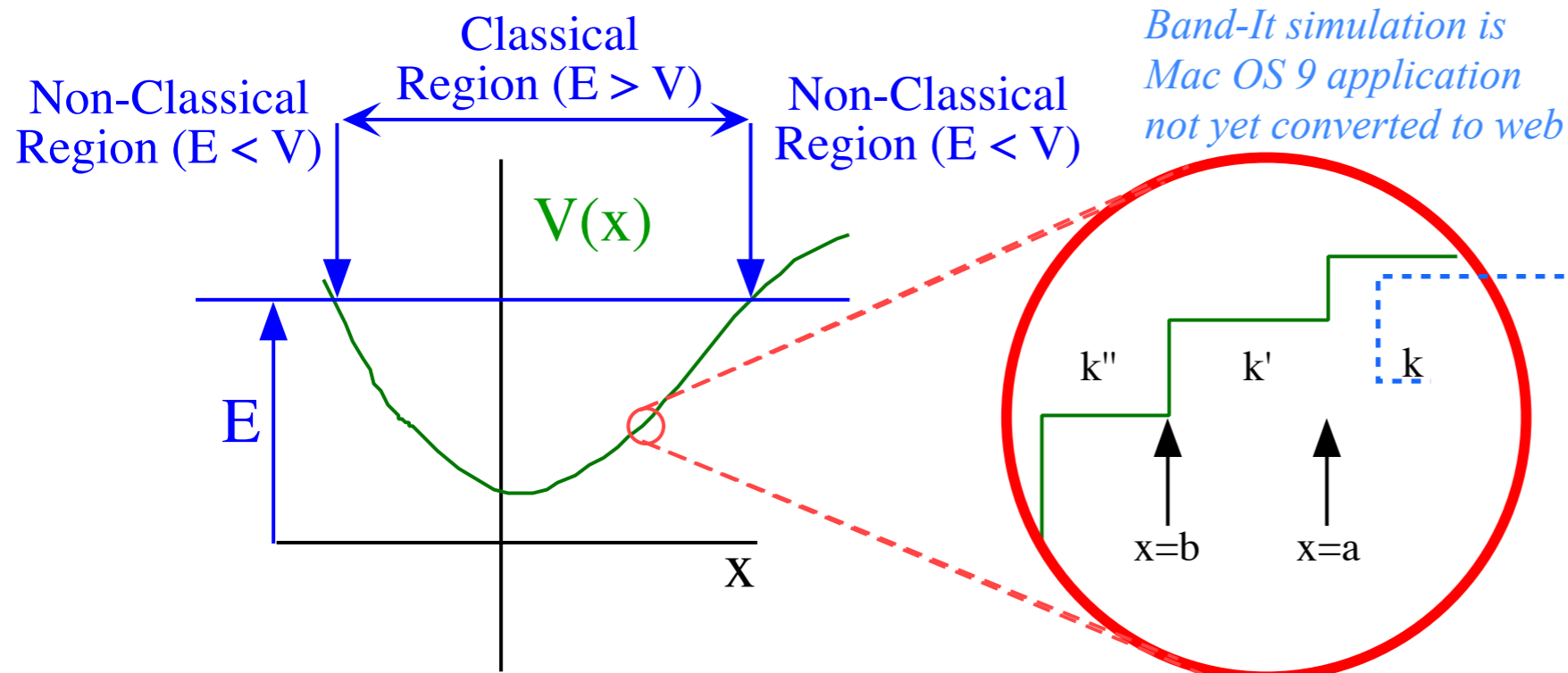


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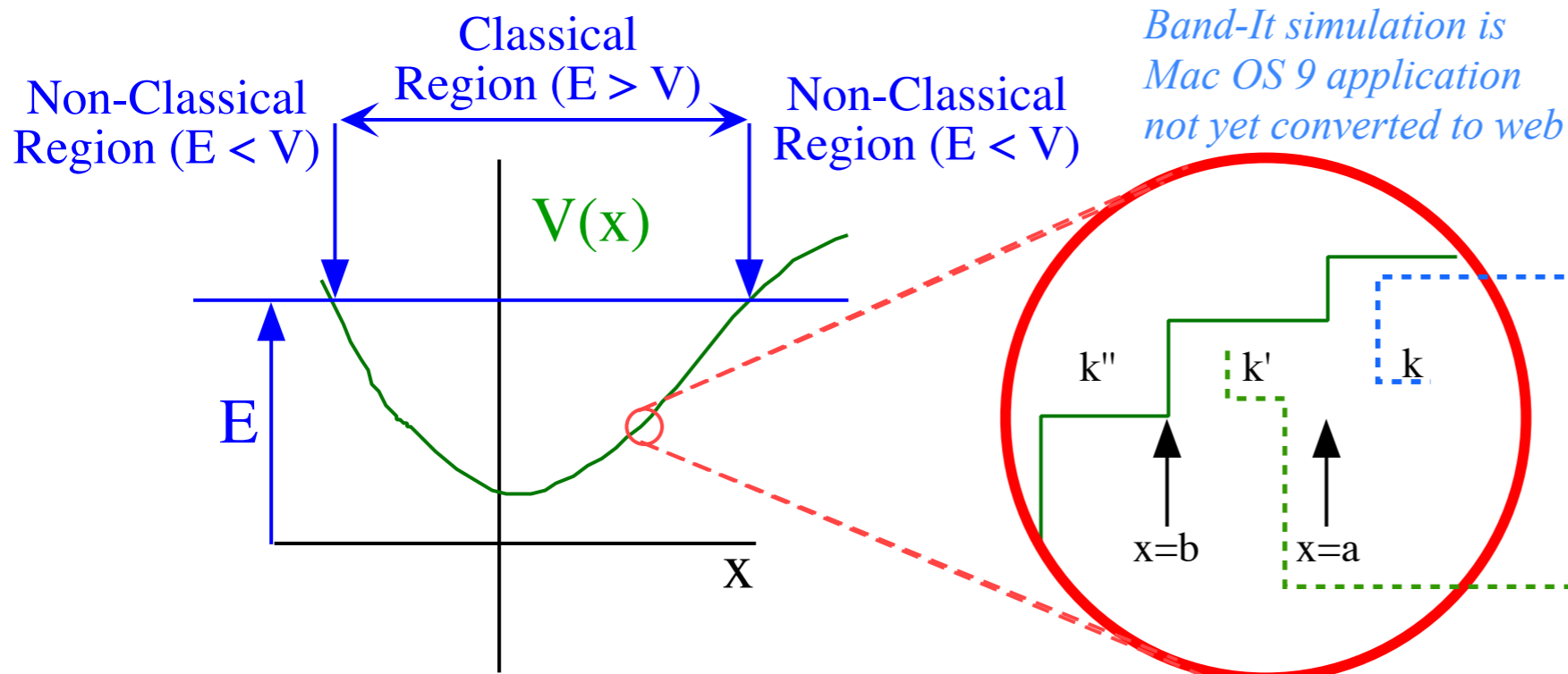


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Relations on the other side of the step boundary just below $x=a$.

$$\begin{pmatrix} \Psi' \\ D\Psi' \end{pmatrix} = \begin{pmatrix} e^{ik'x} & e^{-ik'x} \\ ik'e^{ik'x} & -ik'e^{-ik'x} \end{pmatrix} \begin{pmatrix} R' \\ L' \end{pmatrix}, \quad \begin{pmatrix} R' \\ L' \end{pmatrix} = \frac{i}{2k'} \begin{pmatrix} -ik'e^{-ik'x} & -e^{-ik'x} \\ -ik'e^{ik'x} & e^{ik'x} \end{pmatrix} \begin{pmatrix} \Psi' \\ D\Psi' \end{pmatrix}$$


(Inverted)

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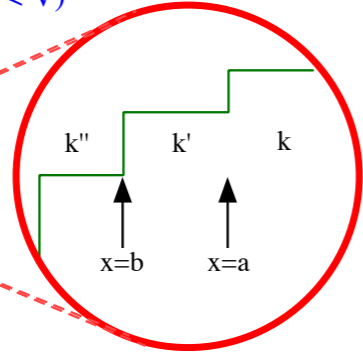
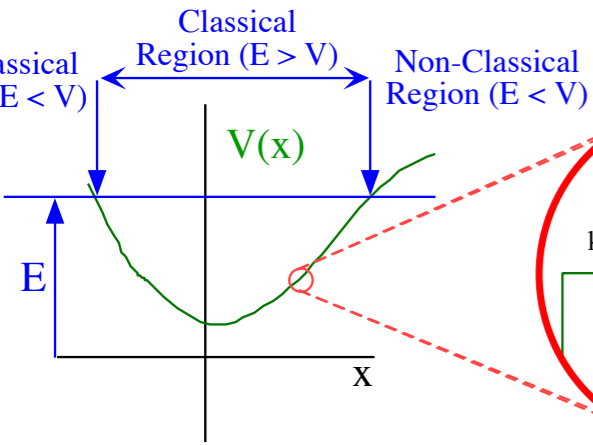
Polygonal geometry of $U(2) \supset C_N$ character spectral function $\chi^j(2\pi/n) = \frac{\sin(\pi(2j+1)/n)}{\sin(\pi/n)}$

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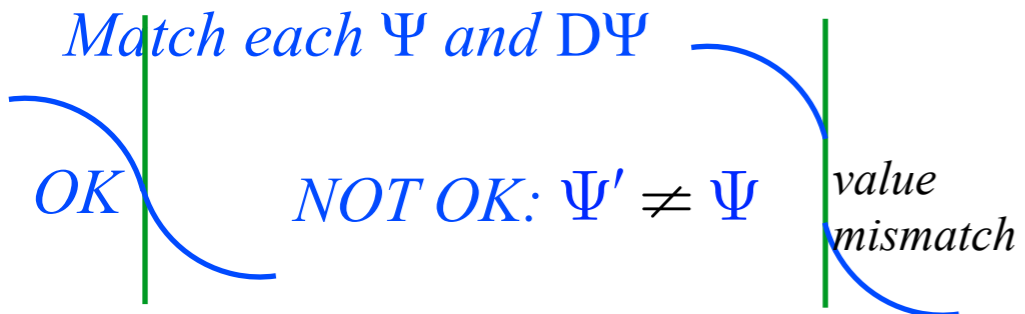
Wave function and derivative at $x=a-\epsilon$ equals that at $x=a+\epsilon$.



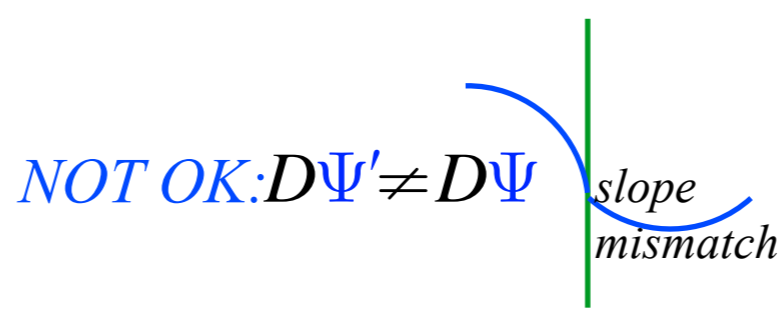
$$\begin{pmatrix} R' \\ L' \end{pmatrix} = \frac{i}{2k'} \begin{pmatrix} -ik'e^{-ik'a} & -e^{-ik'a} \\ -ik'e^{ik'a} & e^{ik'a} \end{pmatrix} \begin{pmatrix} \Psi \\ D\Psi \end{pmatrix}_{x=a}$$

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Match each Ψ and $D\Psi$



NOT OK: $\Psi' \neq \Psi$ value mismatch



NOT OK: $D\Psi' \neq D\Psi$ slope mismatch

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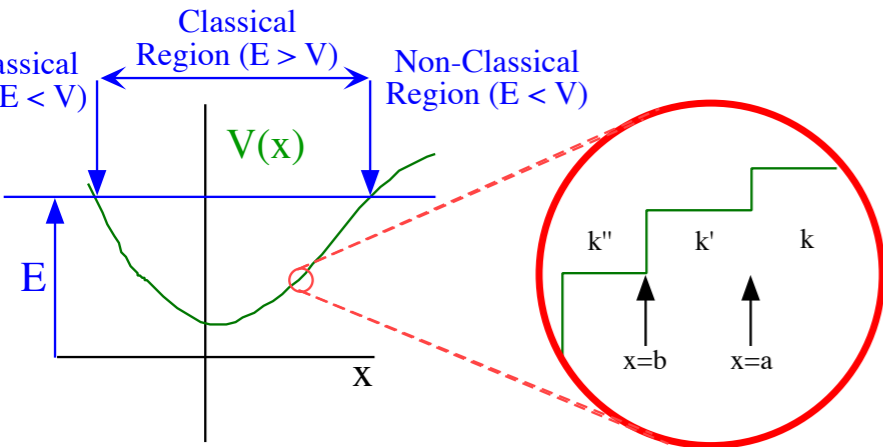
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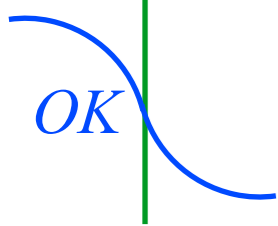
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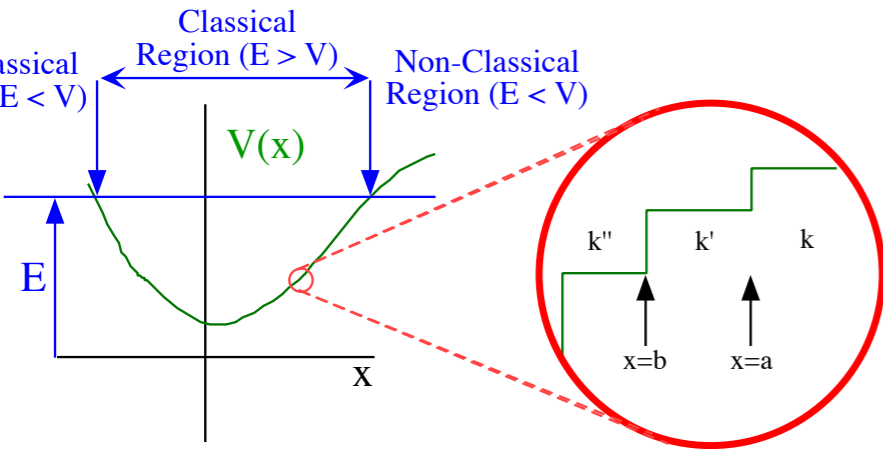
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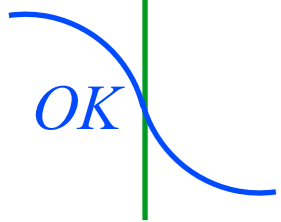
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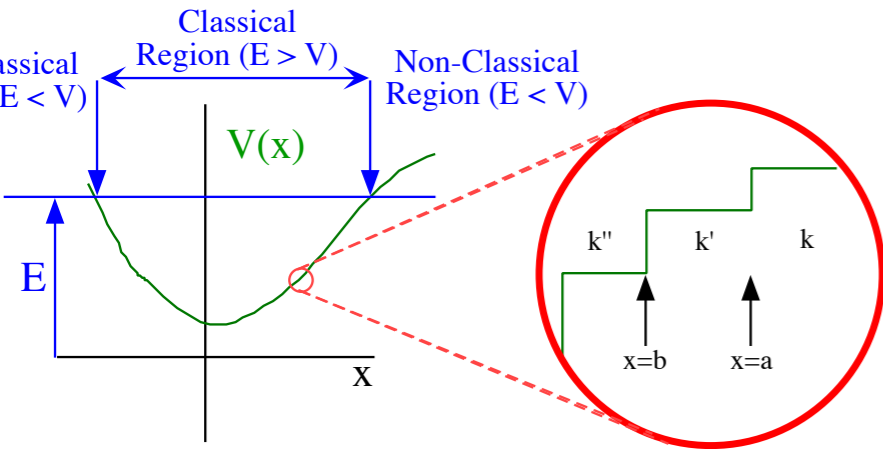
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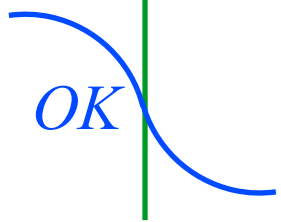
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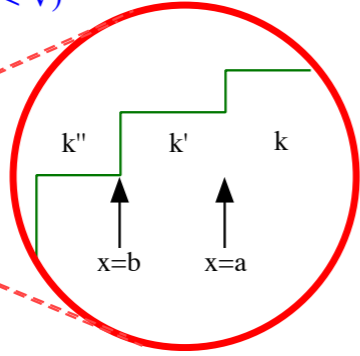
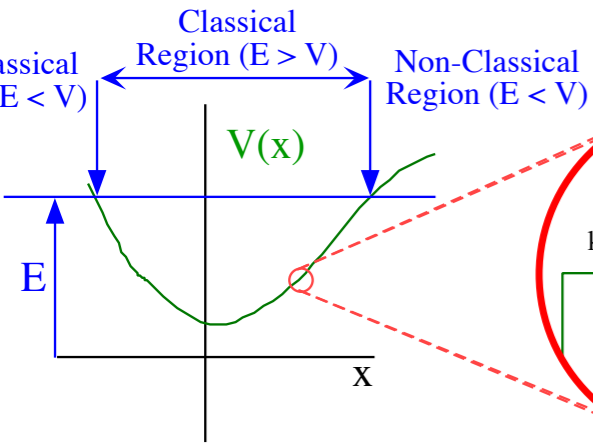
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A special case: *single input conditions* with no sources or reflectors on one side (say, right hand side) so no incoming waves exist there (say, $L=0$ but $R=Outgoing \neq 0$.)

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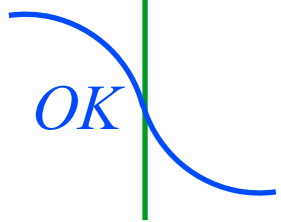
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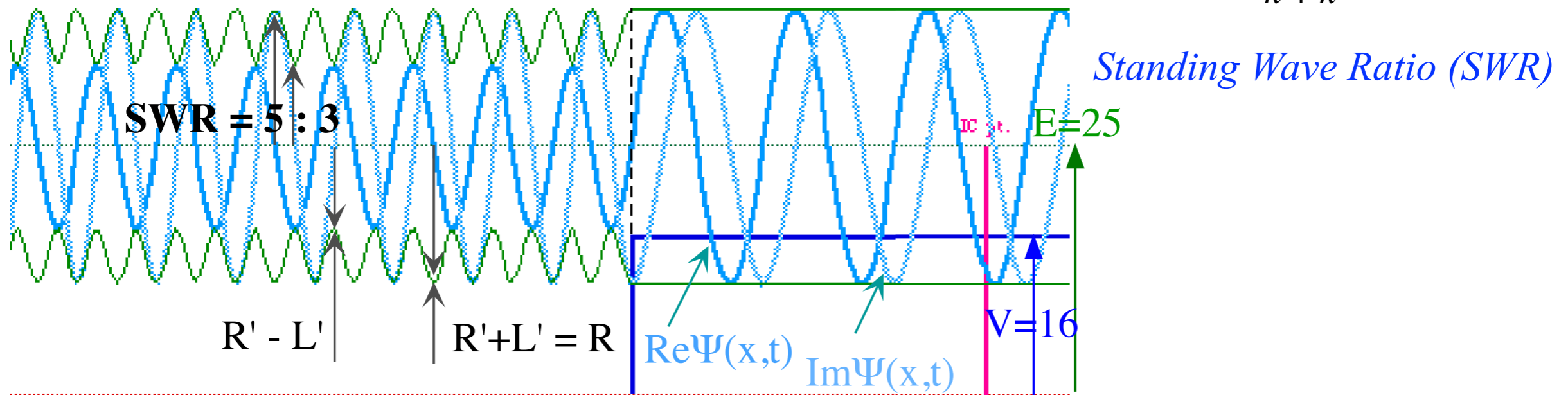
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This gives *transmitted or output amplitude* R and *reflected amplitude* L' given an *input amplitude* R' .

$$R = \frac{2k'}{(k+k')} R' e^{i(k'-k)a}, \quad L' = \frac{(k'-k)}{(k+k')} R' e^{2ik'a}$$

The *transmission coefficient* $T_{transmit}$ and *reflection coefficient* $T_{reflect}$ (for $a=0$)

$$T_{transmit} = \frac{|R|^2}{|R'|^2} = \frac{4|k'|^2}{|k+k'|^2}, \quad T_{reflect} = \frac{|L'|^2}{|R'|^2} = \frac{|k'-k|^2}{|k'+k|^2}, \quad SWR = \frac{L' - R'}{L' + R'} = \frac{\frac{2kR'}{k+k'} - R'}{\frac{2kR'}{k+k'} + R'} = \frac{k}{k'} = \frac{\sqrt{E-V}}{\sqrt{E}}$$



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Geometry

C_{24} lattice reduced to C_{12} symmetry

Fig. 2.7.6 PSDS

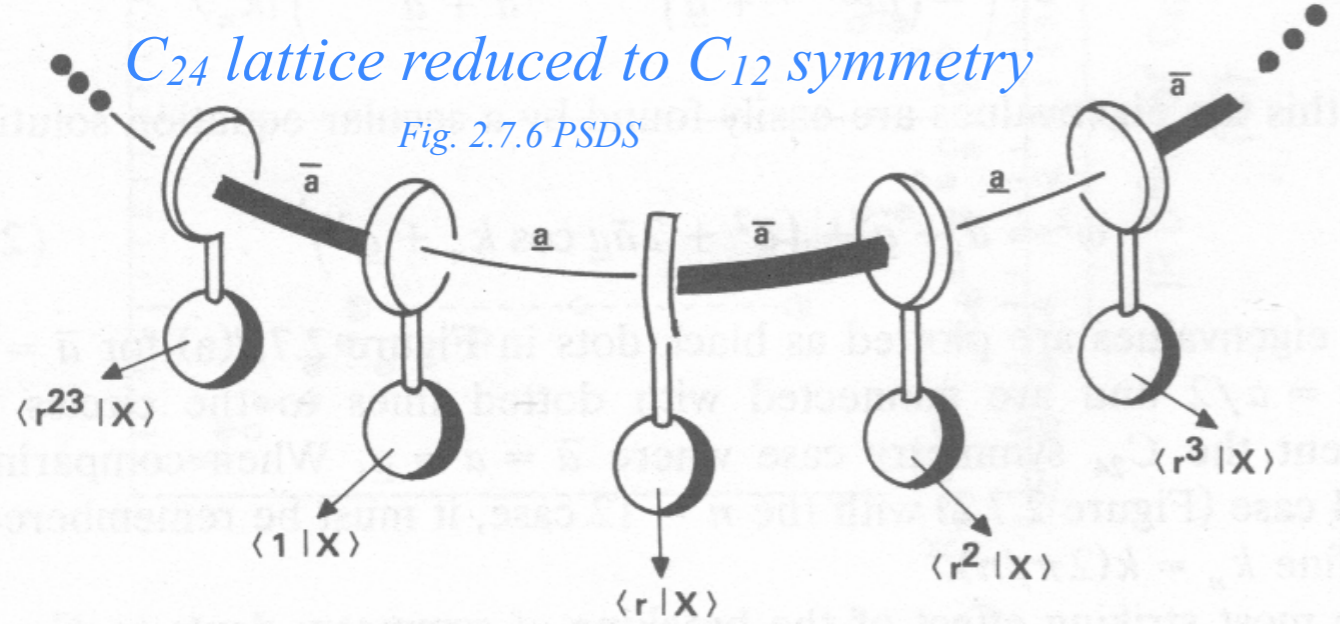
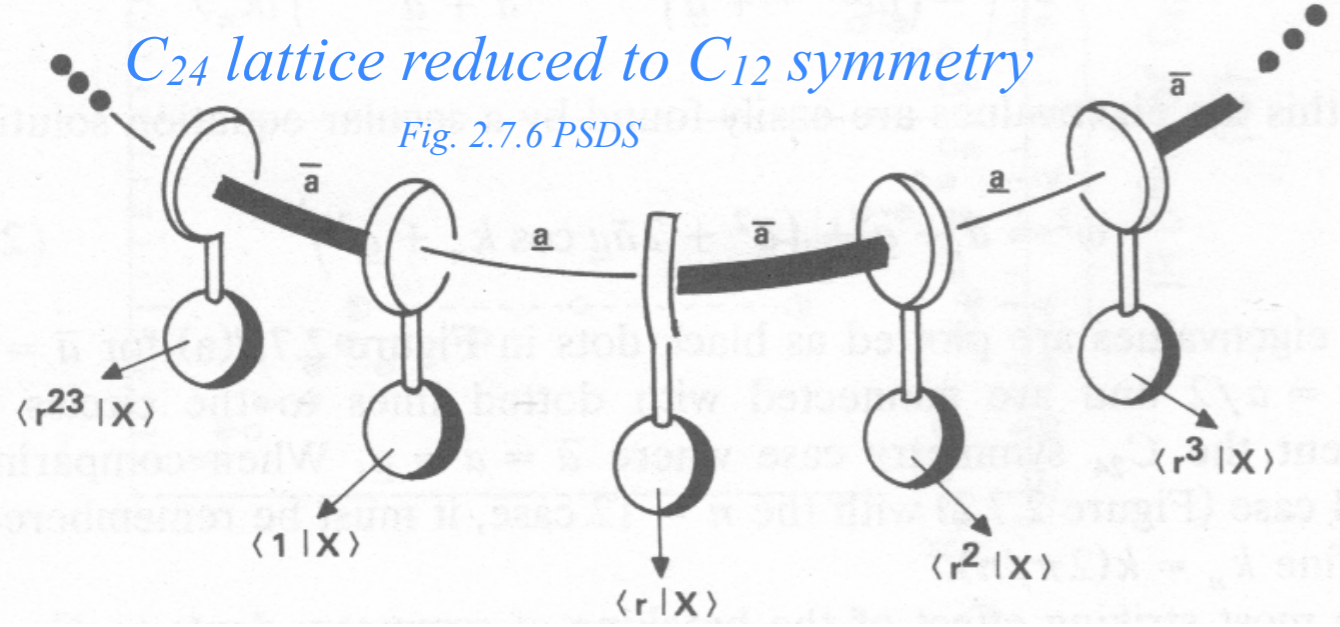


Fig. 2.7.6 Principles Symmetry Dynamics & Spectroscopy

C₂₄ lattice reduced to C₁₂ symmetry

Fig. 2.7.6 PSDS



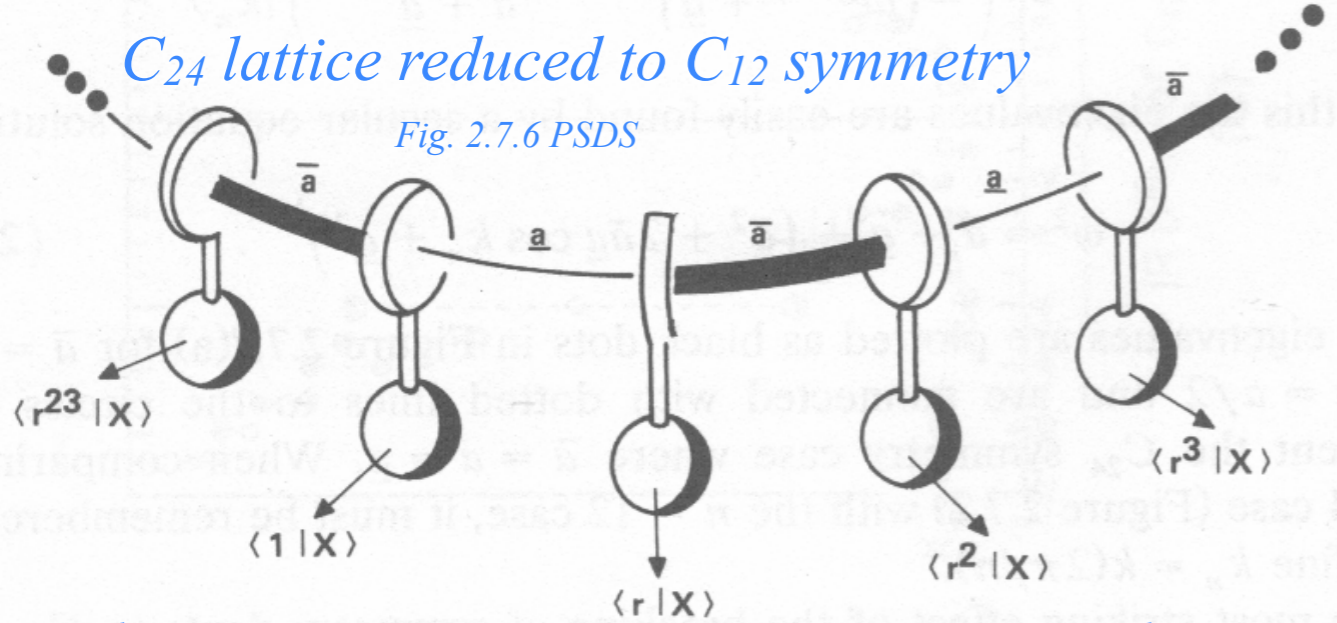
$$\begin{pmatrix} \langle r^0 | \mathbf{K} | r^0 \rangle & \langle r^0 | \mathbf{K} | r^1 \rangle & \langle r^0 | \mathbf{K} | r^2 \rangle & \dots & \langle r^0 | \mathbf{K} | r^{-1} \rangle \\ \langle r^1 | \mathbf{K} | r^0 \rangle & \langle r^1 | \mathbf{K} | r^1 \rangle & \langle r^1 | \mathbf{K} | r^2 \rangle & \dots & \langle r^1 | \mathbf{K} | r^{-1} \rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a} + \bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a} + \bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

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C_{24} lattice reduced to C_{12} symmetry

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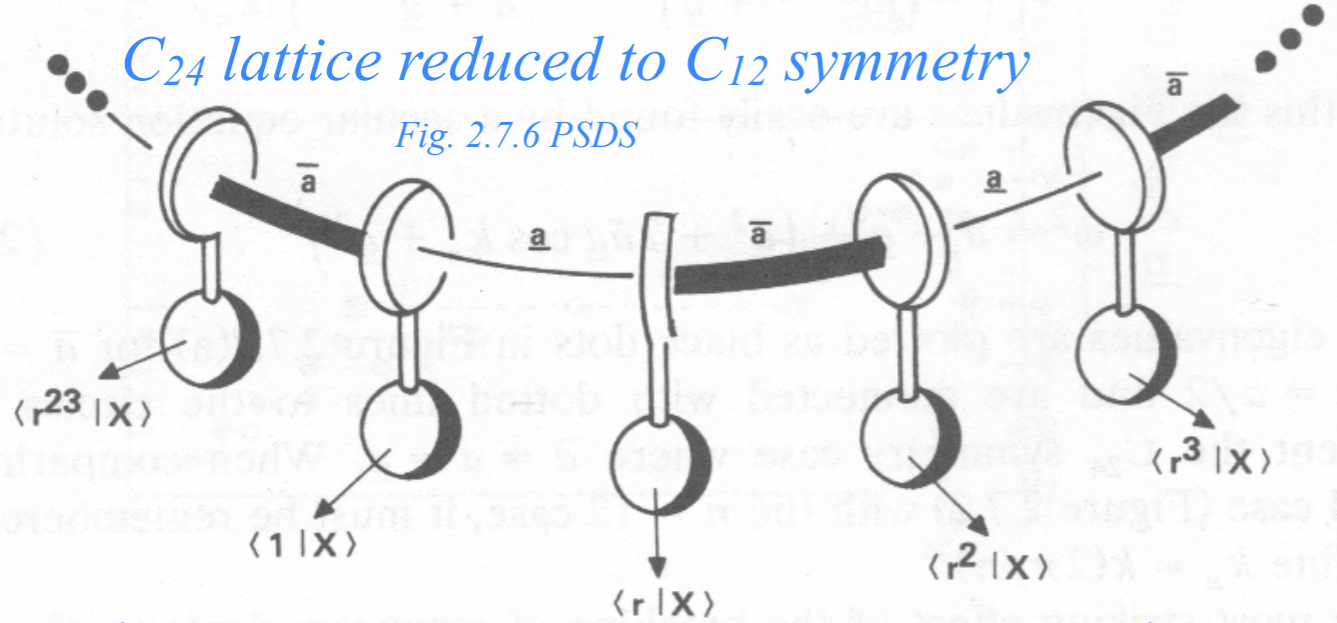
$$\begin{pmatrix} \langle r^0 | \mathbf{K} | r^0 \rangle & \langle r^0 | \mathbf{K} | r^1 \rangle & \langle r^0 | \mathbf{K} | r^2 \rangle & \dots & \langle r^0 | \mathbf{K} | r^{-1} \rangle \\ \langle r^1 | \mathbf{K} | r^0 \rangle & \langle r^1 | \mathbf{K} | r^1 \rangle & \langle r^1 | \mathbf{K} | r^2 \rangle & \dots & \langle r^1 | \mathbf{K} | r^{-1} \rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a} + \bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a} + \bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

Only C_{12} symmetry projectors commute with \mathbf{K} -matrix if $\underline{a} \neq \bar{a}$. Then C_{24} -symmetry is broken!

C_{24} lattice reduced to C_{12} symmetry

Fig. 2.7.6 PSDS



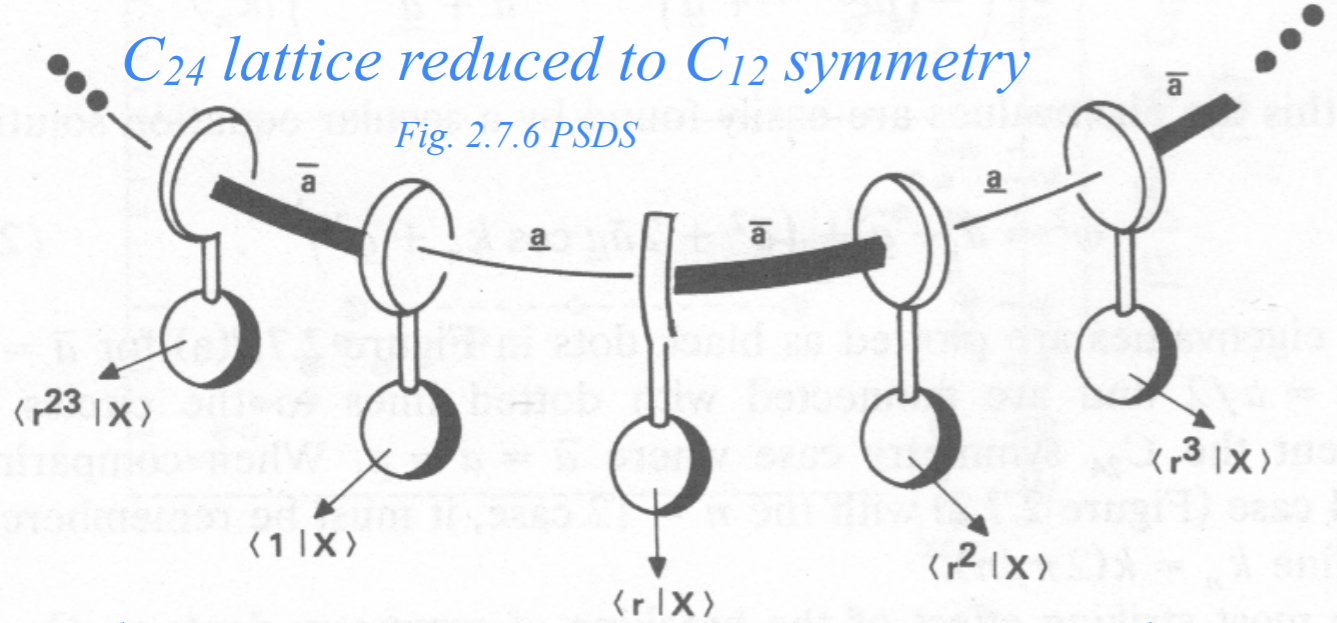
$$\begin{pmatrix} \langle r^0 | \mathbf{K} | r^0 \rangle & \langle r^0 | \mathbf{K} | r^1 \rangle & \langle r^0 | \mathbf{K} | r^2 \rangle & \dots & \langle r^0 | \mathbf{K} | r^{-1} \rangle \\ \langle r^1 | \mathbf{K} | r^0 \rangle & \langle r^1 | \mathbf{K} | r^1 \rangle & \langle r^1 | \mathbf{K} | r^2 \rangle & \dots & \langle r^1 | \mathbf{K} | r^{-1} \rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} = \begin{pmatrix} \underline{a} + \bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a} + \bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

Only C_{12} symmetry projectors commute with \mathbf{K} -matrix if $\underline{a} \neq \bar{a}$. Then C_{24} -symmetry is broken!

$$\mathbf{P}^{(m)} = \frac{1}{12} \left(\mathbf{1} + e^{-ik_m} \mathbf{r}^2 + e^{-2ik_m} \mathbf{r}^4 + e^{-3ik_m} \mathbf{r}^6 + \dots + e^{+2ik_m} \mathbf{r}^{-4} + e^{+ik_m} \mathbf{r}^{-2} \right) \text{ where: } k_m = \frac{2\pi m}{12}$$

C₂₄ lattice reduced to C₁₂ symmetry

Fig. 2.7.6 PSDS



$$\begin{pmatrix} \langle r^0 | \mathbf{K} | r^0 \rangle & \langle r^0 | \mathbf{K} | r^1 \rangle & \langle r^0 | \mathbf{K} | r^2 \rangle & \dots & \langle r^0 | \mathbf{K} | r^{-1} \rangle \\ \langle r^1 | \mathbf{K} | r^0 \rangle & \langle r^1 | \mathbf{K} | r^1 \rangle & \langle r^1 | \mathbf{K} | r^2 \rangle & \dots & \langle r^1 | \mathbf{K} | r^{-1} \rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} = \begin{pmatrix} \underline{a} + \bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a} + \bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

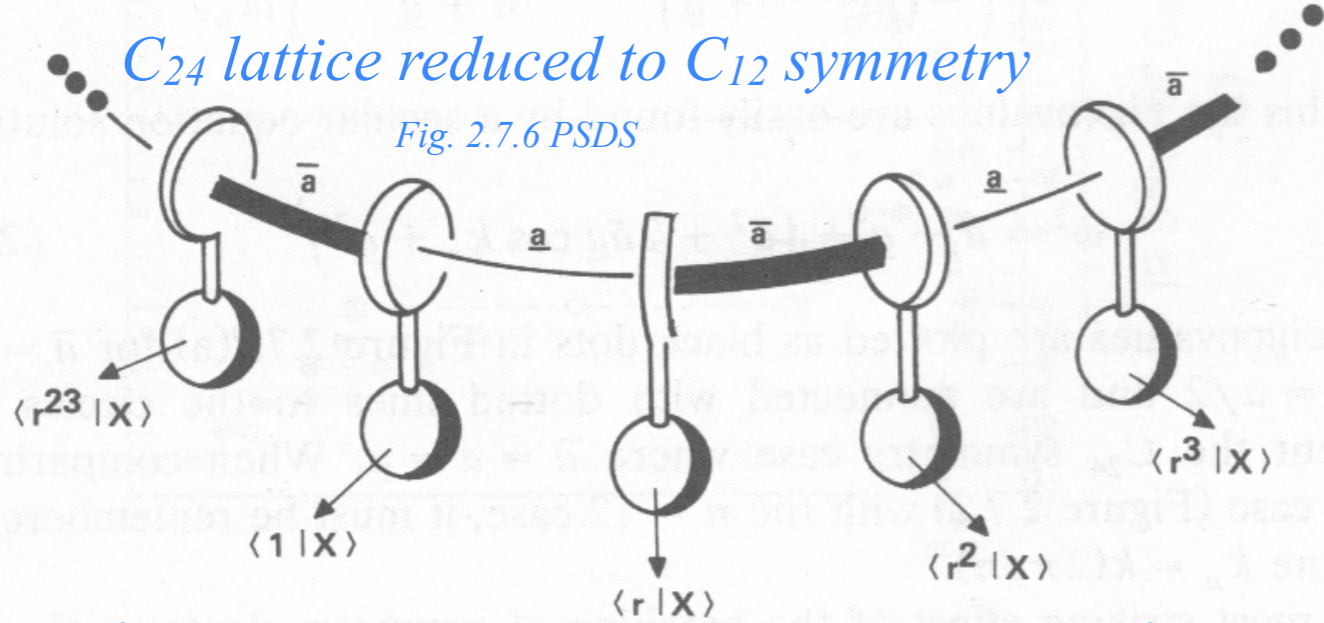
*Only C₁₂ symmetry projectors commute with **K**-matrix if $\underline{a} \neq \bar{a}$. Then C₂₄-symmetry is broken!*

$$\mathbf{P}^{(m)} = \frac{1}{12} \left(\mathbf{1} + e^{-ik_m} \mathbf{r}^2 + e^{-2ik_m} \mathbf{r}^4 + e^{-3ik_m} \mathbf{r}^6 + \dots + e^{+2ik_m} \mathbf{r}^{-4} + e^{+ik_m} \mathbf{r}^{-2} \right) \text{ where: } k_m = \frac{2\pi m}{12}$$

*Two kinds of C₁₂ symmetry m-states are coupled by **K**-matrix.*

C_{24} lattice reduced to C_{12} symmetry

Fig. 2.7.6 PSDS



$$\begin{pmatrix} \langle r^0 | \mathbf{K} | r^0 \rangle & \langle r^0 | \mathbf{K} | r^1 \rangle & \langle r^0 | \mathbf{K} | r^2 \rangle & \dots & \langle r^0 | \mathbf{K} | r^{-1} \rangle \\ \langle r^1 | \mathbf{K} | r^0 \rangle & \langle r^1 | \mathbf{K} | r^1 \rangle & \langle r^1 | \mathbf{K} | r^2 \rangle & \dots & \langle r^1 | \mathbf{K} | r^{-1} \rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} = \begin{pmatrix} \underline{a} + \bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a} + \bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

Only C_{12} symmetry projectors commute with \mathbf{K} -matrix if $\underline{a} \neq \bar{a}$. Then C_{24} -symmetry is broken!

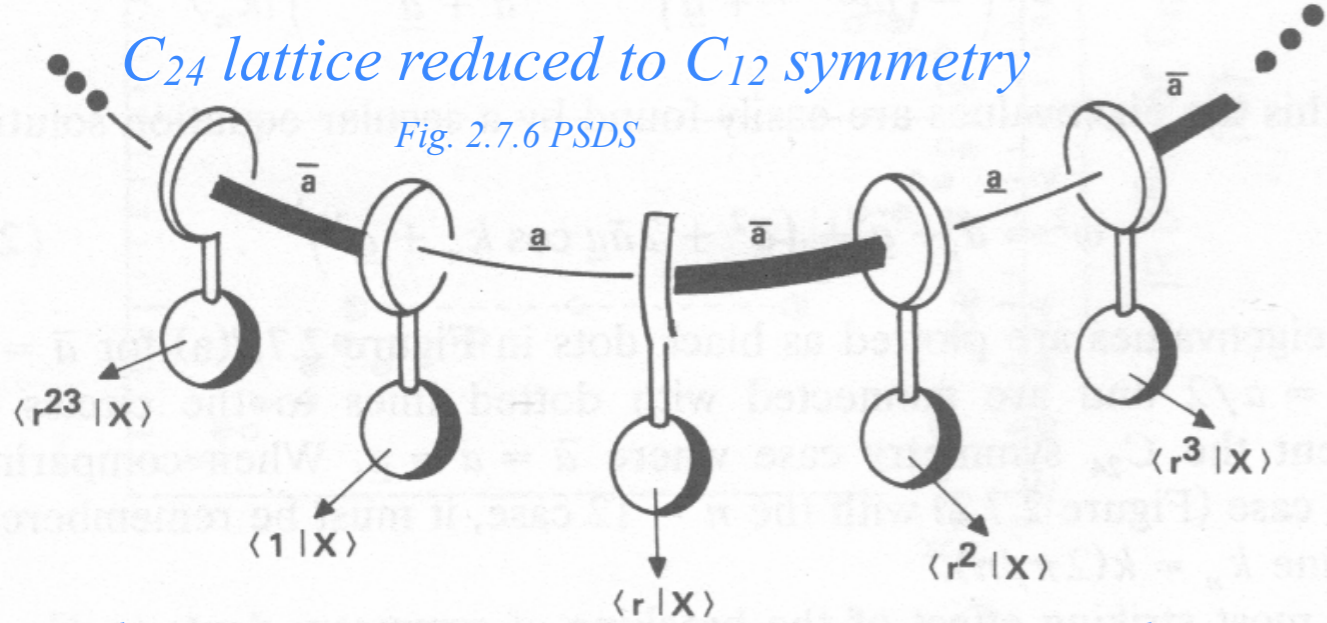
$$\mathbf{P}^{(m)} = \frac{1}{12} \left(\mathbf{1} + e^{-ik_m} \mathbf{r}^2 + e^{-2ik_m} \mathbf{r}^4 + e^{-3ik_m} \mathbf{r}^6 + \dots + e^{+2ik_m} \mathbf{r}^{-4} + e^{+ik_m} \mathbf{r}^{-2} \right) \text{ where: } k_m = \frac{2\pi m}{12}$$

Two kinds of C_{12} symmetry m -states are coupled by \mathbf{K} -matrix: Even $|r^{even}\rangle$ and odd $|r^{odd}\rangle$ p -points.

$$|k_m\rangle = \mathbf{P}^{(m)} |r^0\rangle \cdot \sqrt{12} = (|r^0\rangle + e^{-ik_m} |r^2\rangle + e^{-2ik_m} |r^4\rangle + \dots) / \sqrt{12} \quad |k'_m\rangle = \mathbf{P}^{(m)} |r^1\rangle \cdot \sqrt{12} = (|r^1\rangle + e^{-ik_m} |r^3\rangle + e^{-2ik_m} |r^5\rangle + \dots) / \sqrt{12}$$

C_{24} lattice reduced to C_{12} symmetry

Fig. 2.7.6 PSDS



$$\begin{pmatrix} \langle r^0 | \mathbf{K} | r^0 \rangle & \langle r^0 | \mathbf{K} | r^1 \rangle & \langle r^0 | \mathbf{K} | r^2 \rangle & \dots & \langle r^0 | \mathbf{K} | r^{-1} \rangle \\ \langle r^1 | \mathbf{K} | r^0 \rangle & \langle r^1 | \mathbf{K} | r^1 \rangle & \langle r^1 | \mathbf{K} | r^2 \rangle & \dots & \langle r^1 | \mathbf{K} | r^{-1} \rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} = \begin{pmatrix} \underline{a} + \bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a} + \bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

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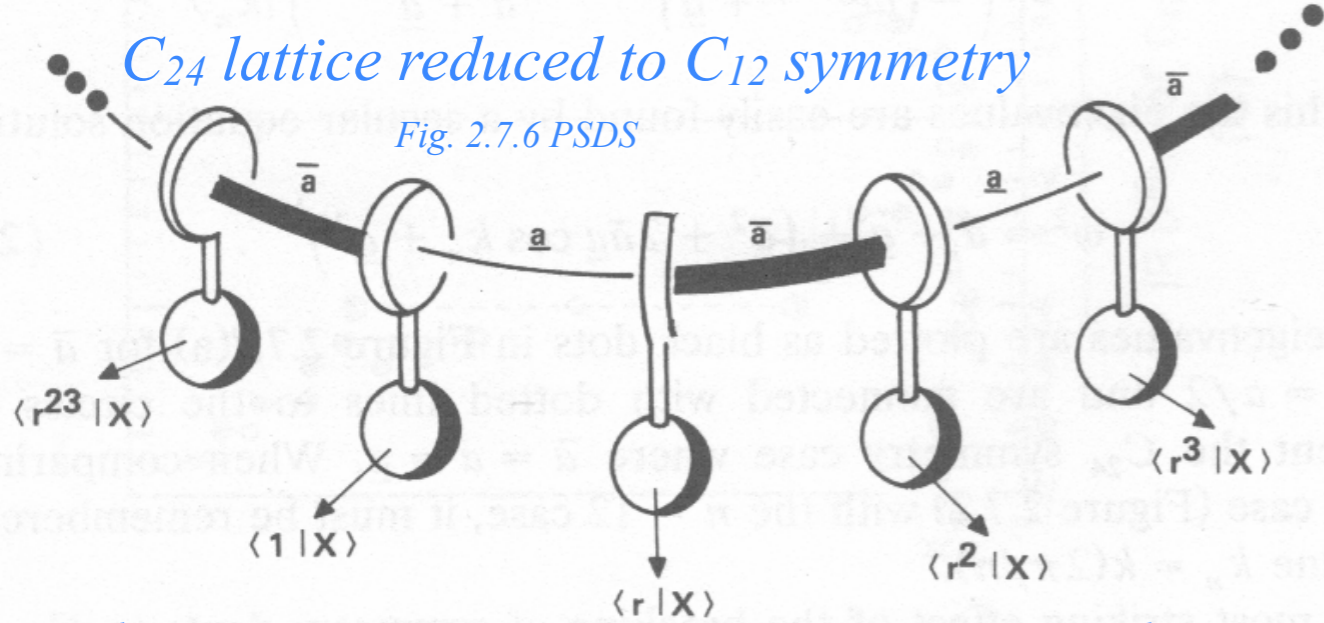
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C_{24} lattice reduced to C_{12} symmetry

Fig. 2.7.6 PSDS



$$\begin{pmatrix} \langle r^0 | \mathbf{K} | r^0 \rangle & \langle r^0 | \mathbf{K} | r^1 \rangle & \langle r^0 | \mathbf{K} | r^2 \rangle & \dots & \langle r^0 | \mathbf{K} | r^{-1} \rangle \\ \langle r^1 | \mathbf{K} | r^0 \rangle & \langle r^1 | \mathbf{K} | r^1 \rangle & \langle r^1 | \mathbf{K} | r^2 \rangle & \dots & \langle r^1 | \mathbf{K} | r^{-1} \rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} = \begin{pmatrix} \underline{a} + \bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a} + \bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

Only C_{12} symmetry projectors commute with \mathbf{K} -matrix if $\underline{a} \neq \bar{a}$. Then C_{24} -symmetry is broken!

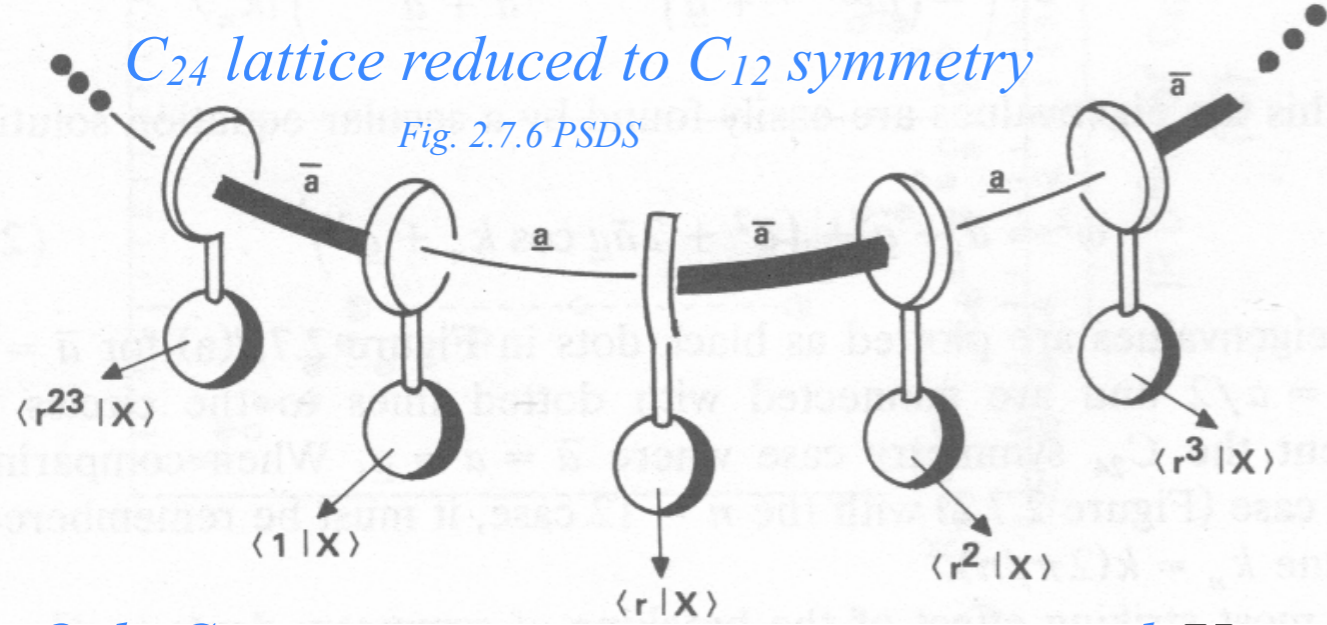
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$$\begin{aligned} \langle k'_m | \mathbf{K} | k_m \rangle &= \langle r^1 | \mathbf{P}^{(m)} \mathbf{K} \mathbf{P}^{(m)} | r^0 \rangle \cdot 12 = \langle r^1 | \mathbf{K} \mathbf{P}^{(m)} | r^0 \rangle \cdot 12 \\ &= \langle r^1 | \mathbf{K} | r^0 \rangle + e^{-ik_m} \langle r^1 | \mathbf{K} | r^2 \rangle + e^{-2ik_m} \langle r^1 | \mathbf{K} | r^4 \rangle + \dots \\ &= -\underline{a} + e^{-ik_m} (-\bar{a}) + 0 + \dots \\ &= -(\underline{a} + e^{-ik_m} \bar{a}) = \langle k_m | \mathbf{K} | k'_m \rangle^* \end{aligned}$$



$$\begin{pmatrix} \langle r^0 | \mathbf{K} | r^0 \rangle & \langle r^0 | \mathbf{K} | r^1 \rangle & \langle r^0 | \mathbf{K} | r^2 \rangle & \dots & \langle r^0 | \mathbf{K} | r^{-1} \rangle \\ \langle r^1 | \mathbf{K} | r^0 \rangle & \langle r^1 | \mathbf{K} | r^1 \rangle & \langle r^1 | \mathbf{K} | r^2 \rangle & \dots & \langle r^1 | \mathbf{K} | r^{-1} \rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} = \begin{pmatrix} \underline{a} + \bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a} + \bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

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$$\begin{aligned} \langle \mathbf{K} \rangle^{k_m} &= \begin{pmatrix} \langle k_m | \mathbf{K} | k_m \rangle & \langle k_m | \mathbf{K} | k'_m \rangle \\ \langle k'_m | \mathbf{K} | k_m \rangle & \langle k'_m | \mathbf{K} | k'_m \rangle \end{pmatrix} \\ &= \begin{pmatrix} \underline{a} + \bar{a} & -(a + e^{+ik_m} \bar{a}) \\ -(a + e^{-ik_m} \bar{a}) & \underline{a} + \bar{a} \end{pmatrix} \end{aligned}$$

$$\begin{aligned} \langle k'_m | \mathbf{K} | k_m \rangle &= \langle r^1 | \mathbf{P}^{(m)} \mathbf{K} \mathbf{P}^{(m)} | r^0 \rangle \cdot 12 = \langle r^1 | \mathbf{K} \mathbf{P}^{(m)} | r^0 \rangle \cdot 12 \\ &= \langle r^1 | \mathbf{K} | r^0 \rangle + e^{-ik_m} \langle r^1 | \mathbf{K} | r^2 \rangle + e^{-2ik_m} \langle r^1 | \mathbf{K} | r^4 \rangle + \dots \\ &= -\underline{a} + e^{-ik_m} (-\bar{a}) + 0 + \dots \\ &= -(a + e^{-ik_m} \bar{a}) = \langle k_m | \mathbf{K} | k'_m \rangle^* \end{aligned}$$

Breaking C_N cyclic coupling into linear chains

Review of 1D-Bohr-ring related to infinite square well

Breaking C_{2N+2} to approximate linear N -chain (Examples $C_2 \leftrightarrow C_6 \leftrightarrow C_{14}$)

Band-It simulation: Intro to scattering approach to quantum symmetry

How Band-It works: Match each Ψ and $D\Psi$, Let $L=0$ at Right end

Breaking C_{2N} cyclic coupling down to C_N symmetry

Acoustical modes vs. Optical modes

Intro to other examples of band theory

Avoided crossing view of band-gaps

Finally! Symmetry groups that are not just C_N

The “4-Group(s)” D_2 and C_{2v}

Spectral decomposition of D_2

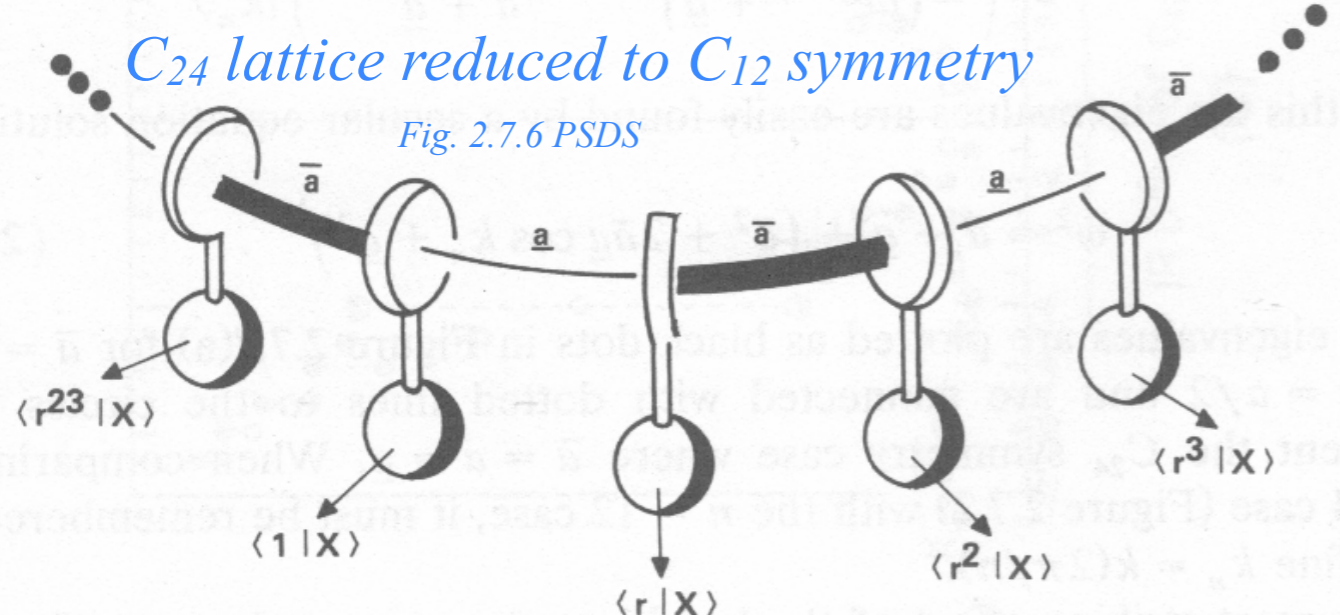
Some D_2 modes

Outer product properties and the Crystal-Point Symmetry Group Zoo

Polygonal geometry of $U(2) \supset C_N$ character spectral function $\chi^j(2\pi/n) = \frac{\sin(\pi(2j+1)/n)}{\sin(\pi/n)}$

Algebra

Geometry



$$\begin{pmatrix} \langle r^0 | \mathbf{K} | r^0 \rangle & \langle r^0 | \mathbf{K} | r^1 \rangle & \langle r^0 | \mathbf{K} | r^2 \rangle & \dots & \langle r^0 | \mathbf{K} | r^{-1} \rangle \\ \langle r^1 | \mathbf{K} | r^0 \rangle & \langle r^1 | \mathbf{K} | r^1 \rangle & \langle r^1 | \mathbf{K} | r^2 \rangle & \dots & \langle r^1 | \mathbf{K} | r^{-1} \rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a} + \bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a} + \bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

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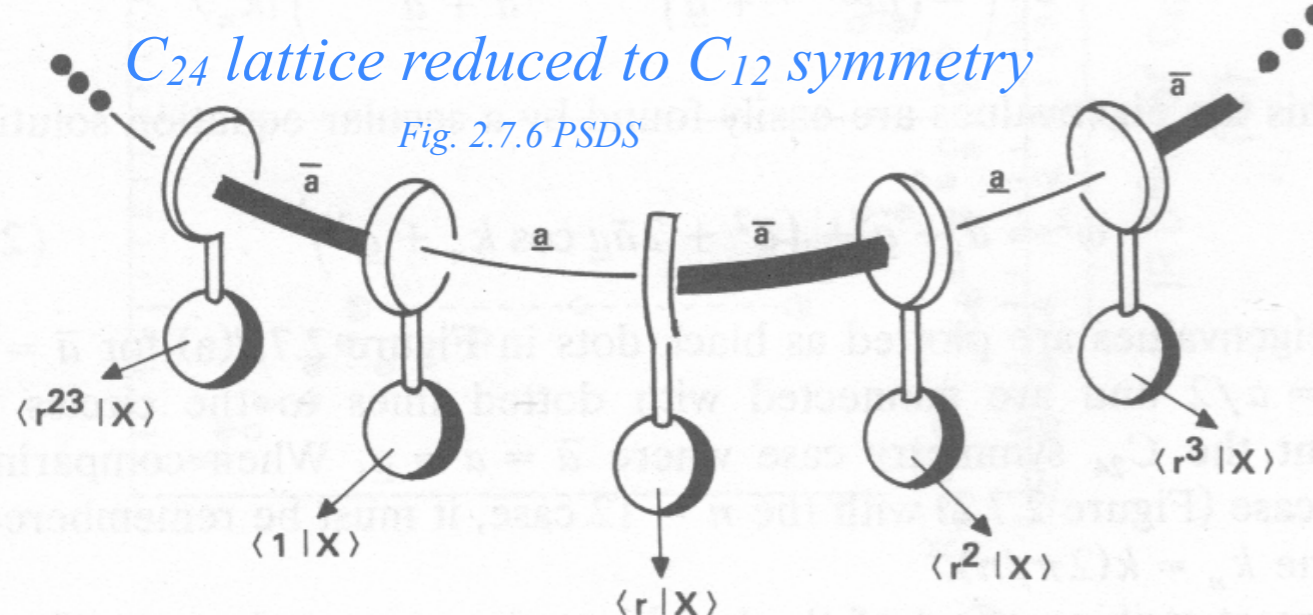
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$$\langle \mathbf{K} \rangle^{k_m} = \begin{pmatrix} \langle k_m | \mathbf{K} | k_m \rangle & \langle k_m | \mathbf{K} | k'_m \rangle \\ \langle k'_m | \mathbf{K} | k_m \rangle & \langle k'_m | \mathbf{K} | k'_m \rangle \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a} + \bar{a} & -(a + e^{+ik_m} \bar{a}) \\ -(a + e^{-ik_m} \bar{a}) & \underline{a} + \bar{a} \end{pmatrix}$$



$$\begin{pmatrix} \langle r^0 | \mathbf{K} | r^0 \rangle & \langle r^0 | \mathbf{K} | r^1 \rangle & \langle r^0 | \mathbf{K} | r^2 \rangle & \dots & \langle r^0 | \mathbf{K} | r^{-1} \rangle \\ \langle r^1 | \mathbf{K} | r^0 \rangle & \langle r^1 | \mathbf{K} | r^1 \rangle & \langle r^1 | \mathbf{K} | r^2 \rangle & \dots & \langle r^1 | \mathbf{K} | r^{-1} \rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

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Secular Eq.:

$$0 = \kappa^2 - \text{Tr} \langle \mathbf{K} \rangle^{k_m} + \text{Det} \langle \mathbf{K} \rangle^{k_m}$$

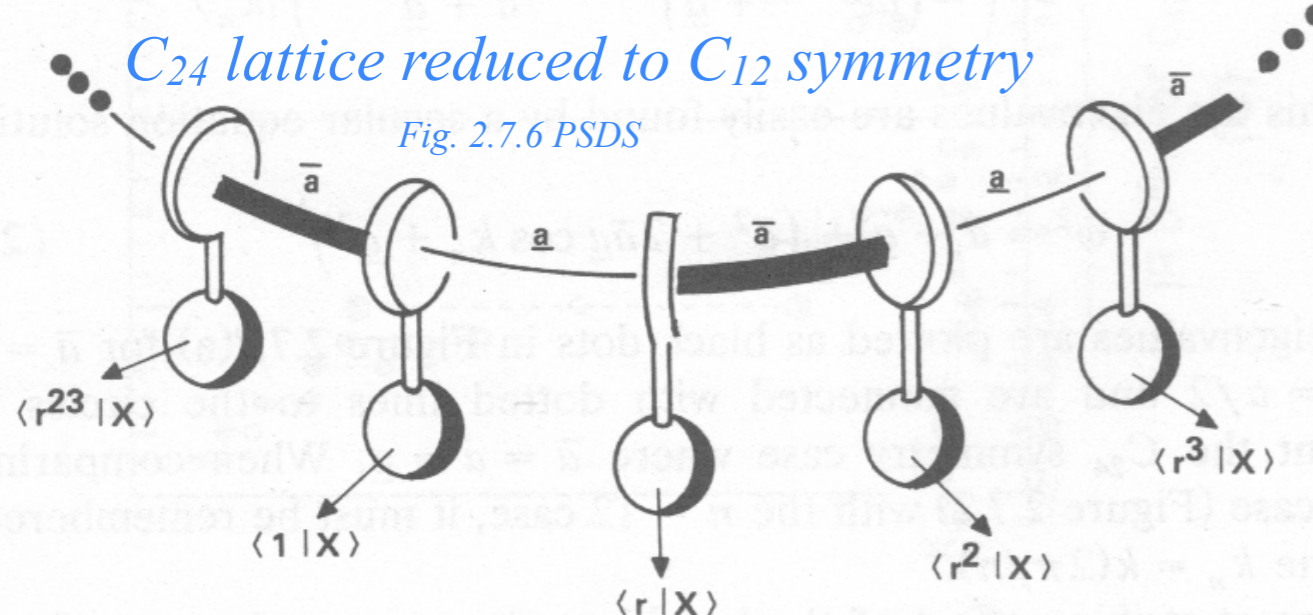
$$0 = \kappa^2 - 2(\underline{a} + \bar{a})\kappa + (\underline{a} + \bar{a})^2 - (\underline{a} + e^{+ik_m} \bar{a})(\underline{a} + e^{-ik_m} \bar{a})$$

$$0 = \kappa^2 - 2(\underline{a} + \bar{a})\kappa + (\underline{a} + \bar{a})^2 - \underline{a}^2 - \bar{a}^2 - 2\bar{a}\underline{a} \cos k_m$$

$$0 = \kappa^2 - 2(\underline{a} + \bar{a})\kappa + 2\bar{a}\underline{a}(1 - \cos k_m)$$

$$\langle \mathbf{K} \rangle^{k_m} = \begin{pmatrix} \langle k_m | \mathbf{K} | k_m \rangle & \langle k_m | \mathbf{K} | k'_m \rangle \\ \langle k'_m | \mathbf{K} | k_m \rangle & \langle k'_m | \mathbf{K} | k'_m \rangle \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a} + \bar{a} & -(\underline{a} + e^{+ik_m} \bar{a}) \\ -(\underline{a} + e^{-ik_m} \bar{a}) & \underline{a} + \bar{a} \end{pmatrix}$$



$$\begin{pmatrix} \langle r^0 | \mathbf{K} | r^0 \rangle & \langle r^0 | \mathbf{K} | r^1 \rangle & \langle r^0 | \mathbf{K} | r^2 \rangle & \dots & \langle r^0 | \mathbf{K} | r^{-1} \rangle \\ \langle r^1 | \mathbf{K} | r^0 \rangle & \langle r^1 | \mathbf{K} | r^1 \rangle & \langle r^1 | \mathbf{K} | r^2 \rangle & \dots & \langle r^1 | \mathbf{K} | r^{-1} \rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a} + \bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a} + \bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

Only C₁₂ symmetry projectors commute with **K**-matrix if $\underline{a} \neq \bar{a}$. Then C₂₄-symmetry is broken!

$$\mathbf{P}^{(m)} = \frac{1}{12} \left(\mathbf{1} + e^{-ik_m} \mathbf{r}^2 + e^{-2ik_m} \mathbf{r}^4 + e^{-3ik_m} \mathbf{r}^6 + \dots + e^{+2ik_m} \mathbf{r}^{-4} + e^{+ik_m} \mathbf{r}^{-2} \right) \text{ where: } k_m = \frac{2\pi m}{12}$$

Two kinds of C₁₂ symmetry m-states are coupled by **K**-matrix: Even $|r^{even}\rangle$ and odd $|r^{odd}\rangle$ p-points.

$$|k_m\rangle = \mathbf{P}^{(m)} |r^0\rangle \cdot \sqrt{12} = (|r^0\rangle + e^{-ik_m} |r^2\rangle + e^{-2ik_m} |r^4\rangle + \dots) / \sqrt{12}$$

$$|k'_m\rangle = \mathbf{P}^{(m)} |r^1\rangle \cdot \sqrt{12} = (|r^1\rangle + e^{-ik_m} |r^3\rangle + e^{-2ik_m} |r^5\rangle + \dots) / \sqrt{12}$$

Secular Eq.:

$$0 = \kappa^2 - \text{Tr} \langle \mathbf{K} \rangle^{k_m} + \text{Det} \langle \mathbf{K} \rangle^{k_m}$$

$$0 = \kappa^2 - 2(\underline{a} + \bar{a})\kappa + (\underline{a} + \bar{a})^2 - (\underline{a} + e^{+ik_m}\bar{a})(\underline{a} + e^{-ik_m}\bar{a})$$

$$0 = \kappa^2 - 2(\underline{a} + \bar{a})\kappa + (\underline{a} + \bar{a})^2 - \underline{a}^2 - \bar{a}^2 - 2\bar{a}\underline{a} \cos k_m$$

$$0 = \kappa^2 - 2(\underline{a} + \bar{a})\kappa + 2\bar{a}\underline{a}(1 - \cos k_m)$$

$$\langle \mathbf{K} \rangle^{k_m} = \begin{pmatrix} \langle k_m | \mathbf{K} | k_m \rangle & \langle k_m | \mathbf{K} | k'_m \rangle \\ \langle k'_m | \mathbf{K} | k_m \rangle & \langle k'_m | \mathbf{K} | k'_m \rangle \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a} + \bar{a} & -(\underline{a} + e^{+ik_m}\bar{a}) \\ -(\underline{a} + e^{-ik_m}\bar{a}) & \underline{a} + \bar{a} \end{pmatrix}$$

Eigenvalues:

$$\kappa = \omega_{k_m}^2 = \underline{a} + \bar{a} \pm \sqrt{\underline{a}^2 + 2\bar{a}\underline{a} \cos k_m + \bar{a}^2}$$

C_{24} lattice reduced to C_{12} symmetry

Fig. 2.7.7 PSDS

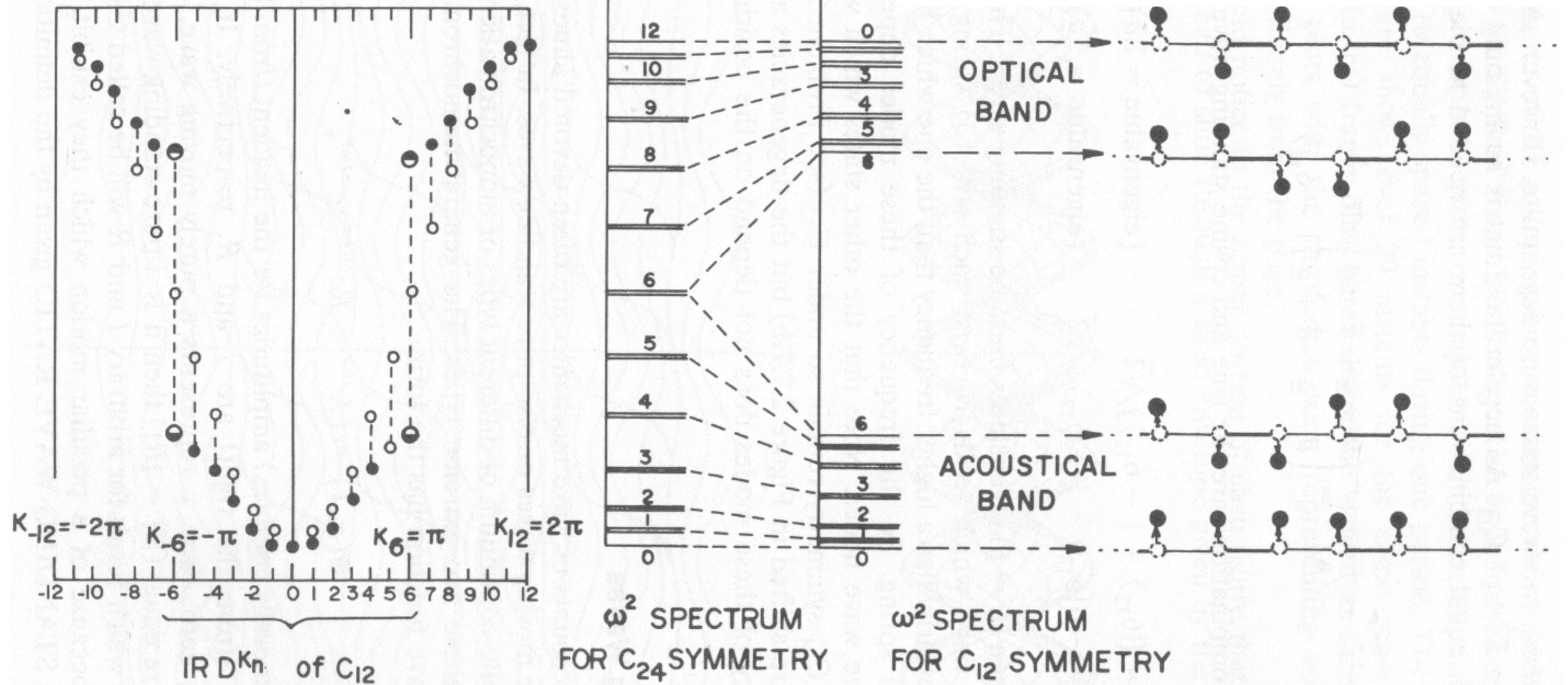


Figure 2.7.7 Band splitting due to $C_{24}-C_{12}$ symmetry breaking.

Eigenvalues:

$$\kappa = \omega_{k_m}^2 = \underline{a} + \bar{a} \pm \sqrt{\underline{a}^2 + 2\underline{a}\bar{a}\cos k_m + \bar{a}^2}$$

$$\begin{aligned} \langle \mathbf{K} \rangle_{k_m} &= \begin{pmatrix} \langle k_m | \mathbf{K} | k_m \rangle & \langle k_m | \mathbf{K} | k'_m \rangle \\ \langle k'_m | \mathbf{K} | k_m \rangle & \langle k'_m | \mathbf{K} | k'_m \rangle \end{pmatrix} \\ &= \begin{pmatrix} \underline{a} + \bar{a} & -(a + e^{+ik_m}\bar{a}) \\ -(a + e^{-ik_m}\bar{a}) & \underline{a} + \bar{a} \end{pmatrix} \end{aligned}$$

C_{24} lattice reduced to C_{12} symmetry

Fig. 2.7.7 PSDS

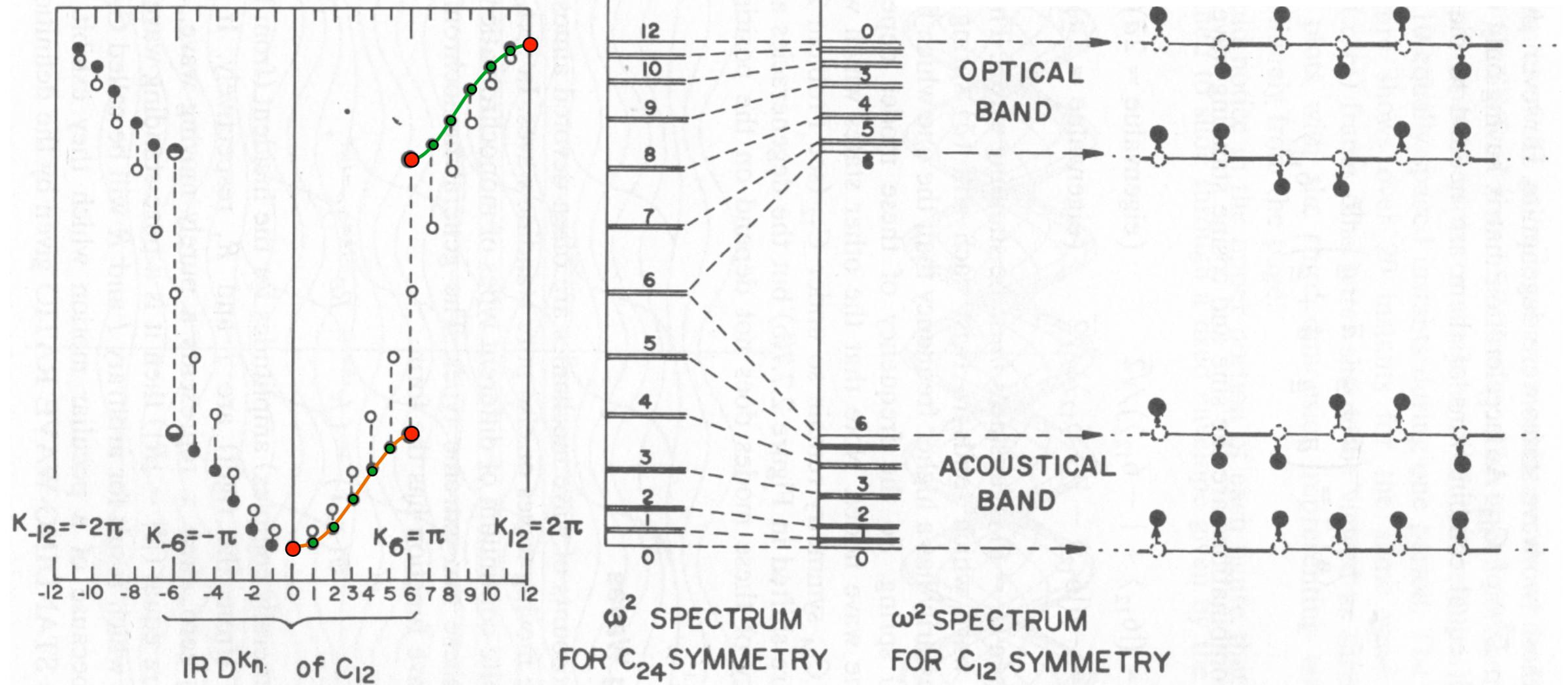


Figure 2.7.7 Band splitting due to C_{24} - C_{12} symmetry breaking.

Eigenvalues:

$$\kappa = \omega_{k_m}^2 = \underline{a} + \bar{a} \pm \sqrt{\underline{a}^2 + 2\underline{a}\bar{a}\cos k_m + \bar{a}^2}$$

$$\langle \mathbf{K} \rangle_{k_m} = \begin{pmatrix} \langle k_m | \mathbf{K} | k_m \rangle & \langle k_m | \mathbf{K} | k'_m \rangle \\ \langle k'_m | \mathbf{K} | k_m \rangle & \langle k'_m | \mathbf{K} | k'_m \rangle \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a} + \bar{a} & -(a + e^{+ik_m} \bar{a}) \\ -(a + e^{-ik_m} \bar{a}) & \underline{a} + \bar{a} \end{pmatrix}$$

C_{24} lattice reduced to C_{12} symmetry

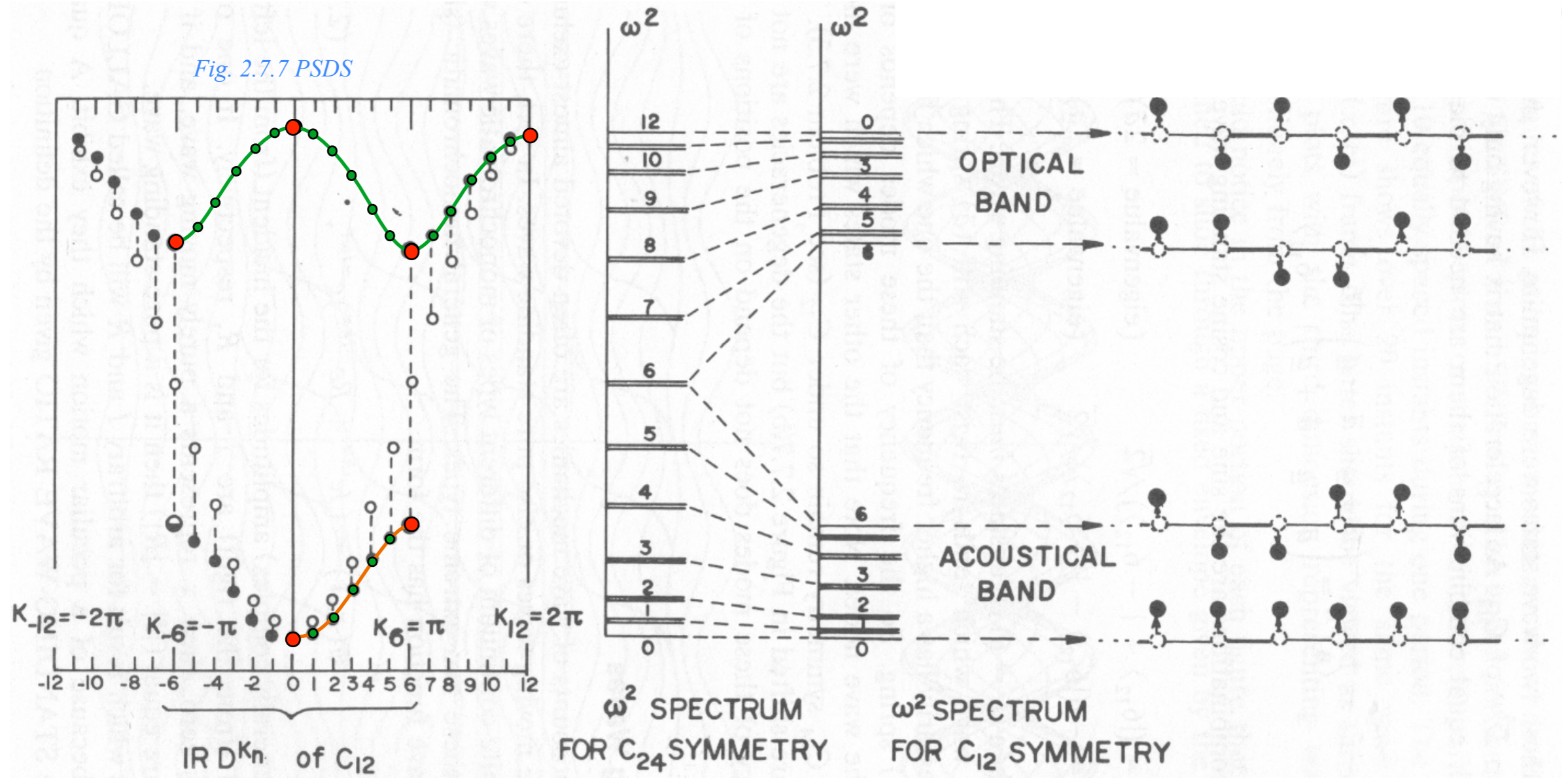


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Eigenvalues:

$$\kappa = \omega_{k_m}^2 = \underline{a} + \bar{a} \pm \sqrt{\underline{a}^2 + 2\underline{a}\bar{a}\cos k_m + \bar{a}^2}$$

$$\langle \mathbf{K} \rangle_{k_m} = \begin{pmatrix} \langle k_m | \mathbf{K} | k_m \rangle & \langle k_m | \mathbf{K} | k'_m \rangle \\ \langle k'_m | \mathbf{K} | k_m \rangle & \langle k'_m | \mathbf{K} | k'_m \rangle \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a} + \bar{a} & -(a + e^{+ik_m} \bar{a}) \\ -(a + e^{-ik_m} \bar{a}) & \underline{a} + \bar{a} \end{pmatrix}$$

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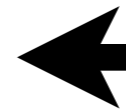
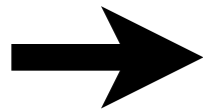
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Algebra

Geometry

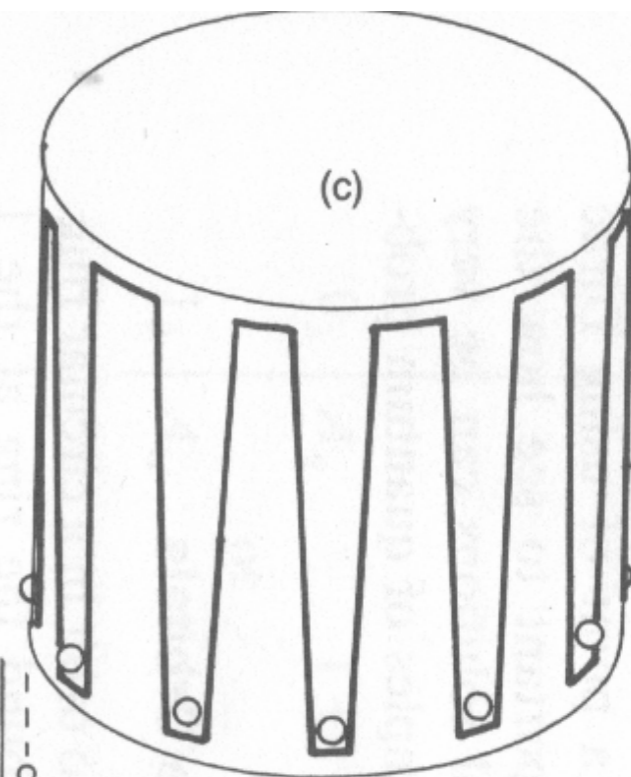
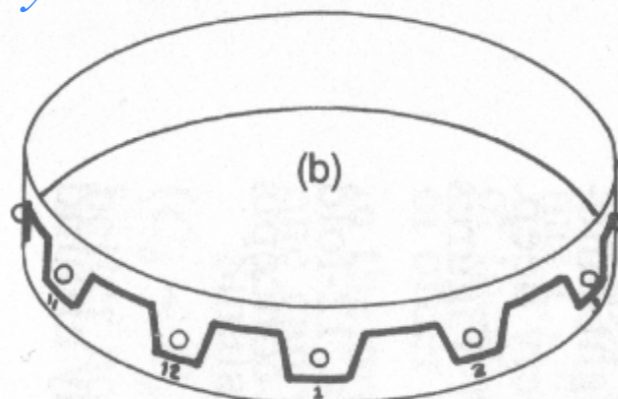
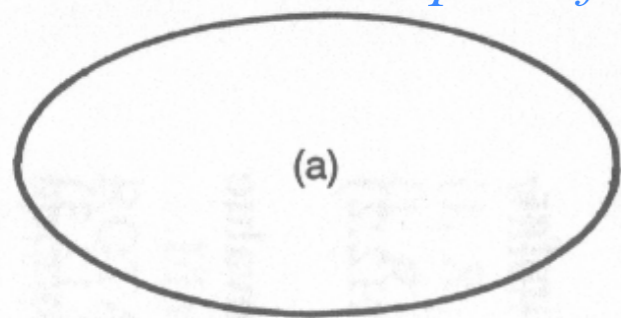
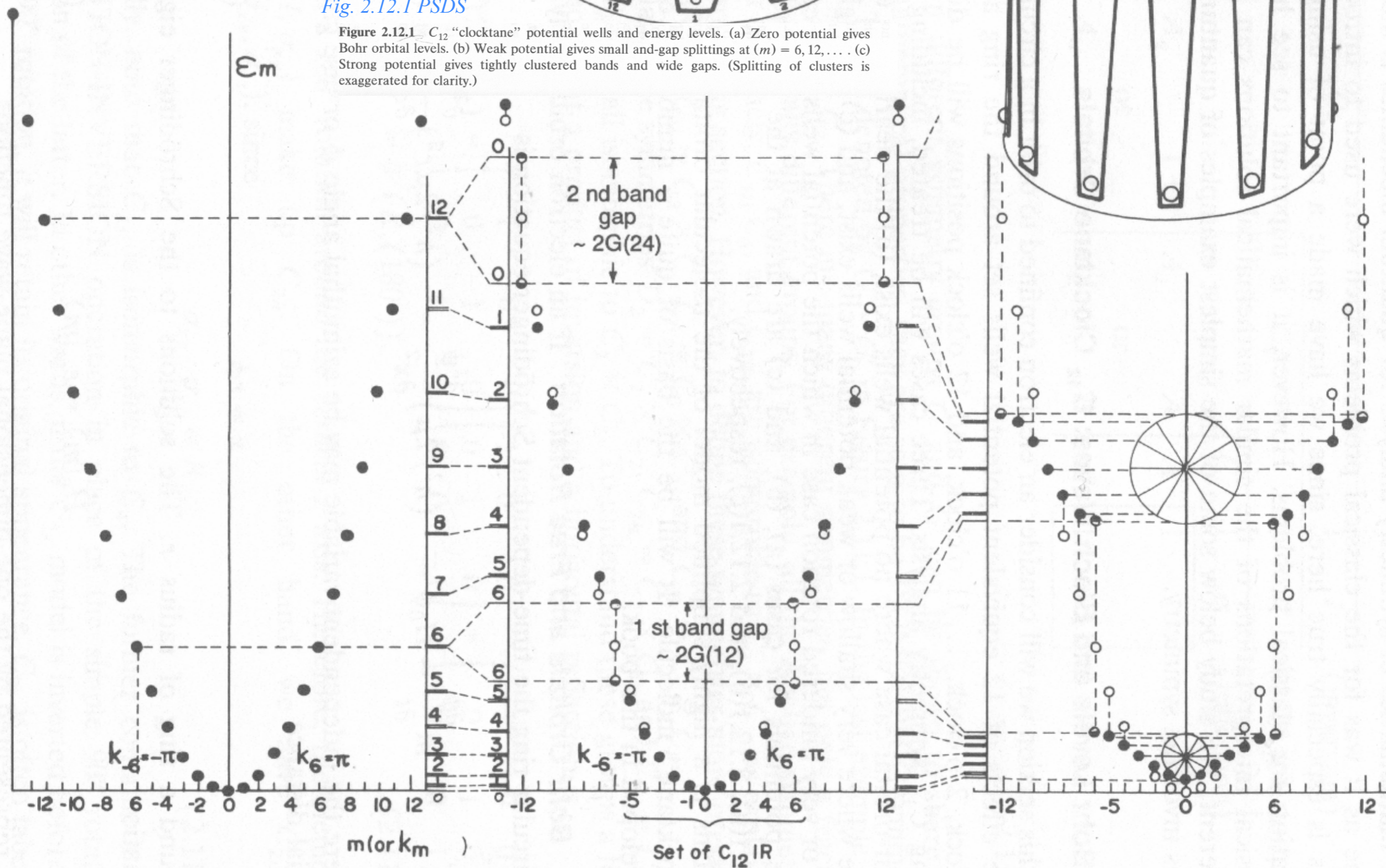


Fig. 2.12.1 PSDS

Figure 2.12.1 C_{12} "clocktane" potential wells and energy levels. (a) Zero potential gives Bohr orbital levels. (b) Weak potential gives small and-gap splittings at $(m) = 6, 12, \dots$. (c) Strong potential gives tightly clustered bands and wide gaps. (Splitting of clusters is exaggerated for clarity.)



Intro to other examples of band theory

Crossing equations for a pair of humps

$$\overbrace{R''e^{ikx} + L''e^{-ikx} \quad R_2'e^{ilx} + L_2'e^{-ilx} \quad R_1'e^{ilx} + L_1'e^{-ilx} \quad Re^{ikx} + Le^{-ikx}}^{}$$

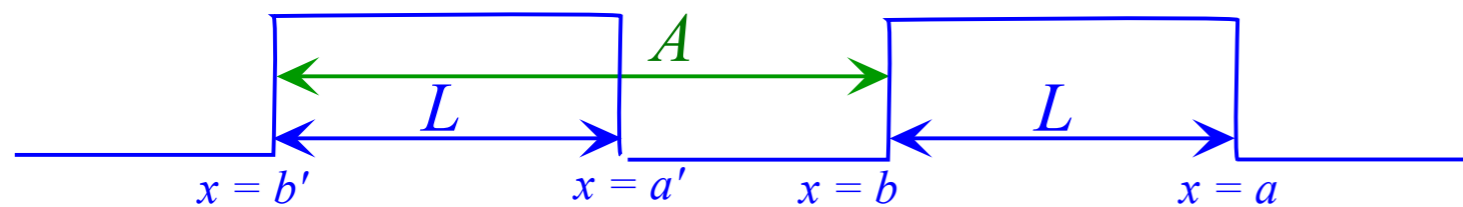


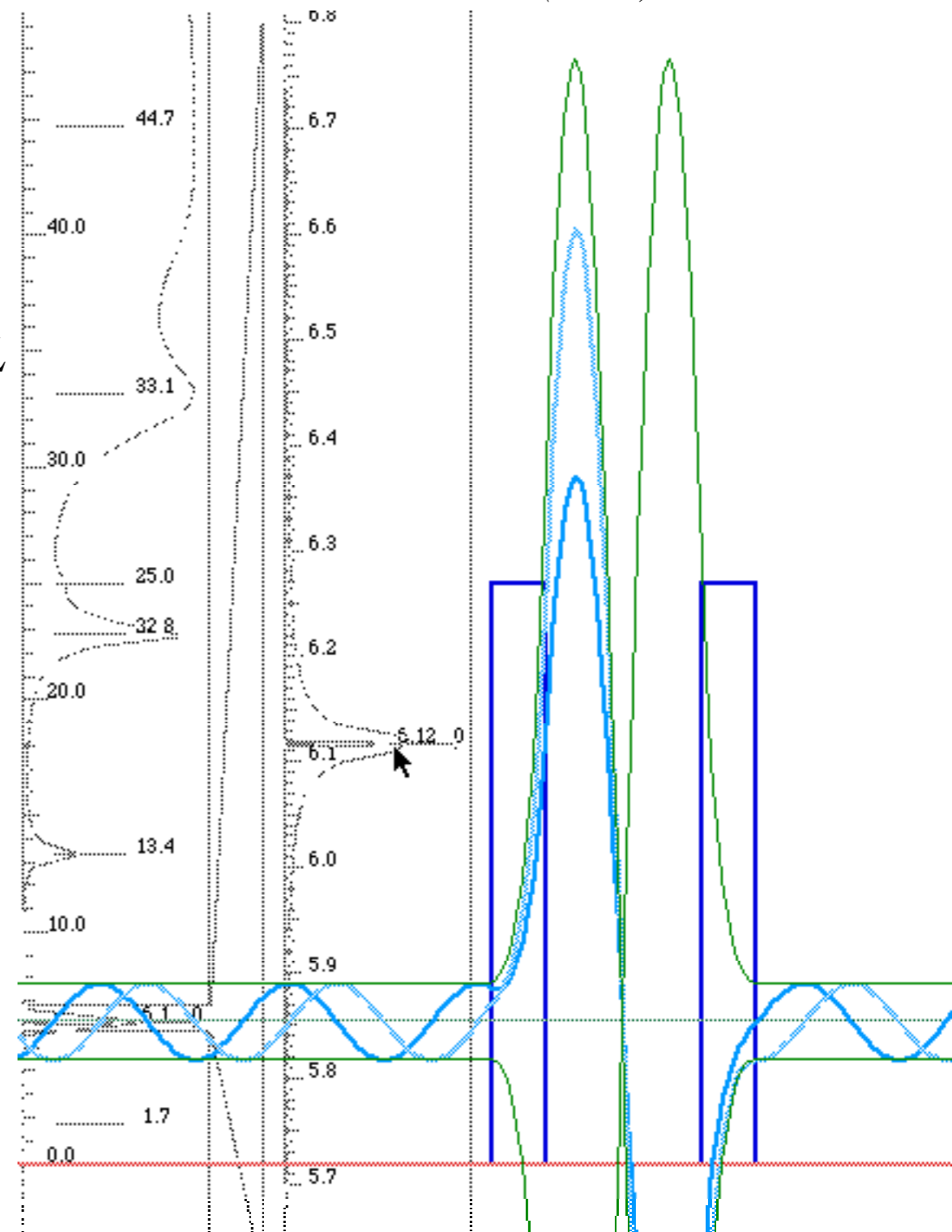
Fig. 14.1.5 C_2 -symmetric double barrier.

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

$\chi = \cosh \kappa L - i \sinh 2\beta \sinh \kappa L$, and: $\xi = \cosh 2\beta \sinh \kappa L$

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

Fig. 14.1.7 Second ($E = 6.117$) resonance in $L = 0.5$ well between two width = 0.5 barriers ($V = 25$).



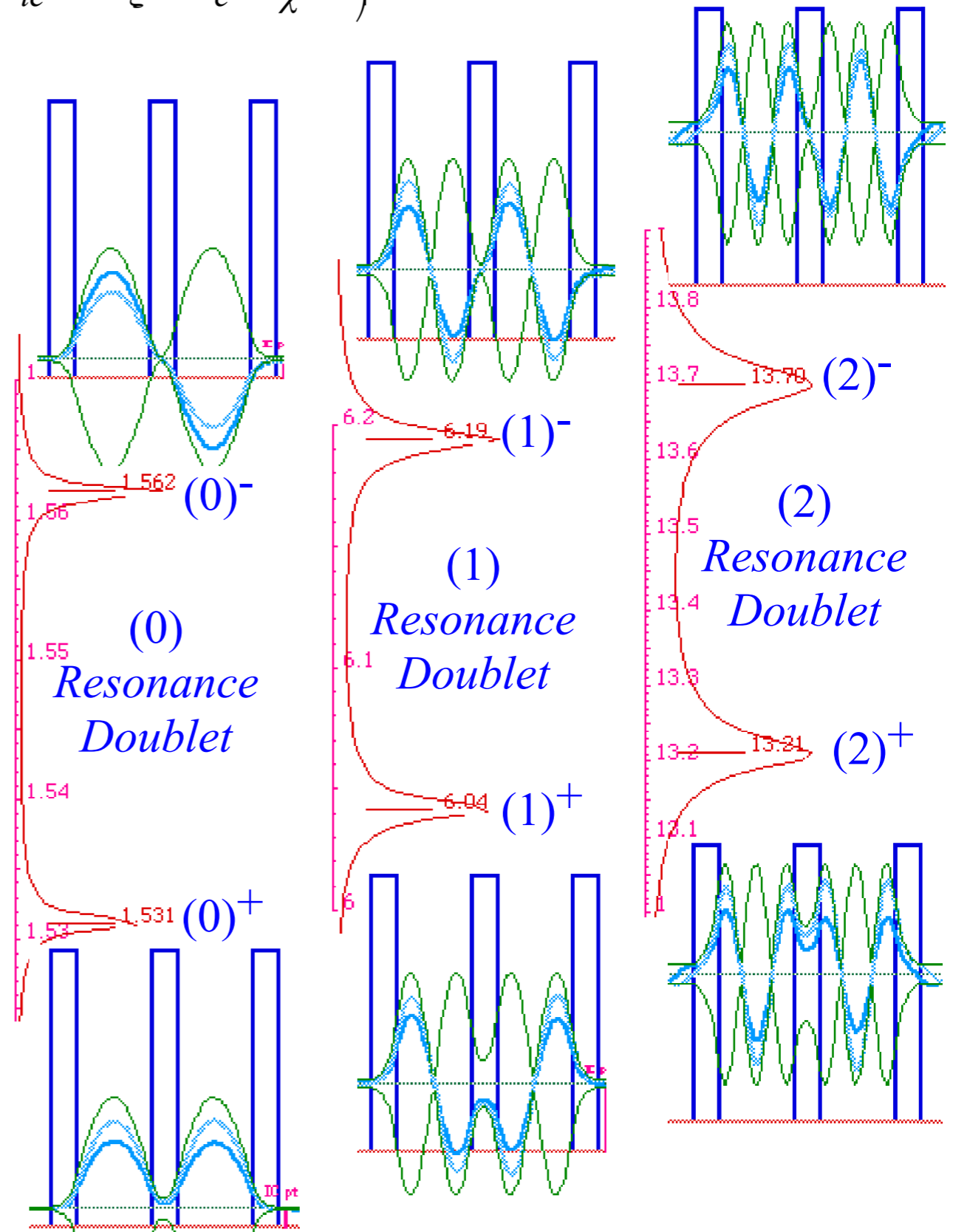
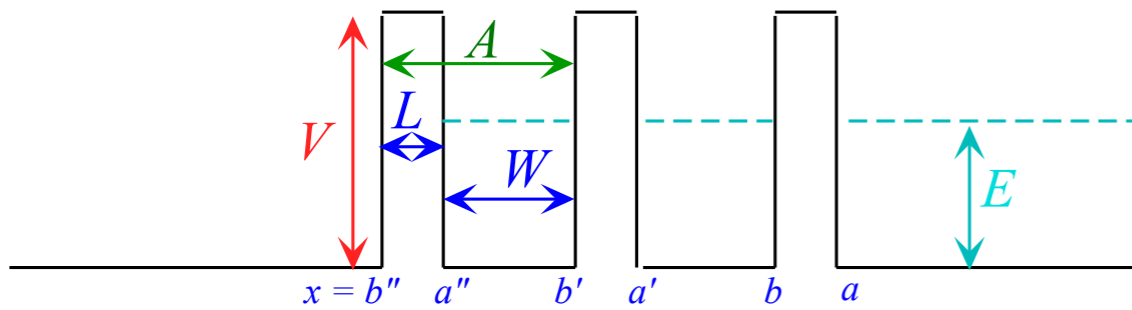
Intro to other examples of band theory

$$C^{3\text{-barrier}} = C'' \cdot C' \cdot C$$

$$= \begin{pmatrix} e^{ikL} \chi^* & -ie^{-ik(a''+b'')\xi} \\ ie^{ik(a''+b'')\xi} & e^{-ikL} \chi \end{pmatrix} \cdot \begin{pmatrix} e^{ikL} \chi^* & -ie^{-ik(a'+b')\xi} \\ ie^{ik(a'+b')\xi} & e^{-ikL} \chi \end{pmatrix} \cdot \begin{pmatrix} e^{ikL} \chi^* & -ie^{-ik(a+b)\xi} \\ ie^{ik(a+b)\xi} & e^{-ikL} \chi \end{pmatrix}$$

Crossing equations for three humps

Fig. 14.1.10 Triple-barrier double-well potential



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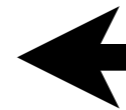
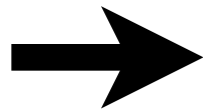
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Geometry

Intro to other examples of band theory

Bohr-It simulations assume ring-periodic-boundary conditions

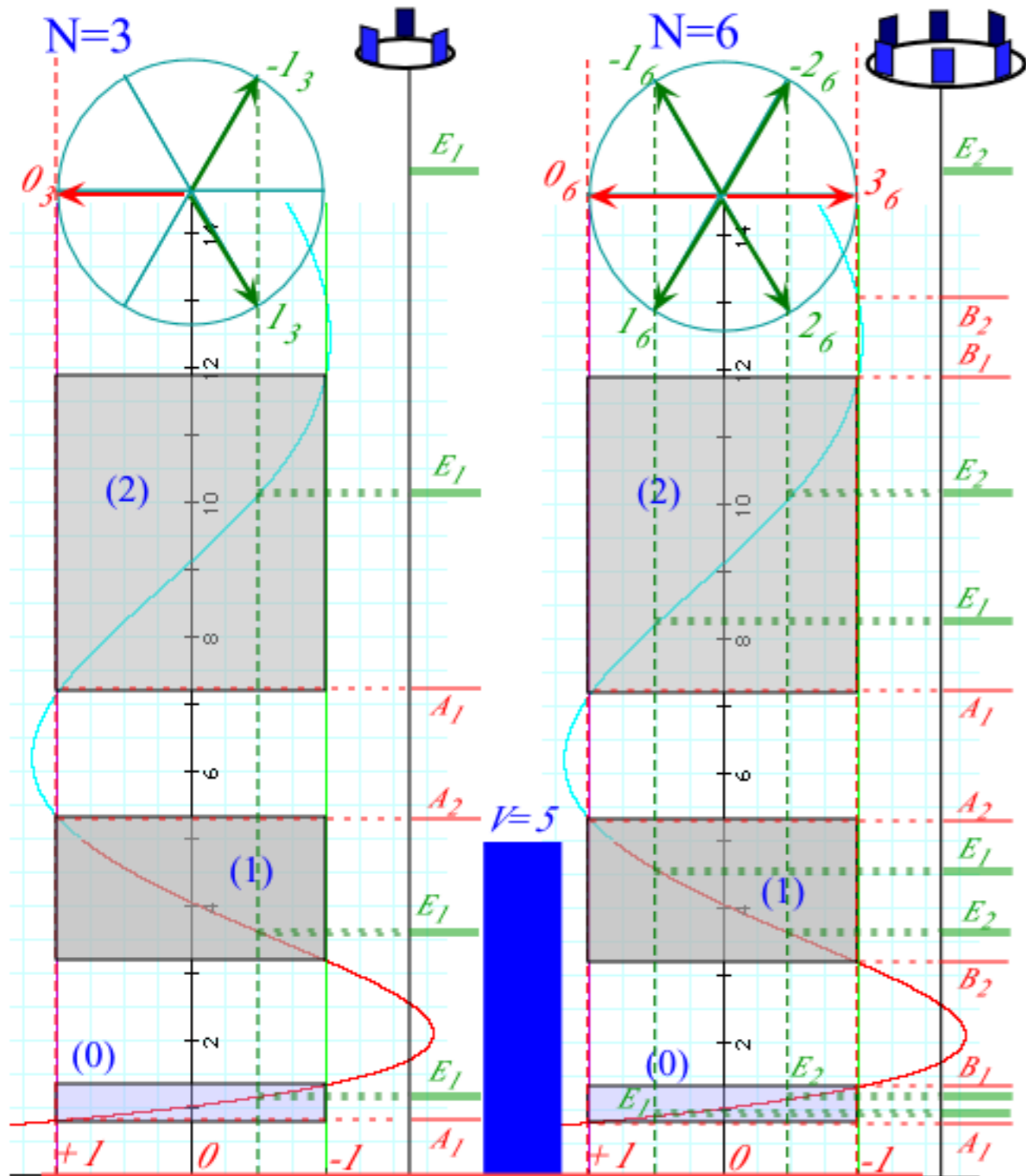


Fig. 14.2.8 Multiplets for $V=5$.
 ($W=15\text{nm}$ well, $L=5\text{nm}$ barrier) for ($N=3$)-ring and ($N=6$)-ring.

Intro to other examples of band theory

Bohr-It simulations assume ring-periodic-boundary conditions

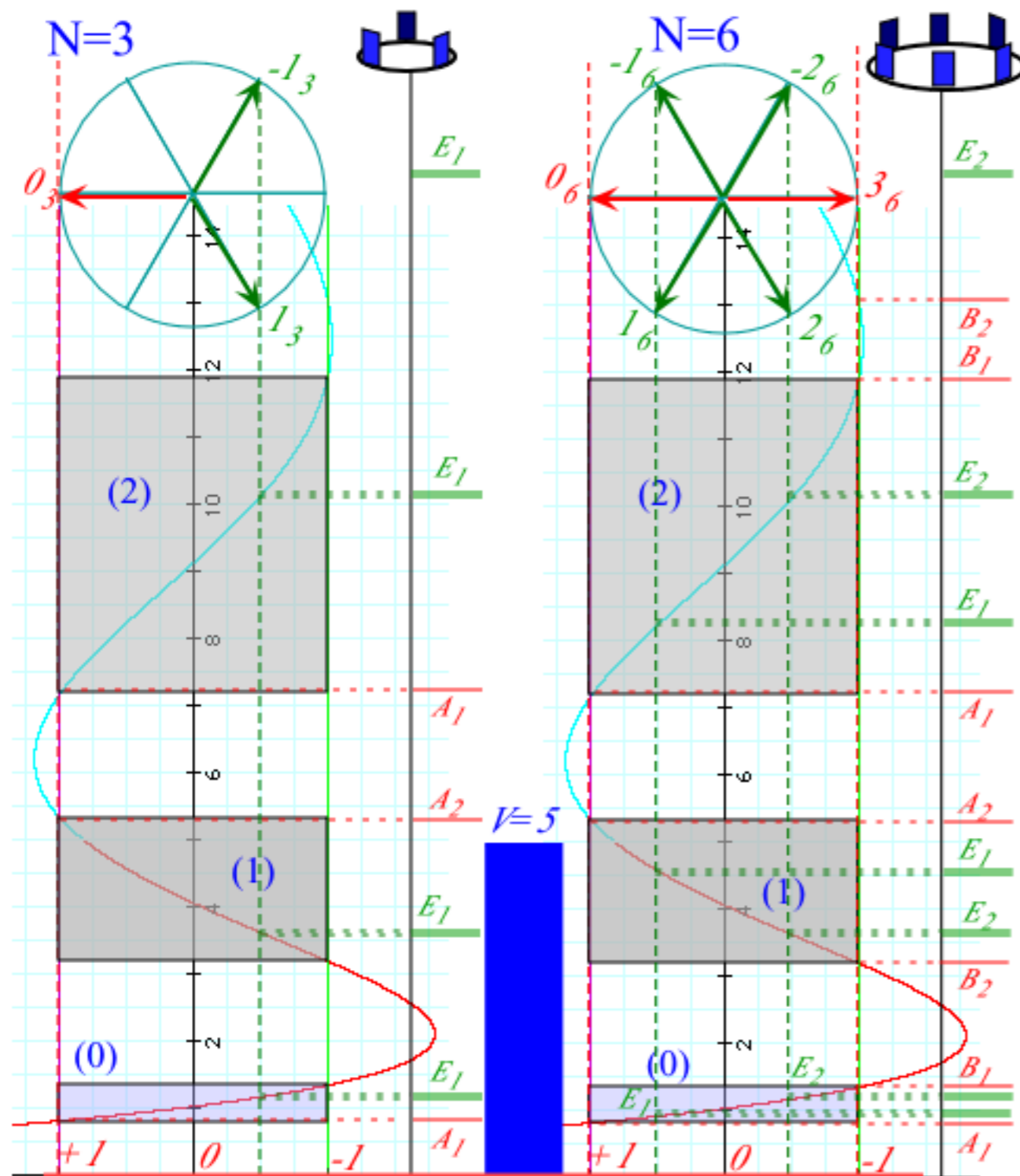


Fig. 14.2.8 Multiplets for $V=5$. ($W=15\text{nm}$ well, $L=5\text{nm}$ barrier) for $(N=3)$ -ring and $(N=6)$ -ring.

Band-It simulations line-non-periodic scattering conditions

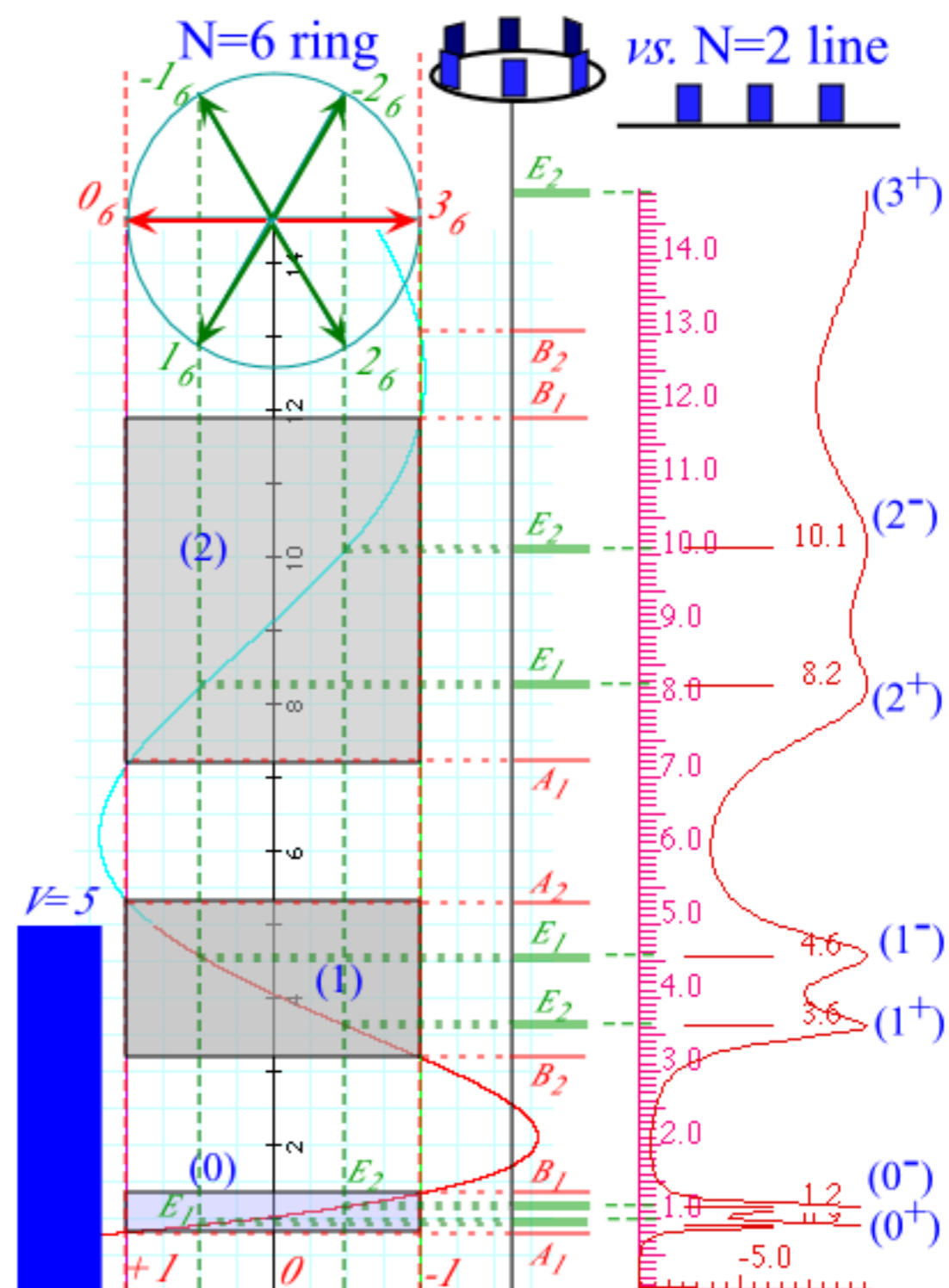


Fig. 14.2.9 $(N=6)$ -ring and $(N=2)$ -line potential. ($V=5$, $W=15\text{nm}$ well, $L=5\text{nm}$ barrier)

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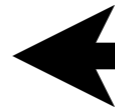
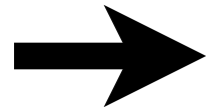
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Algebra

Geometry

Fig. 2.12.7 PSDS

$|X \text{ up} \rangle |X \text{ down} \rangle$

Pure Type-B
Hamiltonian
 NH_3 (Ammonia)

$$\langle H \rangle = \begin{pmatrix} H & -S \\ -S & H \end{pmatrix}$$

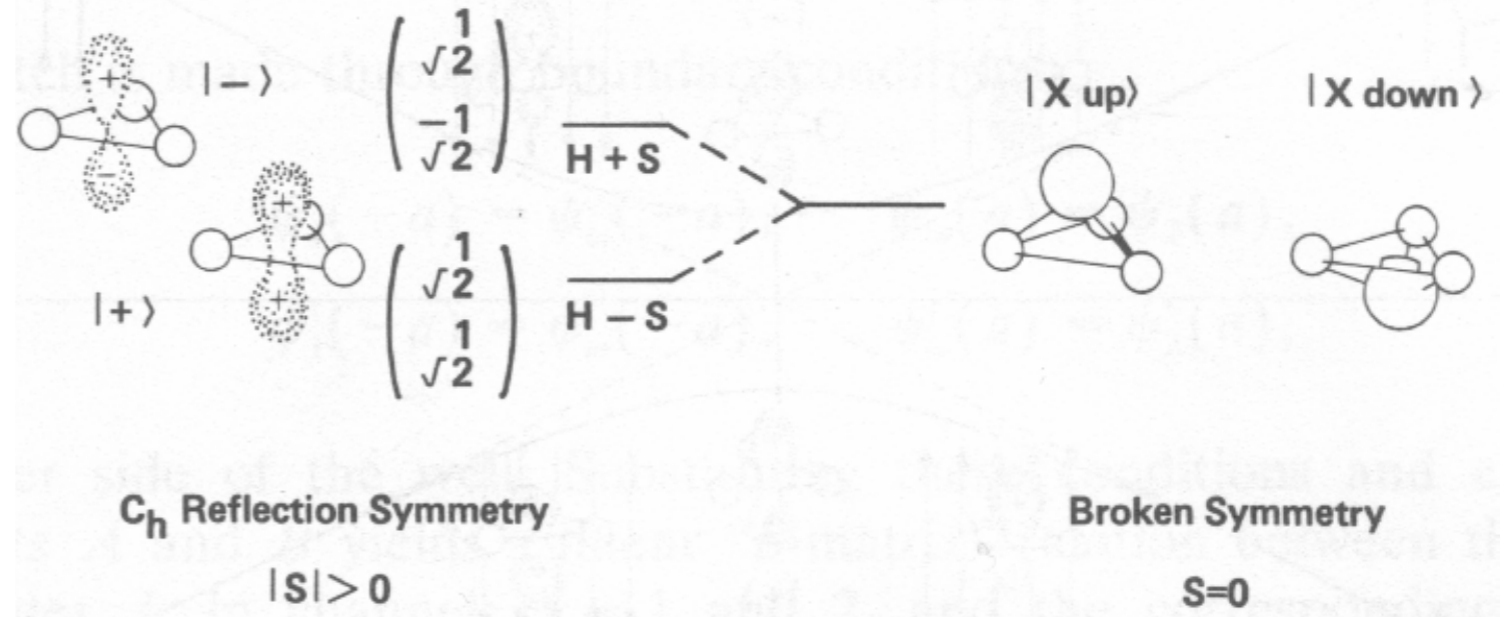
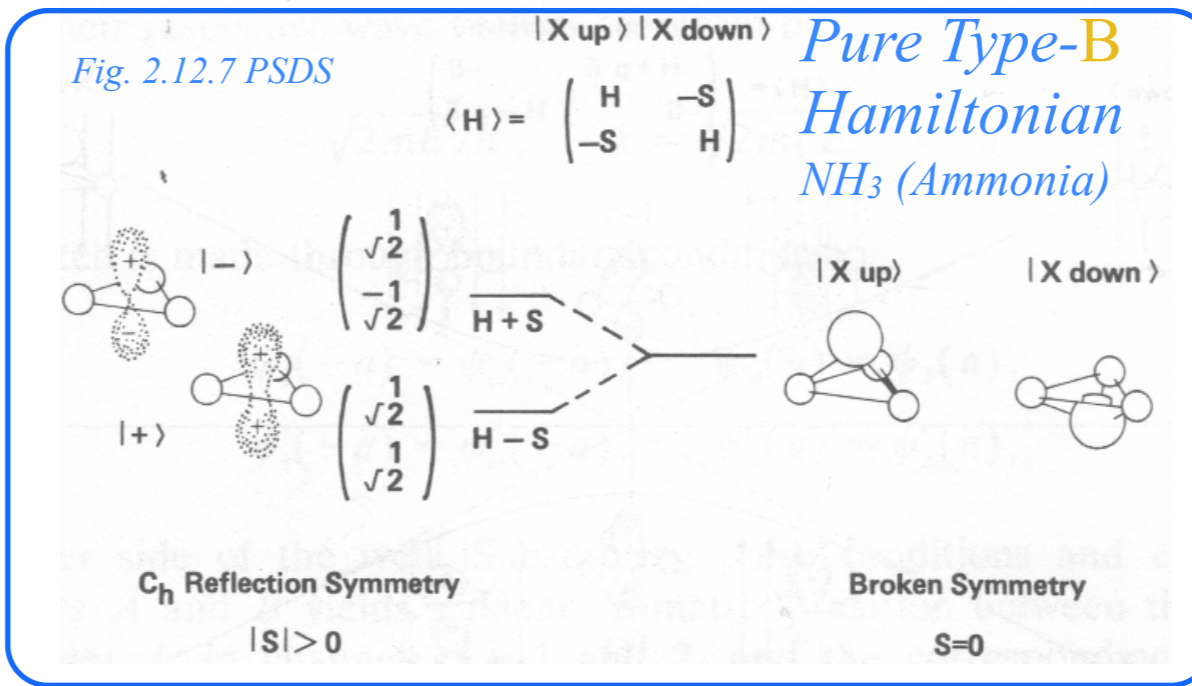


Fig. 2.12.7 PSDS



Type-AB Hamiltonian
NH₃ (with applied E-field)

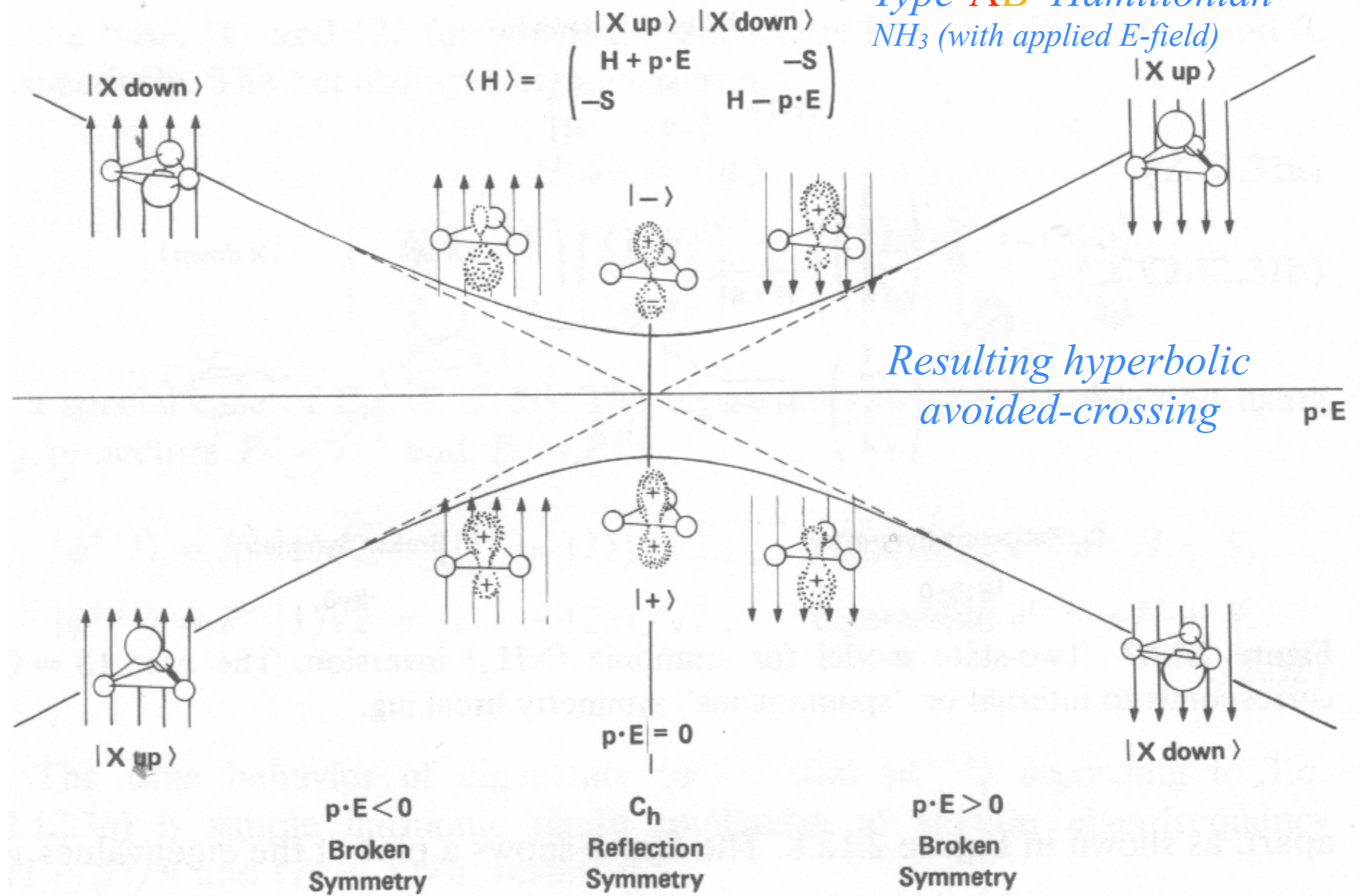


Fig. 2.12.8 PSDS

Transform $\mathbf{H}(A\text{-basis})$ into $\mathbf{H}(B\text{-basis})$

$$\begin{aligned} & \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} +A & B \\ B & -A \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} +A & B \\ B & -A \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} +A+B & B-A \\ +A-B & B+A \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 2B & 2A \\ 2A & -2B \end{pmatrix} \\ &= \begin{pmatrix} +B & A \\ A & -B \end{pmatrix} \end{aligned}$$

Review of
Lecture 10
p. 65 to 73

Fig. 2.12.8 PSDS

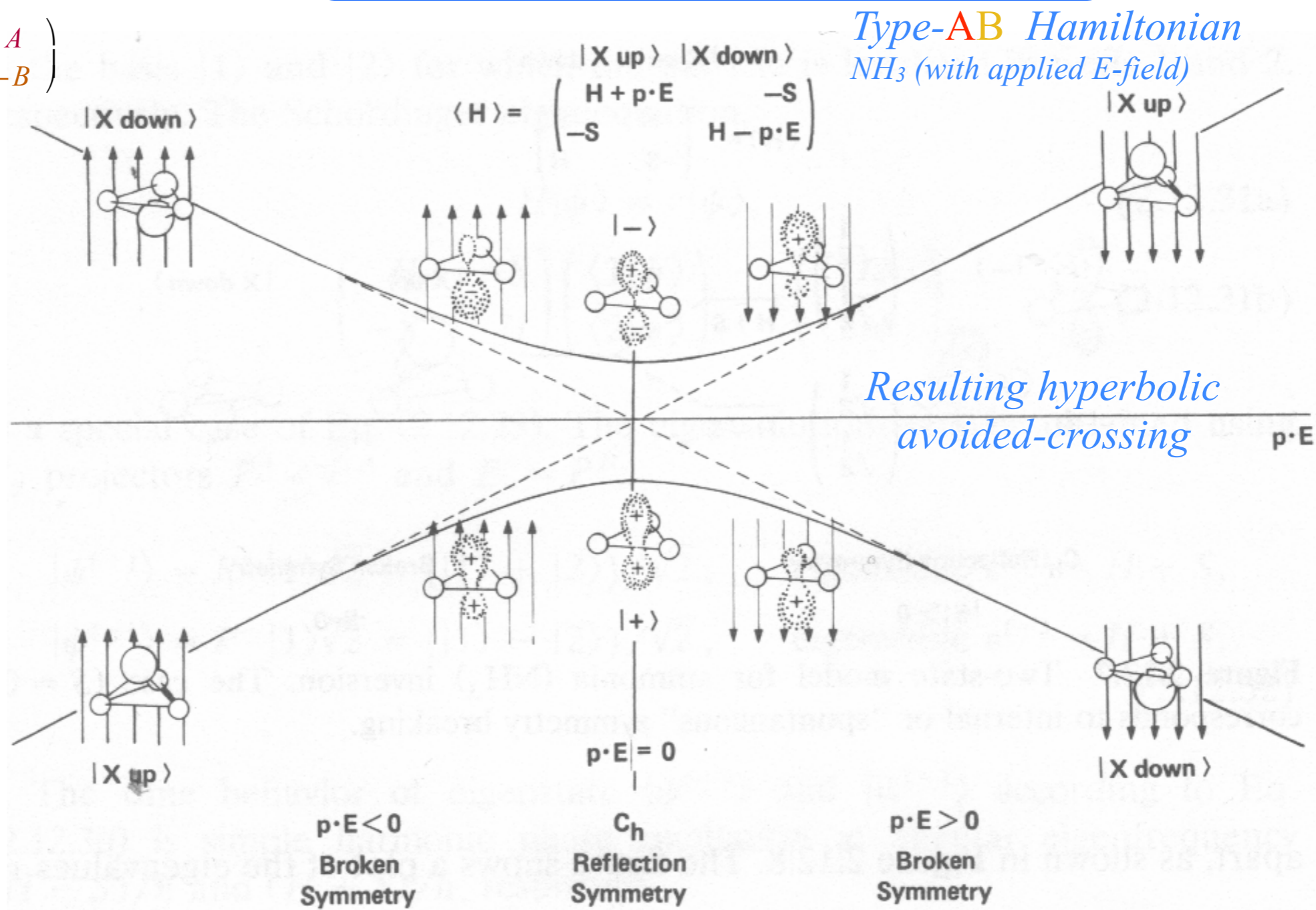
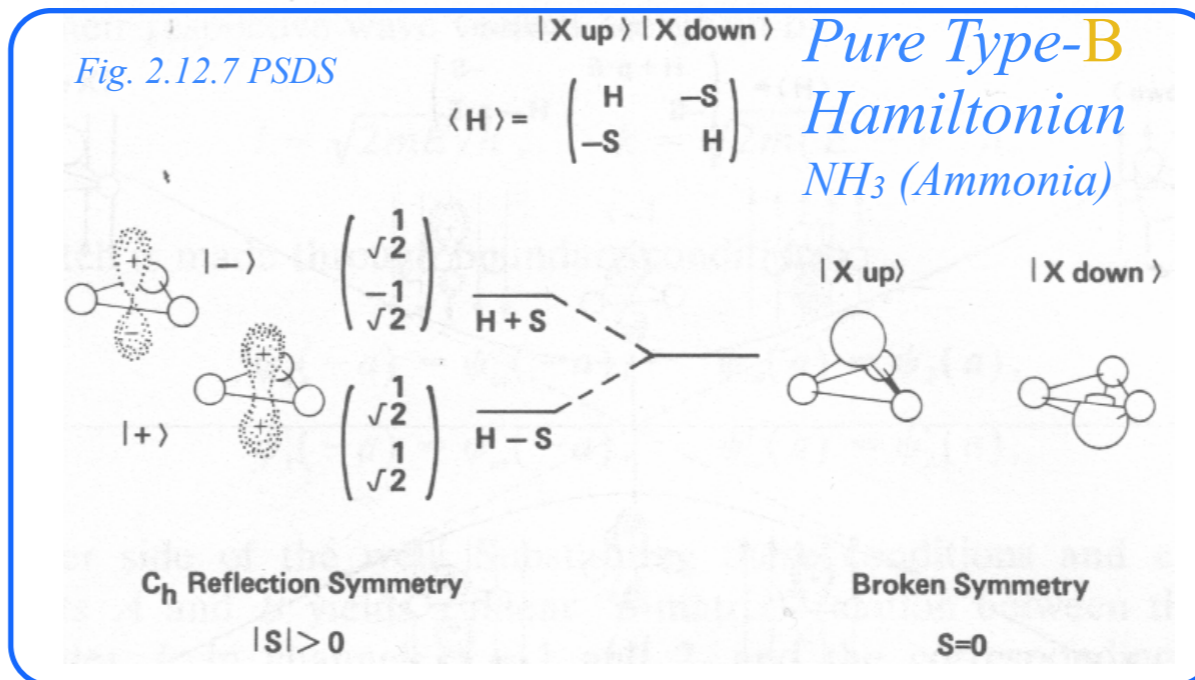


Fig. 2.12.7 PSDS



A to B to A Symmetry breaking described by hyperbolic eigenvalues of $A\sigma_A+B\sigma_B=\mathbf{H}=\begin{pmatrix} +A & B \\ B & -A \end{pmatrix}$

$\mathbf{H}=\begin{pmatrix} +A & B \\ B & -A \end{pmatrix}$ Secular equation: $\varepsilon^2 - 0 \cdot \varepsilon - (A^2 + B^2)$ gives *hyperbolic* energy levels: $\varepsilon = \pm\sqrt{A^2 + B^2}$

$\mathbf{H}(B\text{-basis})$ $\mathbf{H}(A\text{-basis})$

$$\begin{pmatrix} ? & ? \\ ? & ? \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} +A & B \\ B & -A \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} +A & B \\ B & -A \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} +A+B & B-A \\ +A-B & B+A \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 2B & 2A \\ 2A & -2B \end{pmatrix}$$

$$= \begin{pmatrix} +B & A \\ A & -B \end{pmatrix}$$

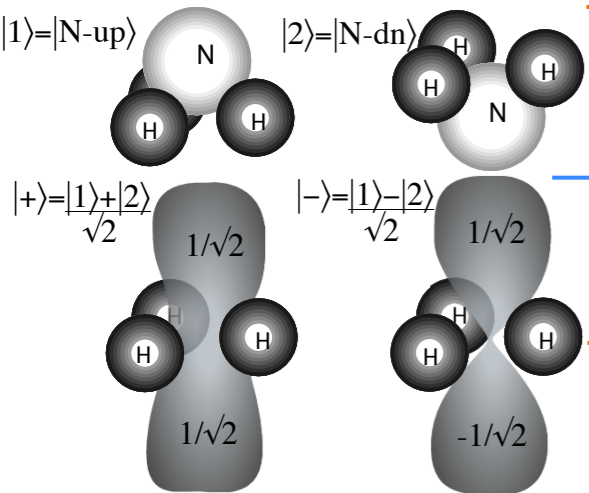
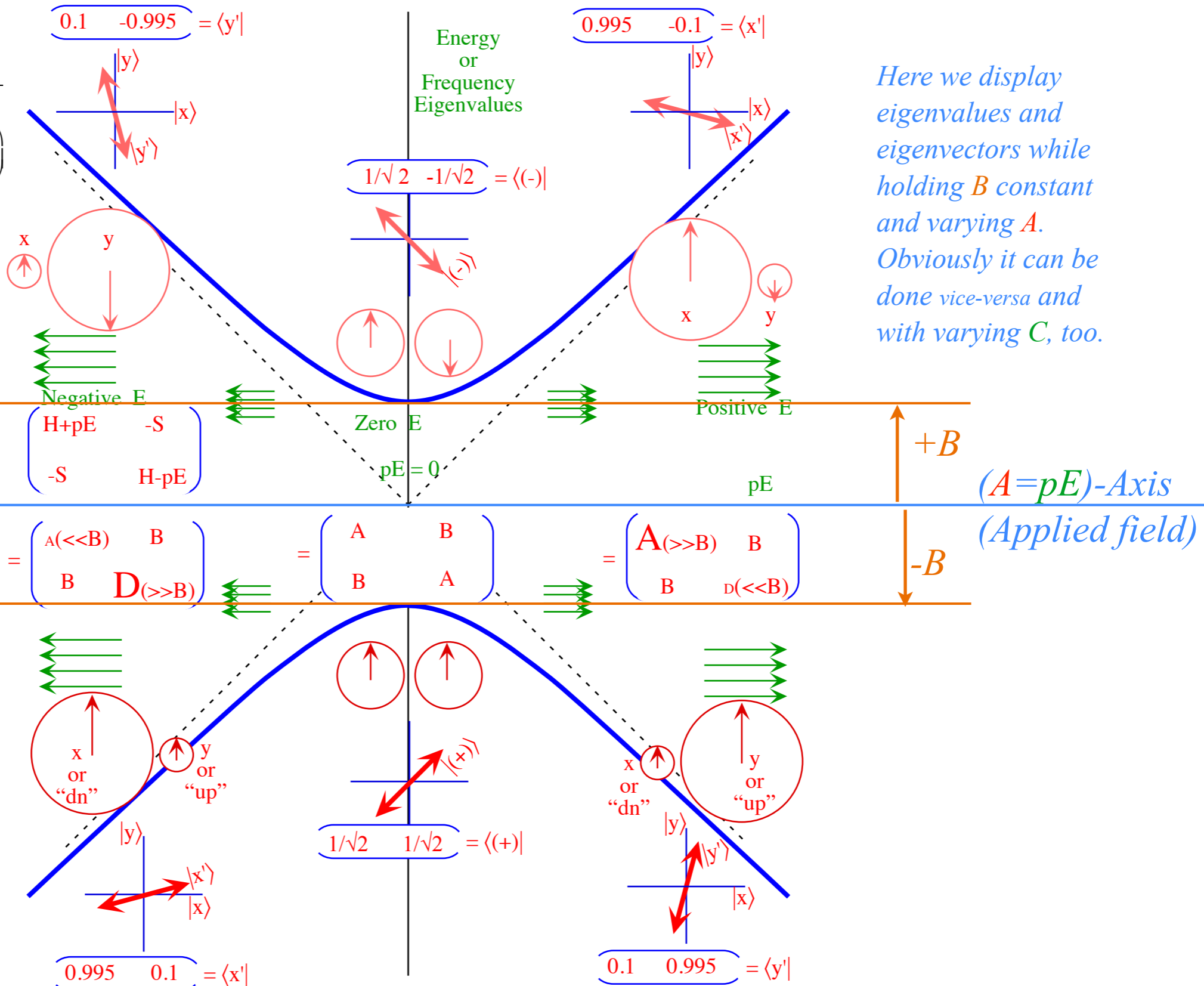


Fig. 10.3.2 Ammonia (NH₃) inversion states
 (a) Base states (b) C₂-Eigenstates



Here we display eigenvalues and eigenvectors while holding *B* constant and varying *A*. Obviously it can be done vice-versa and with varying *C*, too.

Fig. 10.3.1 (b) Wigner avoided level crossing. (Fixed tunneling $B=-S$ and variable $A-D=pE$ field.)

Review of
 Lecture 10
 p. 73

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Algebra

Geometry

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(And some that are)

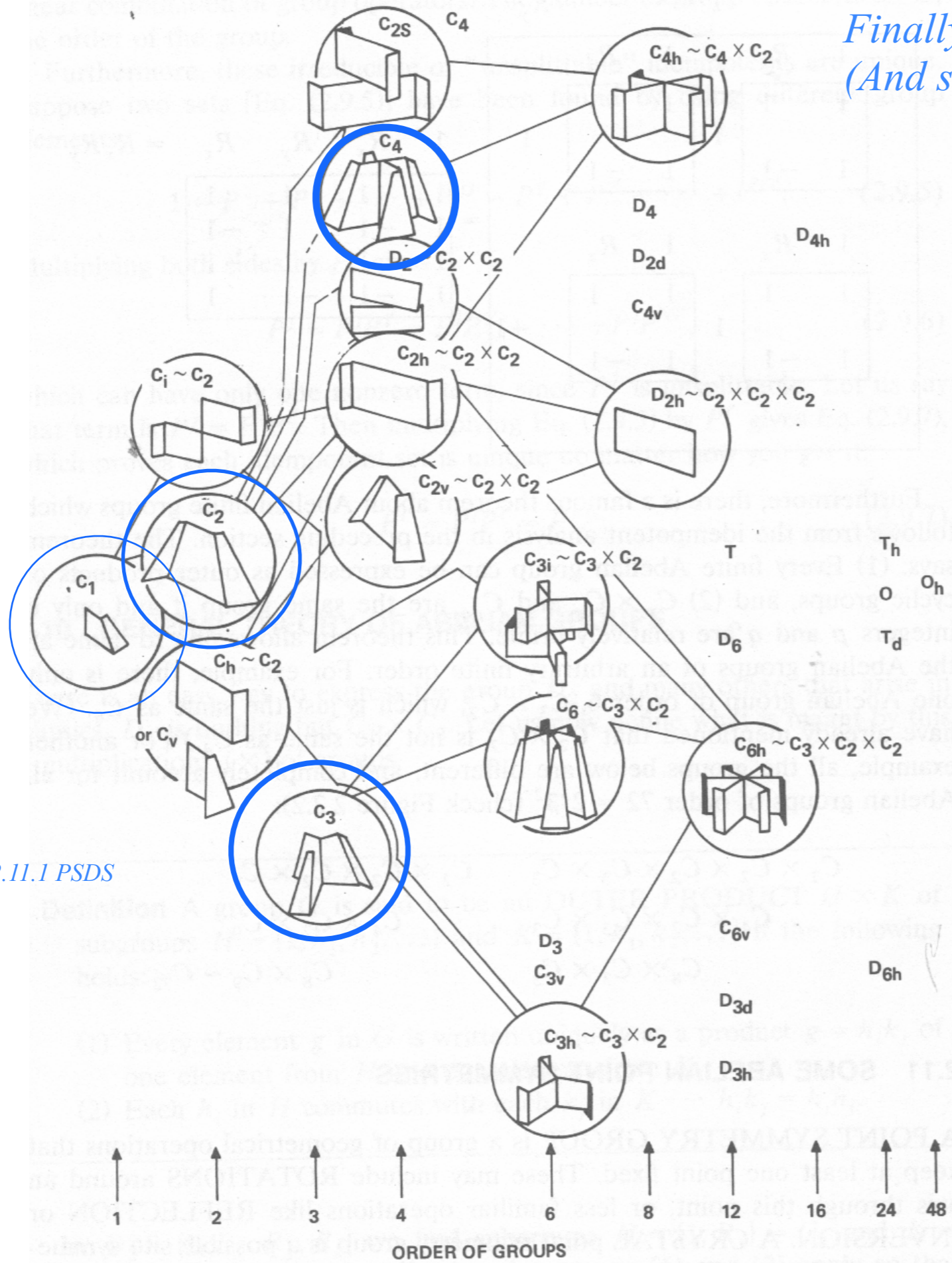


Fig. 2.11.1 PSDS

Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

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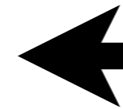
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 (And some that are)
 Starting with D_2*

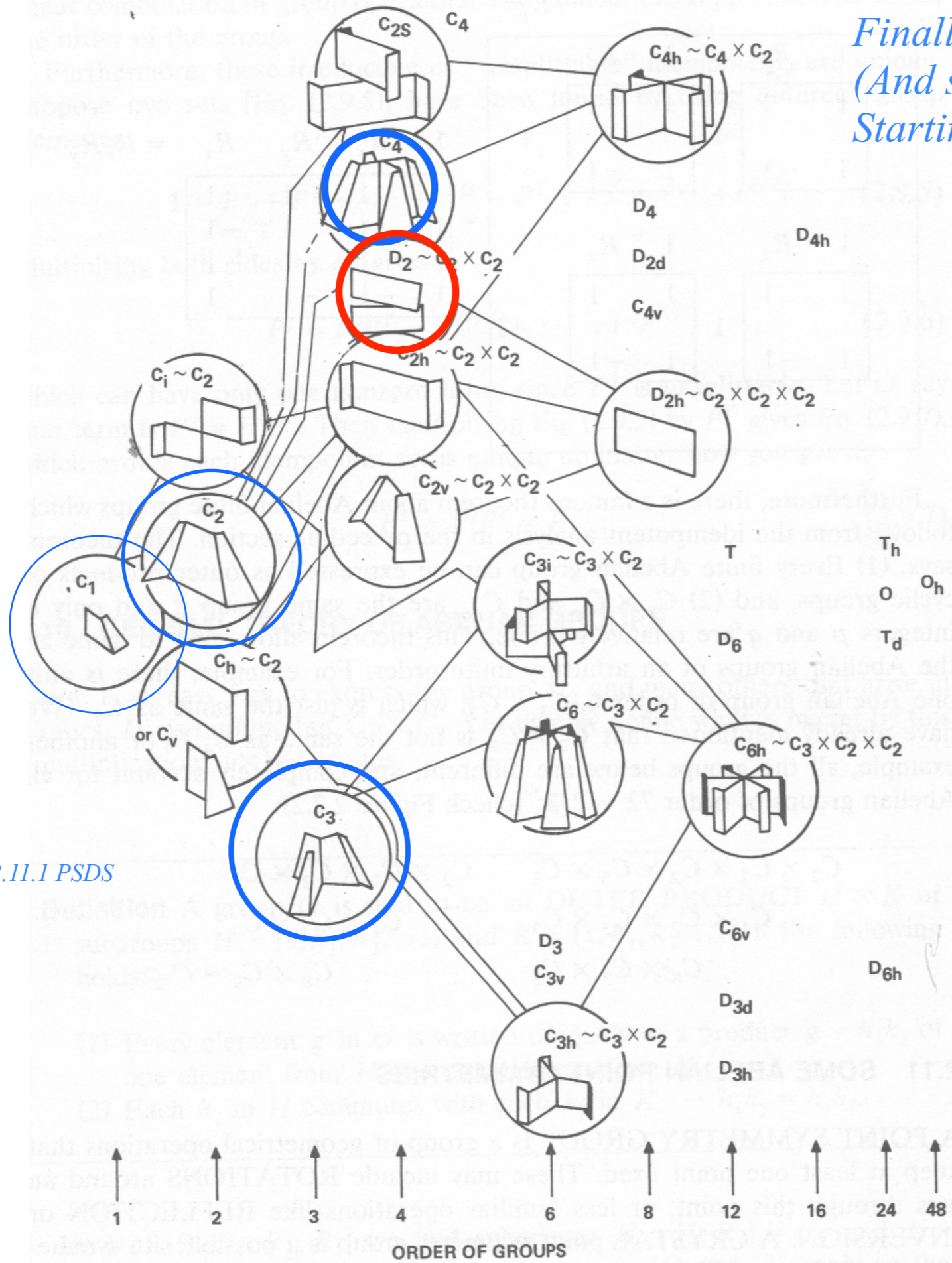


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Finally! Symmetry groups that are not just C_N
 (And some that are)
 Starting with D_2 and C_{2h} and C_{2v}

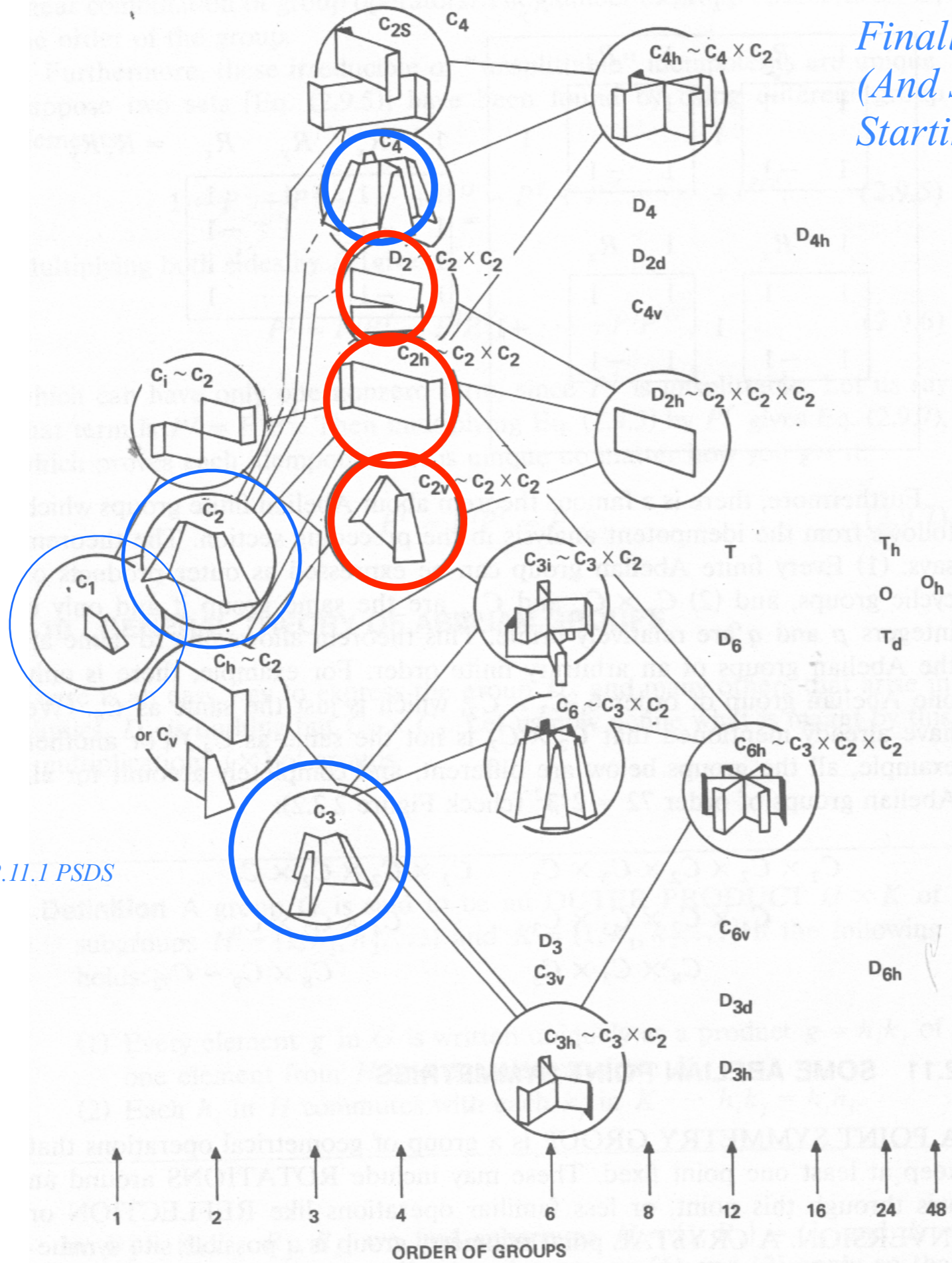


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Some D_2 modes

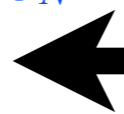
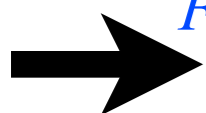
Outer product properties and the Crystal-Point Symmetry Group Zoo

Polygonal geometry of $U(2) \supset C_N$ character spectral function $\chi^j(2\pi/n) = \frac{\sin(\pi(2j+1)/n)}{\sin(\pi/n)}$

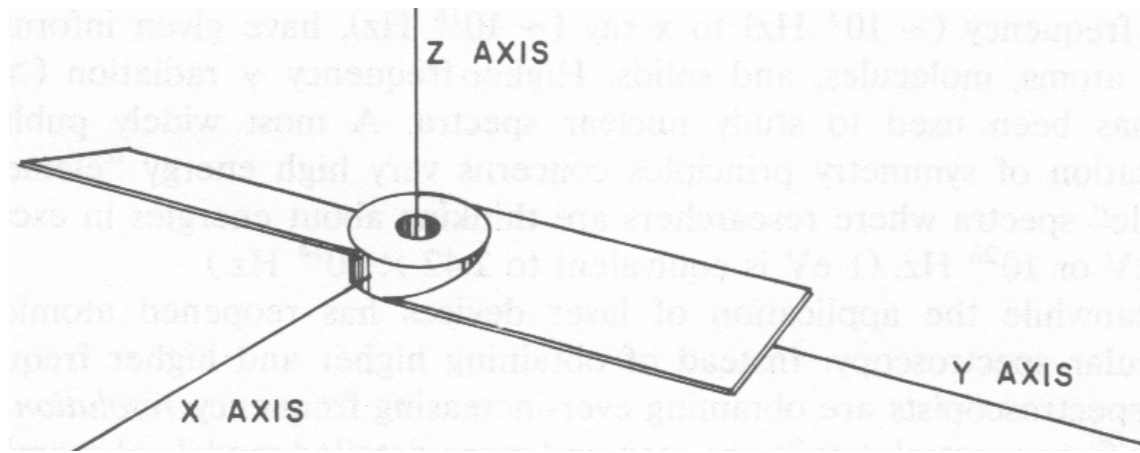
Algebra

Geometry

*The **CPT** subgroup of Lorentz Group*



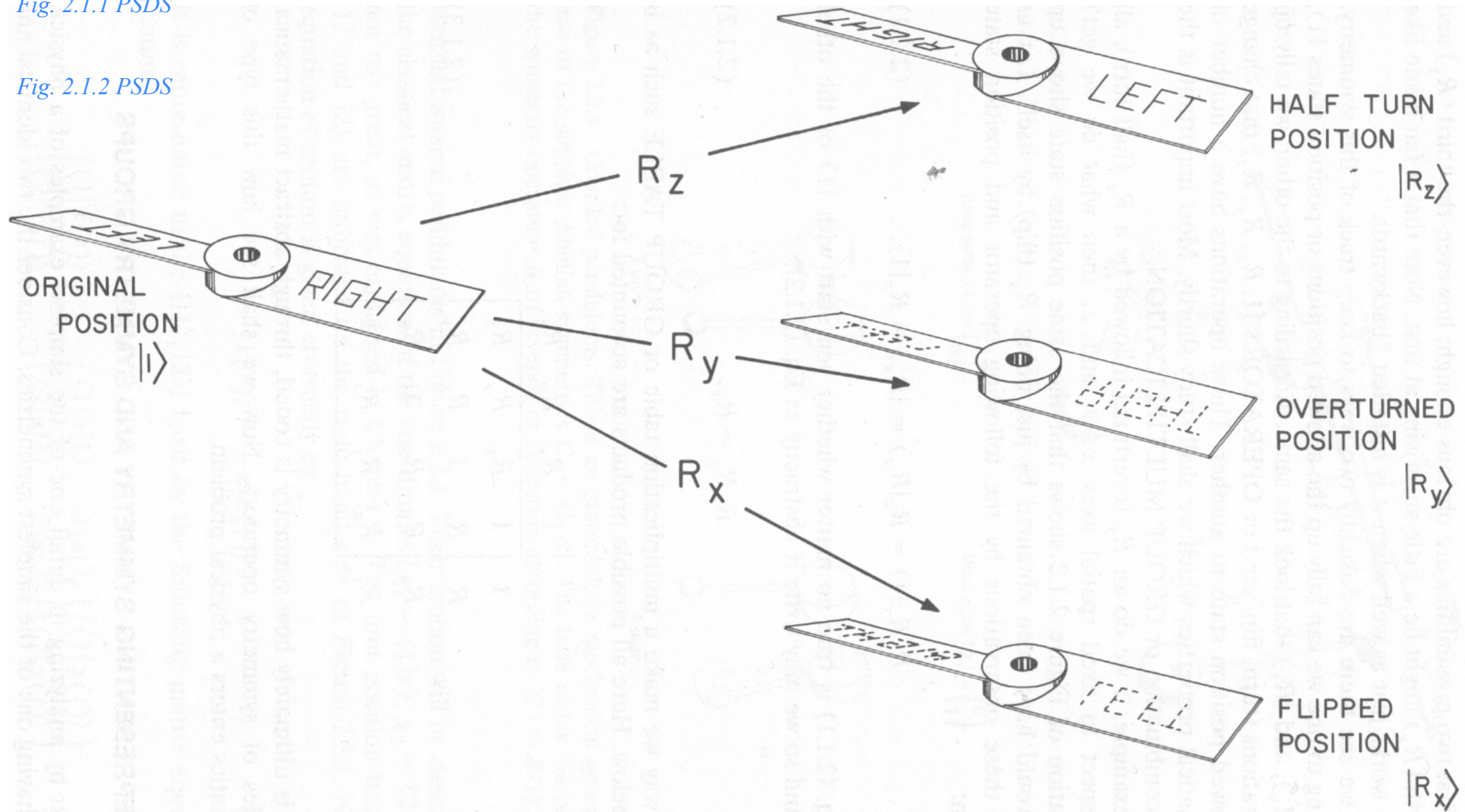
D_2 Symmetry (The 4-Group)



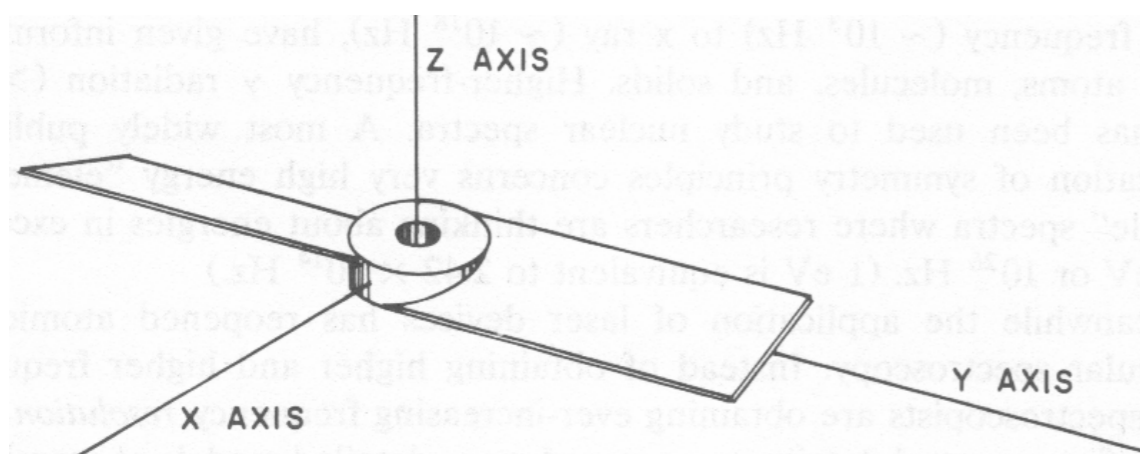
- 1** : THE ORIGINAL POSITION Don't touch the fan blade.
- R_z : THE HALF-TURN POSITION Rotate it by 180° around its axle or the z axis.
- R_y : THE OVERTURNED POSITION Overturn it 180° around the y axis.
- R_x : THE FLIPPED POSITION Flip it 180° around the x axis.

Fig. 2.1.1 PSDS

Fig. 2.1.2 PSDS



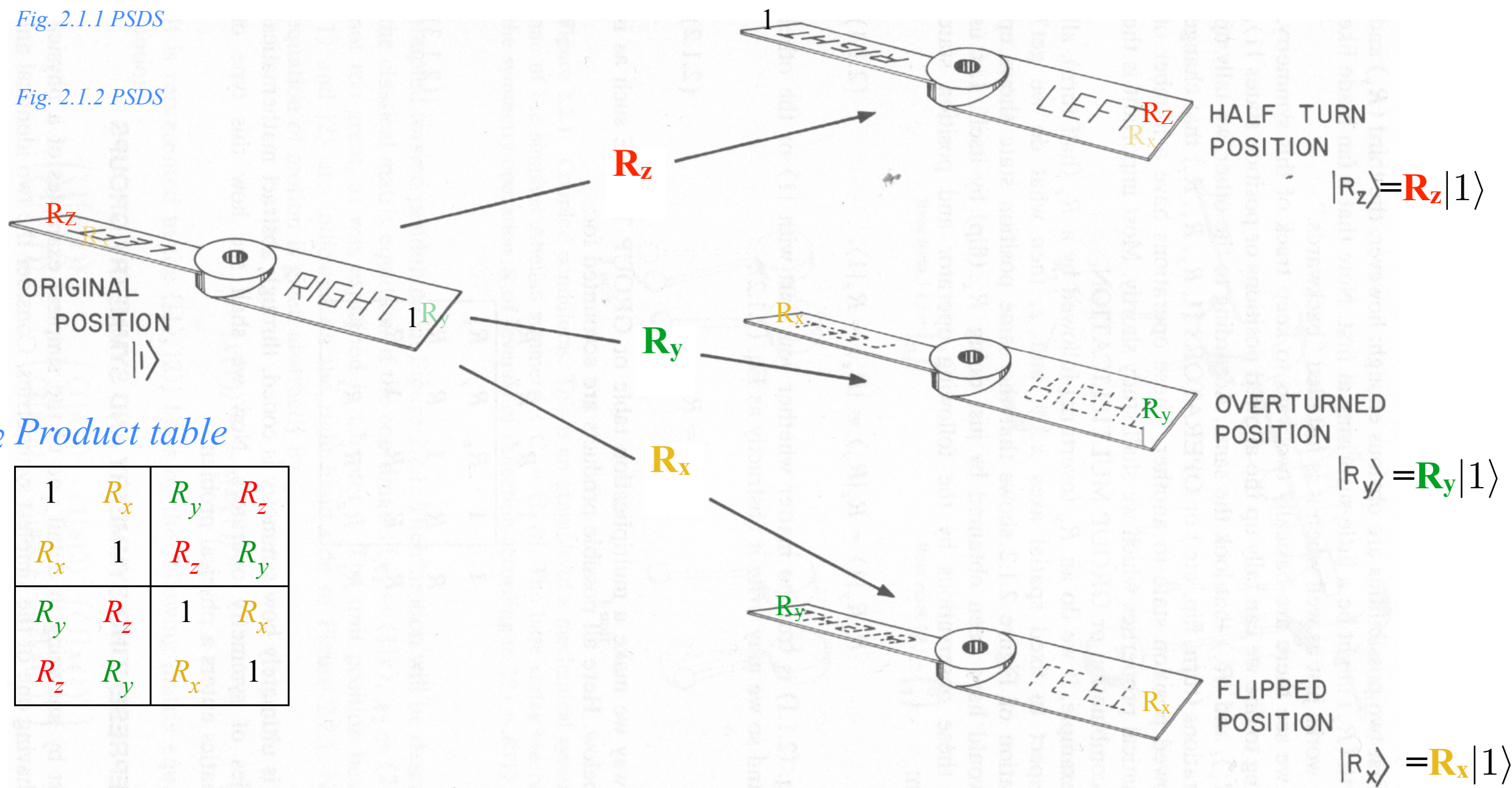
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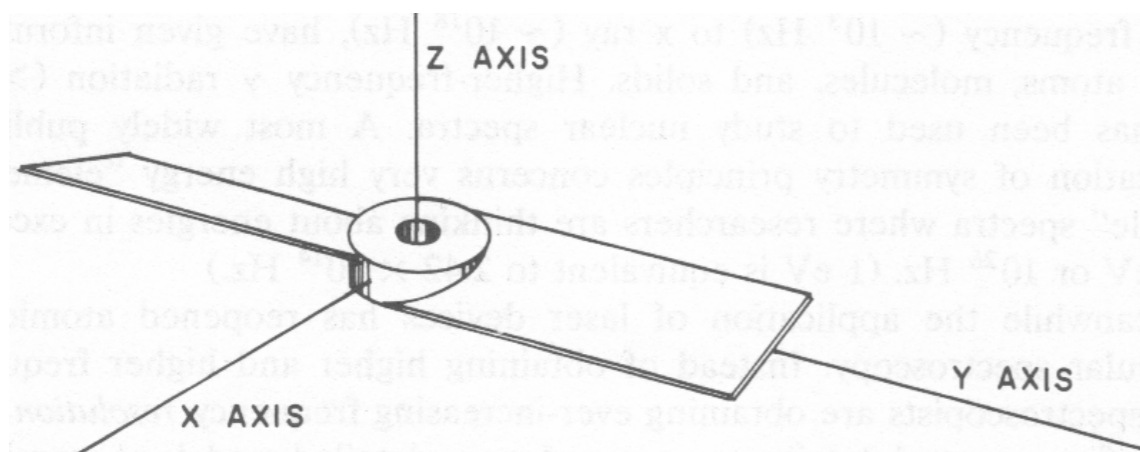
Fig. 2.1.2 PSDS



D_2 Product table

1	R_x	R_y	R_z
R_x	1	R_z	R_y
R_y	R_z	1	R_x
R_z	R_y	R_x	1

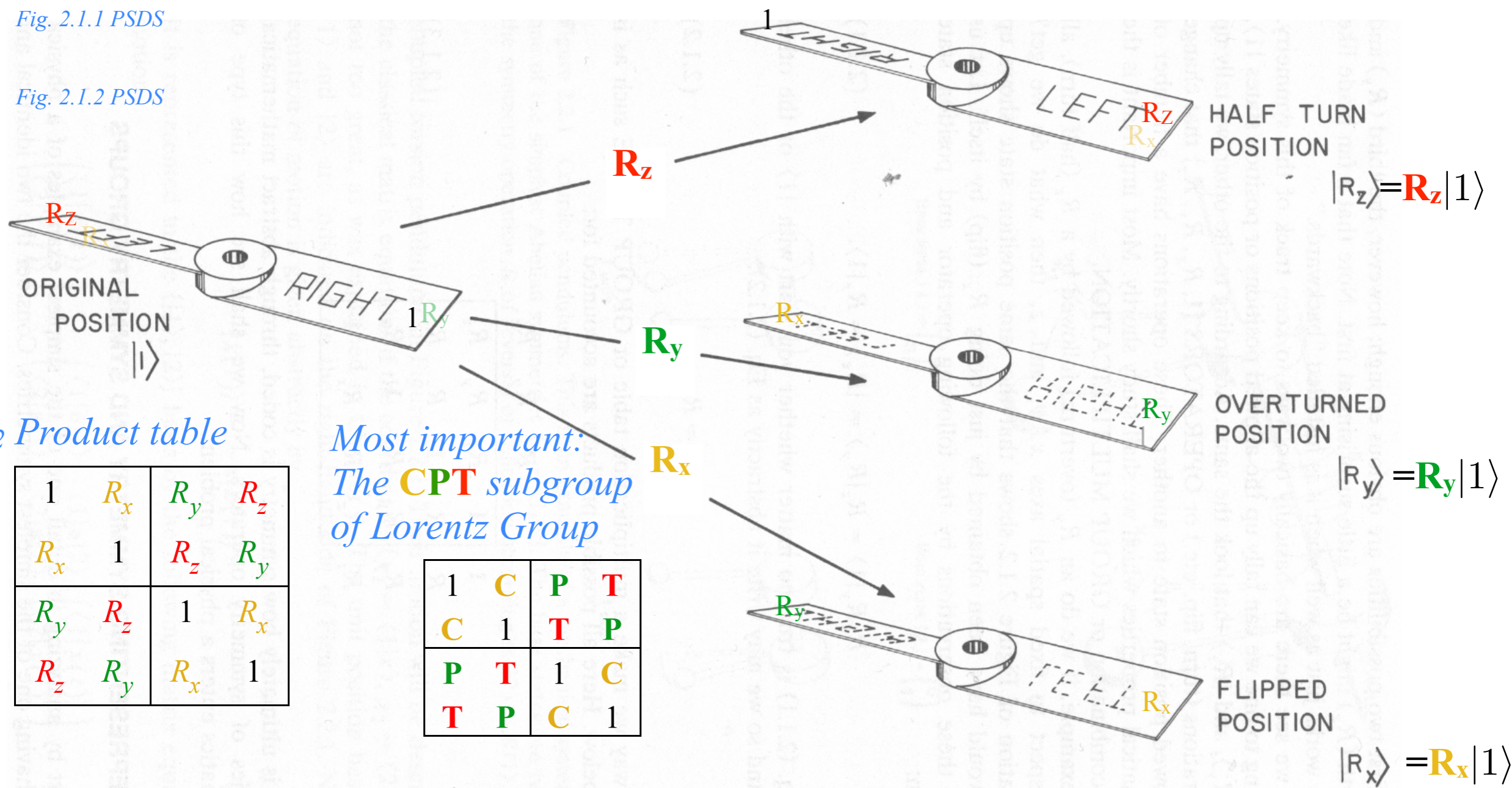
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R_x	1	R_z	R_y
R_y	R_z	1	R_x
R_z	R_y	R_x	1

Most important:
The **CPT** subgroup
of Lorentz Group

1	C	P	T
C	1	T	P
P	T	1	C
T	P	C	1

Breaking C_N cyclic coupling into linear chains

Review of 1D-Bohr-ring related to infinite square well

Breaking C_{2N+2} to approximate linear N -chain (Examples $C_2 \rightleftharpoons C_6 \rightleftharpoons C_{14}$)

Band-It simulation: Intro to scattering approach to quantum symmetry

How Band-It works: Match each Ψ and $D\Psi$, Let $L=0$ at Right end

Breaking C_{2N} cyclic coupling down to C_N symmetry

Acoustical modes vs. Optical modes

Intro to other examples of band theory

Type-AB Avoided crossing view of band-gaps

Finally! Symmetry groups that are not just C_N

*The **CPT** subgroup of Lorentz Group*

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Spectral decomposition of D_2

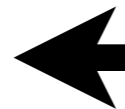
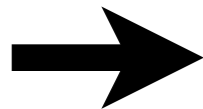
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Algebra

Geometry



D₂ spectral decomposition: The old “1=1•1 trick” again

Two C_2 subgroup minimal equations:

$$\mathbf{R}_x^2 - \mathbf{1} = \mathbf{0},$$

$$\mathbf{R}_y^2 - \mathbf{1} = \mathbf{0}.$$

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Two C₂ subgroup minimal equations and their projectors:

$$\mathbf{R}_x^2 - \mathbf{1} = \mathbf{0},$$

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reducible

$$\mathbf{P}_y^+ = \frac{\mathbf{1} + \mathbf{R}_y}{2}$$

$$\mathbf{P}_x^- = \frac{\mathbf{1} - \mathbf{R}_x}{2}$$

projectors

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Completeness

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Spec. decomps

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The old “1=1•1 trick” $\mathbf{1} = \mathbf{1} \cdot \mathbf{1} = (\mathbf{P}_x^+ + \mathbf{P}_x^-) \cdot (\mathbf{P}_y^+ + \mathbf{P}_y^-) = \mathbf{P}_x^+ \cdot \mathbf{P}_y^+ + \mathbf{P}_x^- \cdot \mathbf{P}_y^+ + \mathbf{P}_x^+ \cdot \mathbf{P}_y^- + \mathbf{P}_x^- \cdot \mathbf{P}_y^-$ *gives irrep projectors*

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$$\mathbf{P}^{++} \equiv \mathbf{P}_x^+ \cdot \mathbf{P}_y^+ = \frac{(\mathbf{1} + \mathbf{R}_x) \cdot (\mathbf{1} + \mathbf{R}_y)}{2 \cdot 2} = \frac{1}{4} (\mathbf{1} + \mathbf{R}_x + \mathbf{R}_y + \mathbf{R}_z)$$

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(completeness is first)

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(then R_x eigenvalues)

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(...and so forth)

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Completeness

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Spec. decomps

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$$\mathbf{R}_z = (+1)\mathbf{P}^{++} + (-1)\mathbf{P}^{-+} + (-1)\mathbf{P}^{+-} + (+1)\mathbf{P}^{--}$$

$$\begin{array}{c|cc} C_2^x & \mathbf{1} & \mathbf{R}_x \\ \hline + & 1 & 1 \\ - & 1 & -1 \end{array} \times \begin{array}{c|cc} C_2^y & \mathbf{1} & \mathbf{R}_y \\ \hline + & 1 & 1 \\ - & 1 & -1 \end{array} =$$

$C_2^x \times C_2^y$	$\mathbf{1} \cdot \mathbf{1}$	$\mathbf{R}_x \cdot \mathbf{1}$	$\mathbf{1} \cdot \mathbf{R}_y$	$\mathbf{R}_x \cdot \mathbf{R}_y$
+•+	1•1	1•1	1•1	1•1
-•+	1•1	-1•1	1•1	-1•1
+•-	1•1	1•1	1•(-1)	1•(-1)
-•-	1•1	-1•1	1•(-1)	-1•(-1)

Shortcut notation for getting D₂ character table

D₂ spectral decomposition: The old “1=1•1 trick” again

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$$\mathbf{R}_x = \mathbf{P}_x^+ - \mathbf{P}_x^- \quad \text{Spec. decomps}$$

$$\mathbf{R}_y = \mathbf{P}_y^+ - \mathbf{P}_y^-$$

$$\begin{array}{c|cc} C_2^x & \mathbf{1} & \mathbf{R}_x \\ \hline + & 1 & 1 \\ - & 1 & -1 \end{array} \times \begin{array}{c|cc} C_2^y & \mathbf{1} & \mathbf{R}_y \\ \hline + & 1 & 1 \\ - & 1 & -1 \end{array}$$

$$= \begin{array}{c|cccc} C_2^x \times C_2^y & \mathbf{1} \cdot \mathbf{1} & \mathbf{R}_x \cdot \mathbf{1} & \mathbf{1} \cdot \mathbf{R}_y & \mathbf{R}_x \cdot \mathbf{R}_y \\ \hline + \cdot + & 1 \cdot 1 & 1 \cdot 1 & 1 \cdot 1 & 1 \cdot 1 \\ - \cdot + & 1 \cdot 1 & -1 \cdot 1 & 1 \cdot 1 & -1 \cdot 1 \\ + \cdot - & 1 \cdot 1 & 1 \cdot 1 & 1 \cdot (-1) & 1 \cdot (-1) \\ - \cdot - & 1 \cdot 1 & -1 \cdot 1 & 1 \cdot (-1) & -1 \cdot (-1) \end{array}$$

$$= \begin{array}{c|cccc} D_2 & \mathbf{1} & \mathbf{R}_x & \mathbf{R}_y & \mathbf{R}_z \\ \hline + \cdot + & 1 & 1 & 1 & 1 \\ - \cdot + & 1 & -1 & 1 & -1 \\ + \cdot - & 1 & 1 & -1 & -1 \\ - \cdot - & 1 & -1 & -1 & 1 \end{array}$$

The old “1=1•1 trick” $\mathbf{1} = \mathbf{1} \cdot \mathbf{1} = (\mathbf{P}_x^+ + \mathbf{P}_x^-) \cdot (\mathbf{P}_y^+ + \mathbf{P}_y^-) = \mathbf{P}_x^+ \cdot \mathbf{P}_y^+ + \mathbf{P}_x^- \cdot \mathbf{P}_y^+ + \mathbf{P}_x^+ \cdot \mathbf{P}_y^- + \mathbf{P}_x^- \cdot \mathbf{P}_y^-$ gives irrep projectors

$$\mathbf{P}^{++} \equiv \mathbf{P}_x^+ \cdot \mathbf{P}_y^+ = \frac{(\mathbf{1} + \mathbf{R}_x) \cdot (\mathbf{1} + \mathbf{R}_y)}{2 \cdot 2} = \frac{1}{4} (\mathbf{1} + \mathbf{R}_x + \mathbf{R}_y + \mathbf{R}_z)$$

(completeness is first)

$$\mathbf{P}^{-+} \equiv \mathbf{P}_x^- \cdot \mathbf{P}_y^+ = \frac{(\mathbf{1} - \mathbf{R}_x) \cdot (\mathbf{1} + \mathbf{R}_y)}{2 \cdot 2} = \frac{1}{4} (\mathbf{1} - \mathbf{R}_x + \mathbf{R}_y - \mathbf{R}_z)$$

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$$\mathbf{R}_z = (+1)\mathbf{P}^{++} + (-1)\mathbf{P}^{-+} + (-1)\mathbf{P}^{+-} + (+1)\mathbf{P}^{--}$$

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$$= \begin{array}{c|cccc} D_2 & \mathbf{1} & \mathbf{R}_x & \mathbf{R}_y & \mathbf{R}_z \\ \hline ++ = A_1 & 1 & 1 & 1 & 1 \\ -+ = A_2 & 1 & -1 & 1 & -1 \\ +- = B_1 & 1 & 1 & -1 & -1 \\ -- = B_2 & 1 & -1 & -1 & 1 \end{array} \quad \text{Note common notation}$$

The old “1=1•1 trick” $\mathbf{1} = \mathbf{1} \cdot \mathbf{1} = (\mathbf{P}_x^+ + \mathbf{P}_x^-) \cdot (\mathbf{P}_y^+ + \mathbf{P}_y^-) = \mathbf{P}_x^+ \cdot \mathbf{P}_y^+ + \mathbf{P}_x^- \cdot \mathbf{P}_y^+ + \mathbf{P}_x^+ \cdot \mathbf{P}_y^- + \mathbf{P}_x^- \cdot \mathbf{P}_y^-$ gives irrep projectors

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Breaking C_N cyclic coupling into linear chains

Review of 1D-Bohr-ring related to infinite square well

Breaking C_{2N+2} to approximate linear N -chain (Examples $C_2 \rightleftharpoons C_6 \rightleftharpoons C_{14}$)

Band-It simulation: Intro to scattering approach to quantum symmetry

How Band-It works: Match each Ψ and $D\Psi$, Let $L=0$ at Right end

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Acoustical modes vs. Optical modes

Intro to other examples of band theory

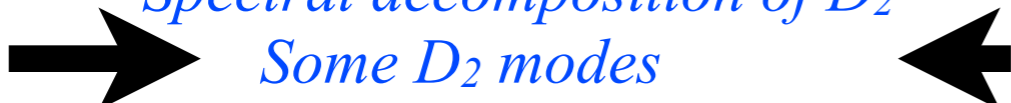
Type-AB Avoided crossing view of band-gaps

Finally! Symmetry groups that are not just C_N

*The **CPT** subgroup of Lorentz Group*

The “4-Group(s)” D_2 and C_{2v}

Spectral decomposition of D_2

 *Some D_2 modes*

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Polygonal geometry of $U(2) \supset C_N$ character spectral function $\chi^j(2\pi/n) = \frac{\sin(\pi(2j+1)/n)}{\sin(\pi/n)}$

Algebra

Geometry

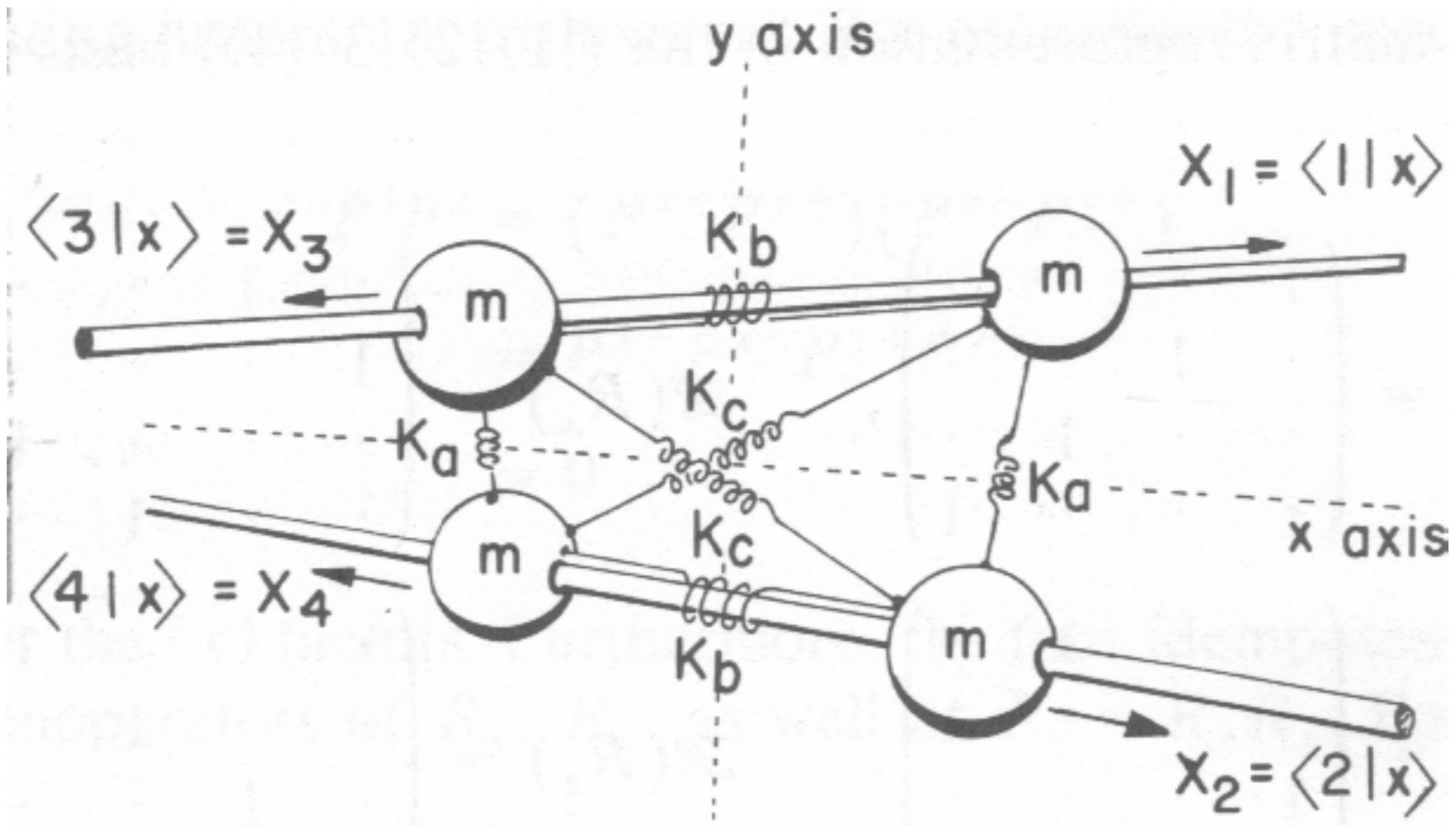


Fig. 2.8.1 PSDS

$$\begin{pmatrix} \langle 1 | \ddot{x} \rangle \\ \langle 2 | \ddot{x} \rangle \\ \langle 3 | \ddot{x} \rangle \\ \langle 4 | \ddot{x} \rangle \end{pmatrix} = \begin{pmatrix} A & a & b & c \\ a & A & c & b \\ b & c & A & a \\ c & b & a & A \end{pmatrix} \begin{pmatrix} \langle 1 | x \rangle \\ \langle 2 | x \rangle \\ \langle 3 | x \rangle \\ \langle 4 | x \rangle \end{pmatrix}$$

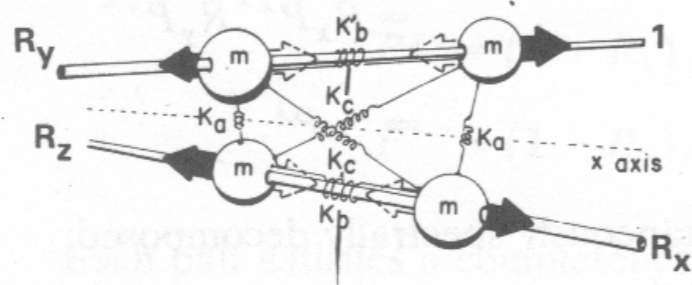
$$\begin{aligned}
 A &= -(k_a \cos^2(a, b) + k_b + k_c \cos^2(b, c)) / m, \\
 a &= -k_a \cos^2(a, b) / m, \\
 b &= -k_b / m, \\
 c &= -k_c \cos^2(b, c) / m.
 \end{aligned}$$

$$|e^{A_1}\rangle \equiv |e^1\rangle = P^1|1\rangle\sqrt{4} = (|1\rangle + |2\rangle + |3\rangle + |4\rangle)/2,$$

$$|e^{B_2}\rangle \equiv |e^2\rangle = P^2|1\rangle\sqrt{4} = (|1\rangle - |2\rangle + |3\rangle - |4\rangle)/2,$$

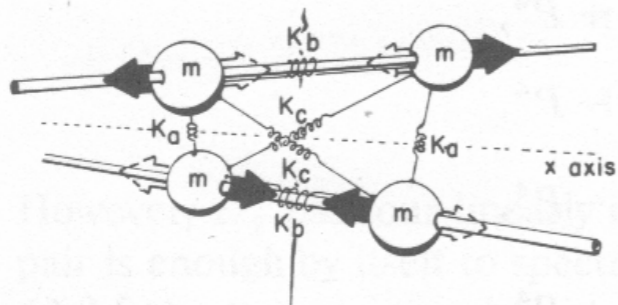
$$|e^{B_1}\rangle \equiv |e^3\rangle = P^3|1\rangle\sqrt{4} = (|1\rangle + |2\rangle - |3\rangle - |4\rangle)/2,$$

$$|e^{A_2}\rangle \equiv |e^4\rangle = P^4|1\rangle\sqrt{4} = (|1\rangle - |2\rangle - |3\rangle + |4\rangle)/2,$$



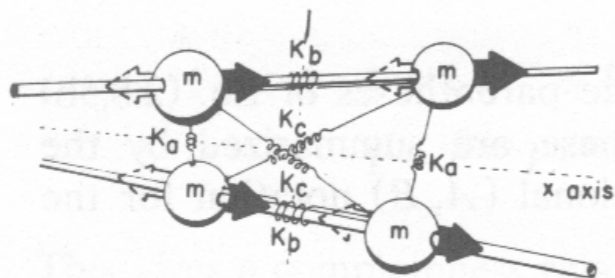
$$\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} / 2$$

$$(A+a+b+c)^{1/2}$$



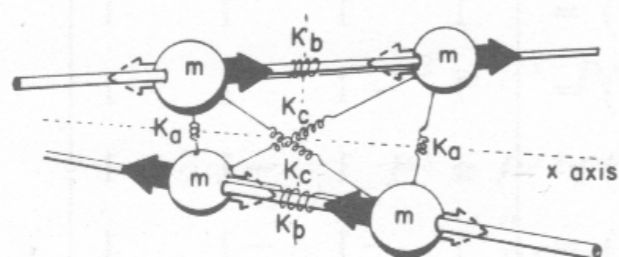
$$\begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} / 2$$

$$(A-a+b-c)^{1/2}$$



$$\begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix} / 2$$

$$(A+a-b-c)^{1/2}$$



$$\begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix} / 2$$

$$(A-a-b+c)^{1/2}$$

Fig. 2.8.2 PSDS

Breaking C_N cyclic coupling into linear chains

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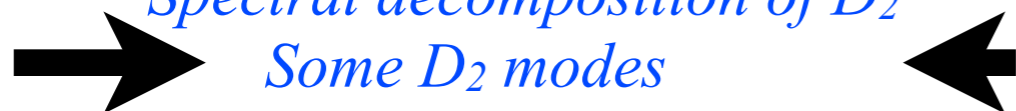
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Algebra

Geometry

Crystal-Point Group Zoo
 having 32 groups
 (Showing
 16 Abelian
 Crystal Groups)

Fig. 2.11.1 PSDS

The other 16
 crystal-point groups
 are
Non-Abelian

Abelian
 means
 all its elements
 commute

Non-Abelian
 means
 some elements
 do not commute

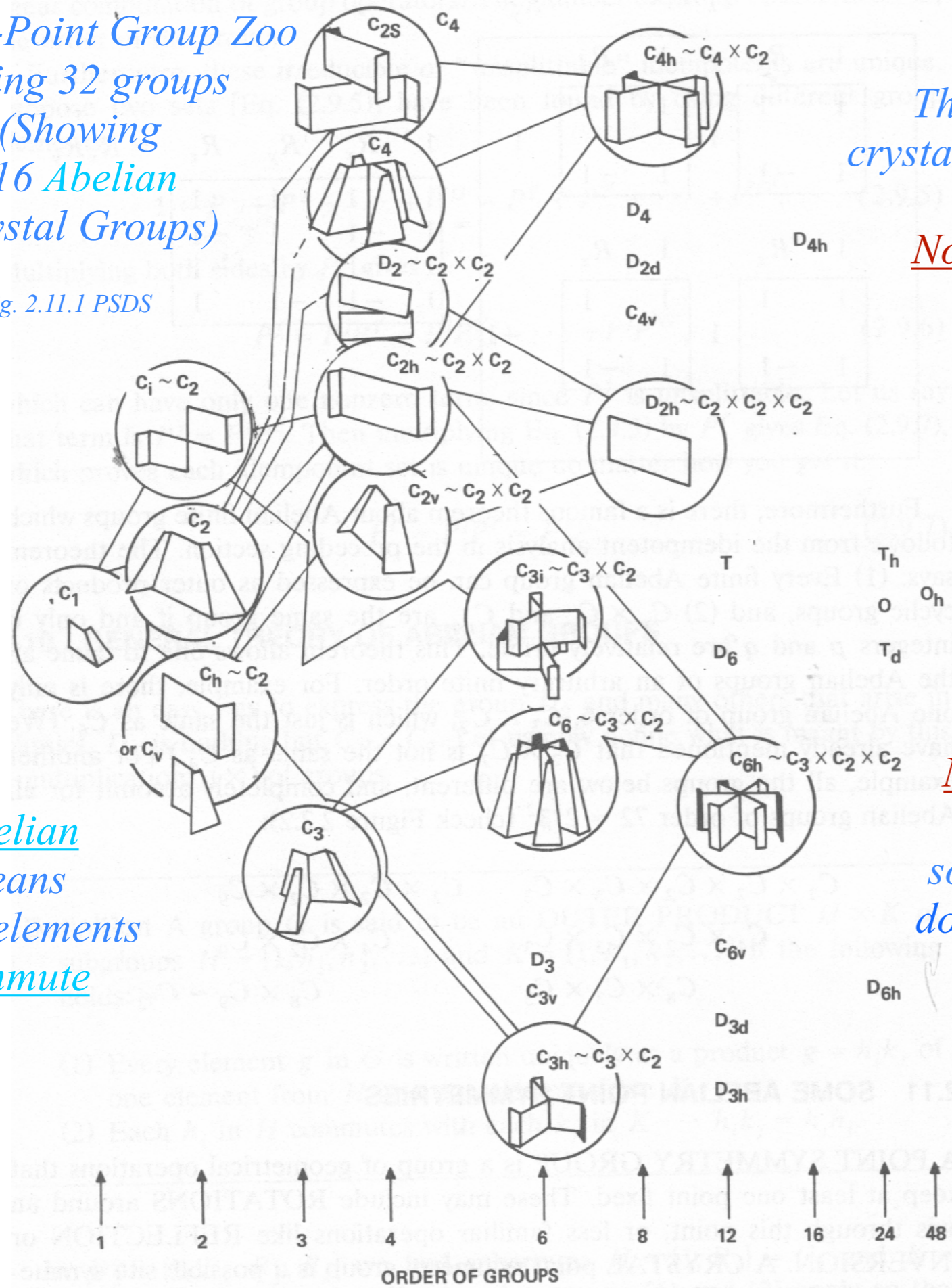
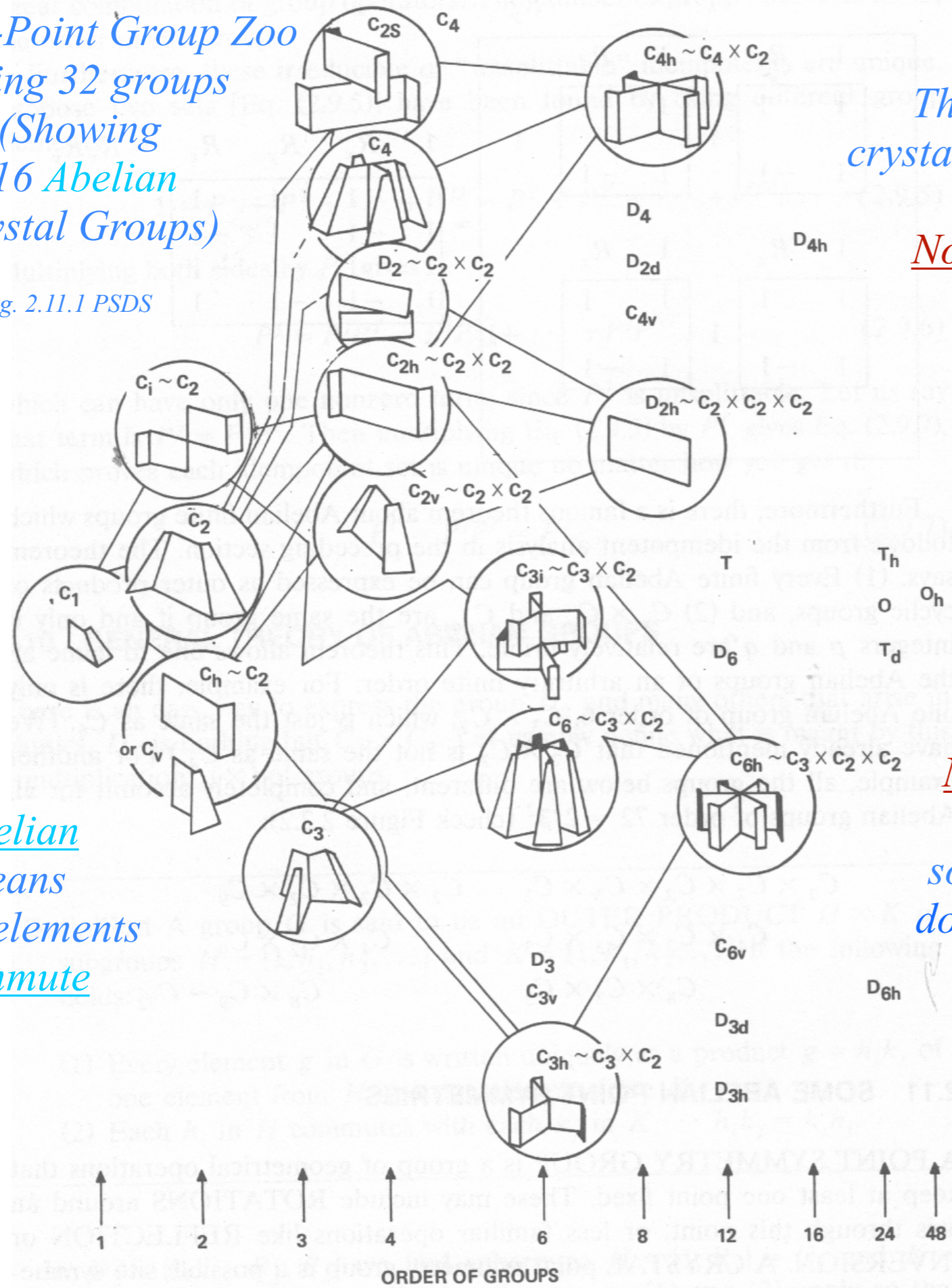


Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

Crystal-Point Group Zoo
 having 32 groups
 (Showing
 16 Abelian
 Crystal Groups)

Fig. 2.11.1 PSDS



The other 16
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 are
Non-Abelian

From p. 93-101
 Character Trace of
 n-fold rotation
 where: $\ell^j = 2j+1$
 is U(2) irrep dimension

$$\chi^j\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{\pi}{n}(2j+1)}{\sin\frac{\pi}{n}} = \frac{\sin\frac{\pi\ell^j}{n}}{\sin\frac{\pi}{n}}$$

Abelian
 means
 all its elements
 commute

Non-Abelian
 means
 some elements
 do not commute

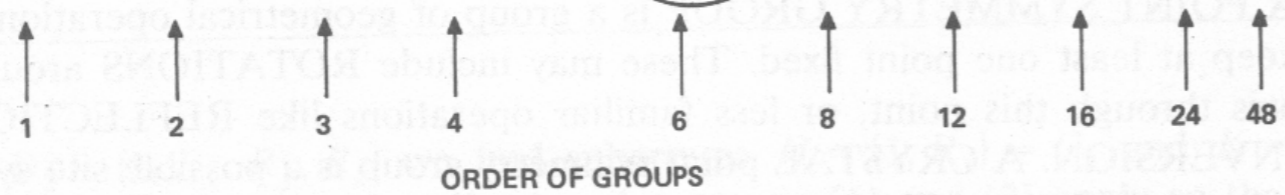
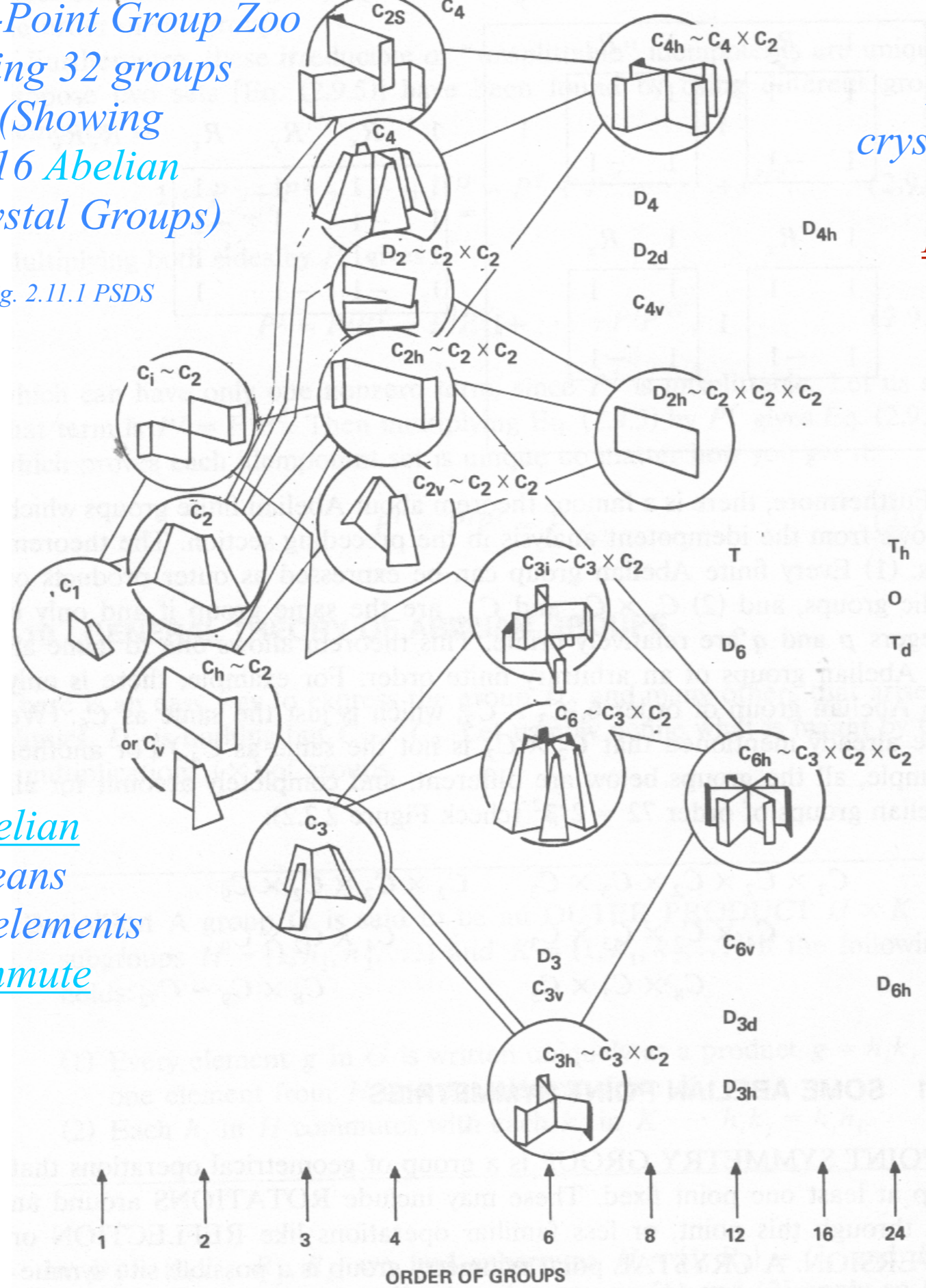


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To be a crystal-point group
 the Character Trace of
 n-fold vector rotation
 for: $\ell^1 = 2+1=3$
 must be an integer

$$\chi^1\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{\pi}{n}(2j+1)}{\sin\frac{\pi}{n}} = \frac{\sin\frac{3\pi}{n}}{\sin\frac{\pi}{n}} = \text{integer}$$

Non-Abelian
 means
 some elements
 do not commute

Abelian
 means
 all its elements
 commute

- $\frac{\sin\frac{3\pi}{2}}{\sin\frac{\pi}{2}} = -1$ (n=2 ok)
- $\frac{\sin\frac{3\pi}{3}}{\sin\frac{\pi}{3}} = +1$ (n=3 ok)
- $\frac{\sin\frac{3\pi}{4}}{\sin\frac{\pi}{4}} = +1$ (n=4 ok)
- $\frac{\sin\frac{3\pi}{5}}{\sin\frac{\pi}{5}} = G^+$ (n=5 NO!)
- $\frac{\sin\frac{3\pi}{6}}{\sin\frac{\pi}{6}} = +2$ (n=6 ok)

...But,
 n=7 to ∞
 are not ok

Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

*Crystal-Point Group Zoo
having 32 groups
(Showing
16 Abelian
Crystal Groups)*

Fig. 2.11.1 PSDS

Abelian
means
all its elements
commute

The other 16
crystal-point groups
are
Non-Abelian

Non-Abelian
means
some elements
do not commute

Log-histogram of
all groups of order
 $^{\circ}G=1$ to 64

Abelian shown in **Black**
Non-Abelian in White

Group "census"

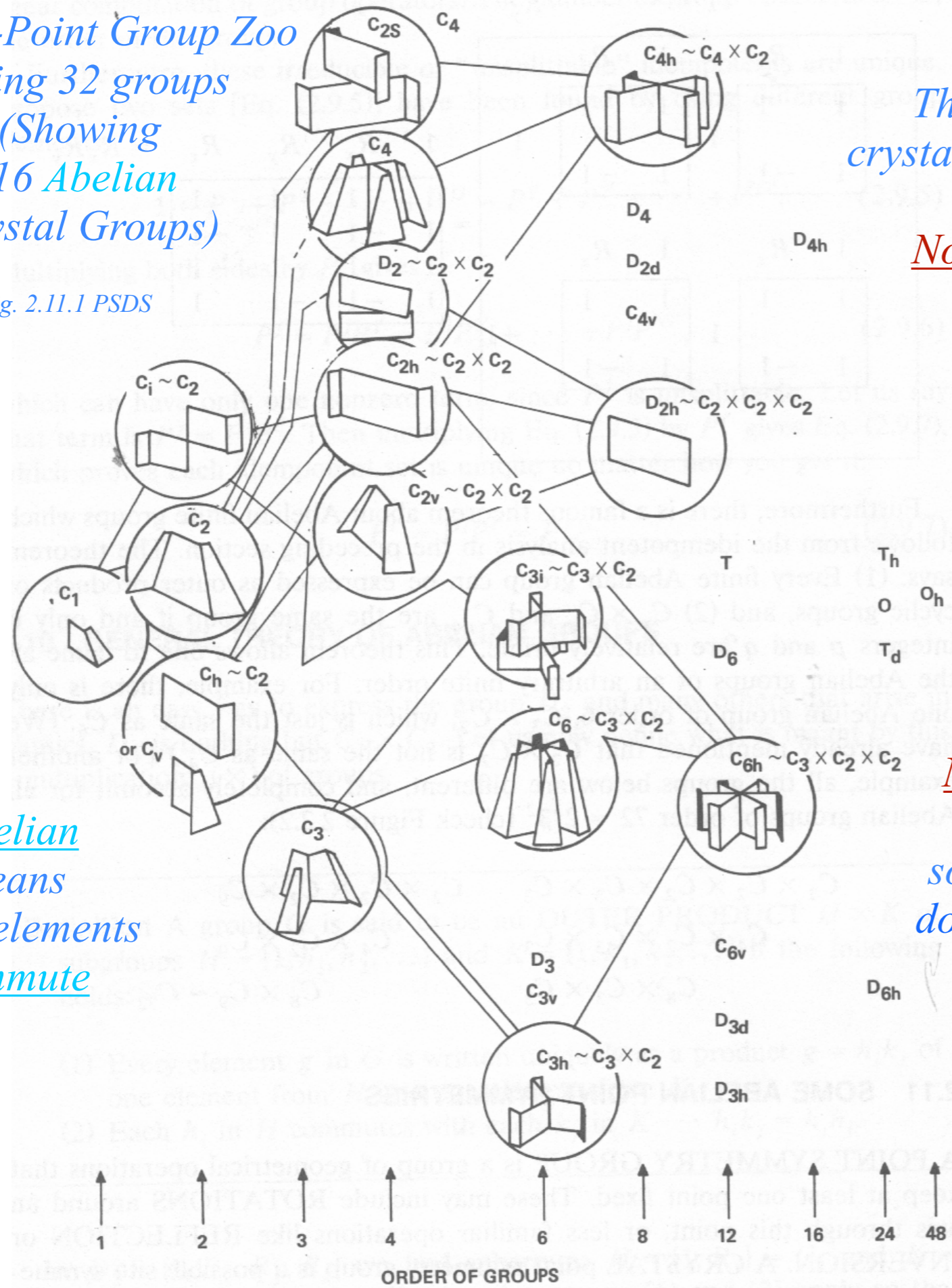
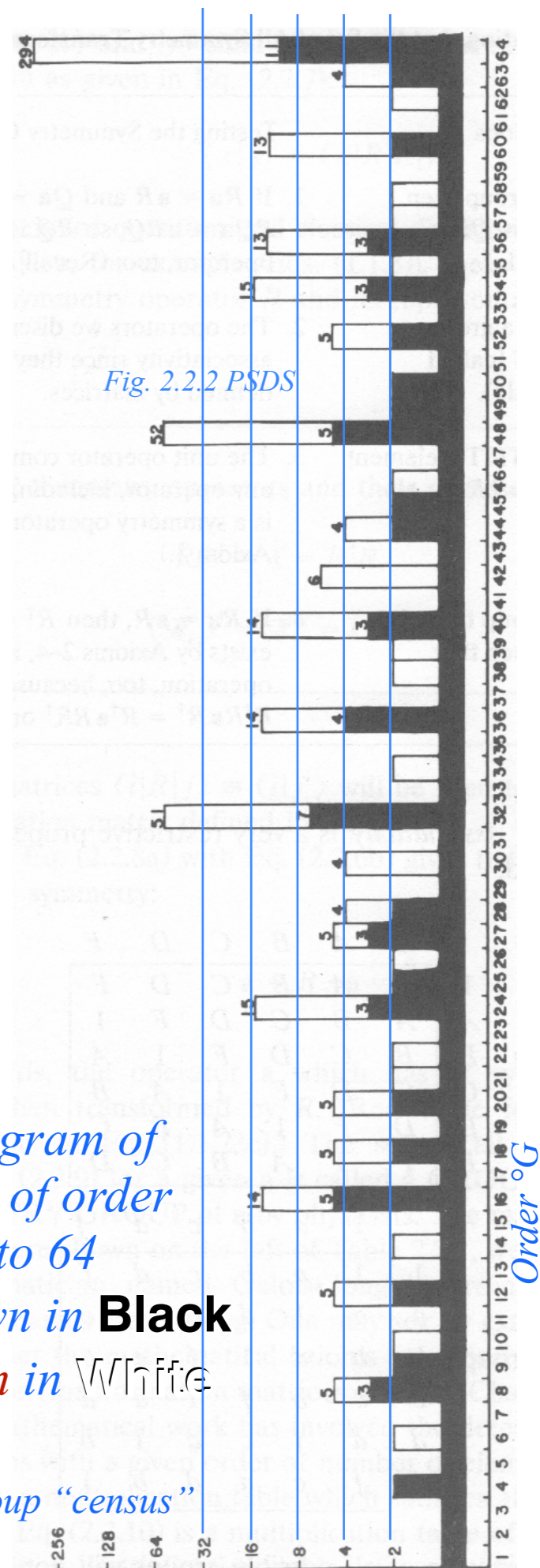


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*Crystal-Point Group Zoo
having 32 groups
(Showing
16 Non-Abelian
Crystal Groups)*

*The other 16
crystal-point groups
are
Abelian*

*Abelian
means
all its elements
commute*

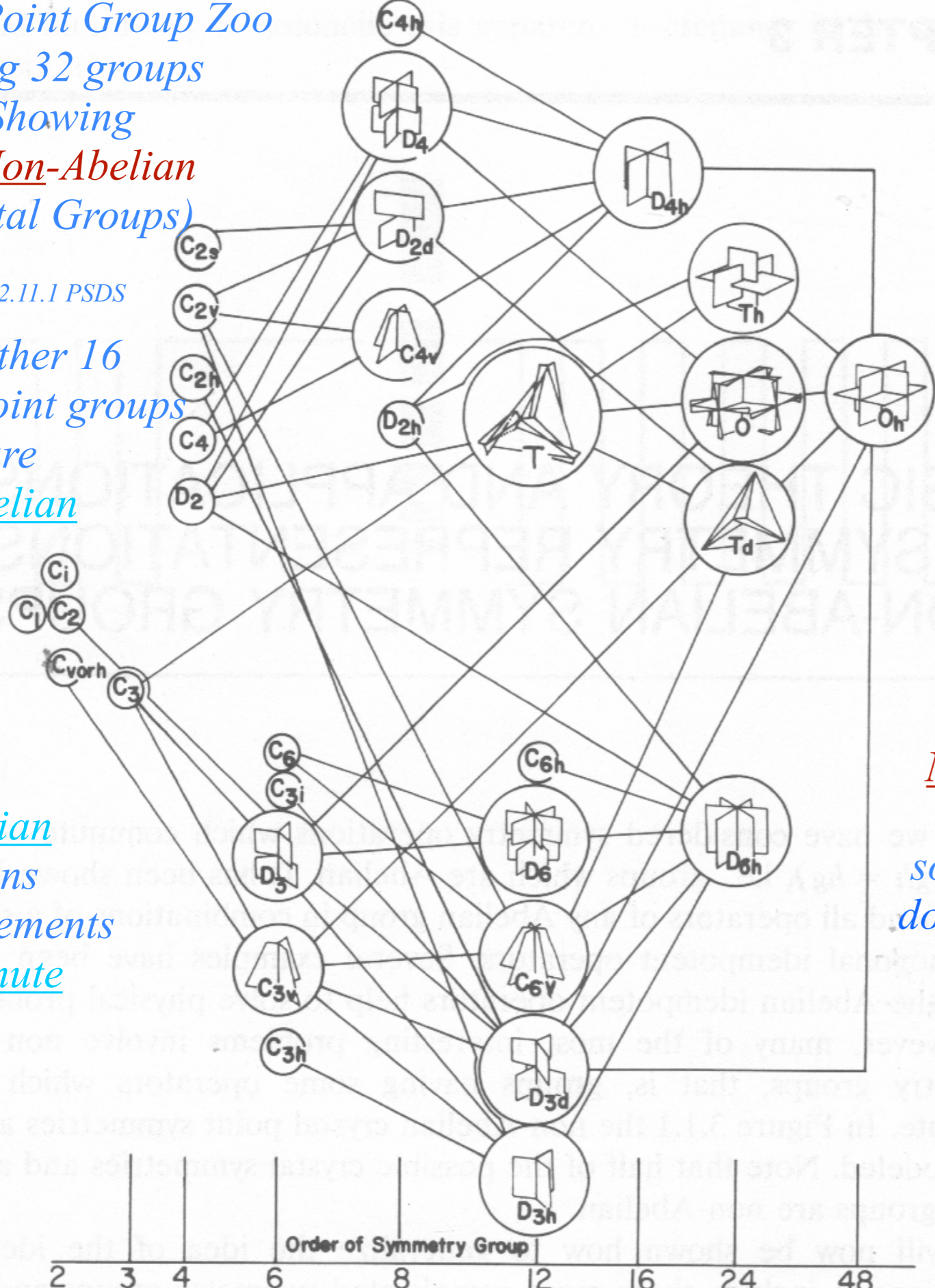


Figure 3.1.1 Crystal point symmetry groups. Models are sketched in circles for the 16 non-Abelian groups. (See also Figure 2.11.1.)

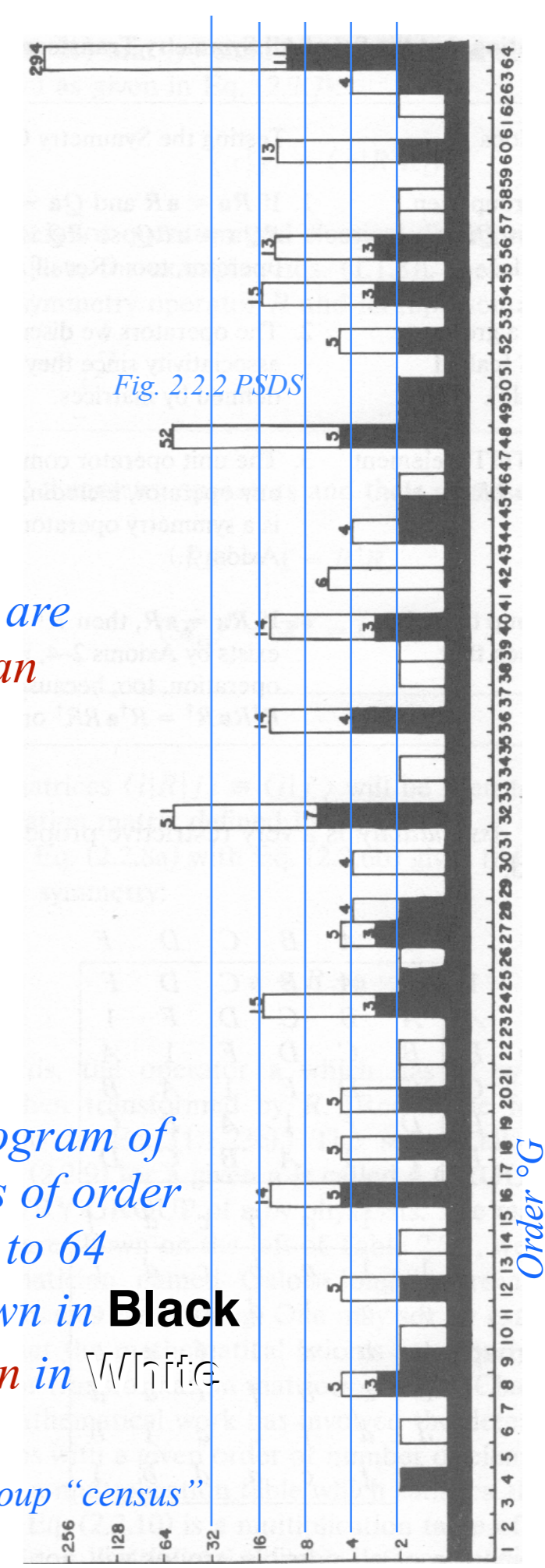


Fig. 2.2.2 PSDS

*Clearly
most groups are
Non-Abelian*

*Non-Abelian
means
some elements
do not commute*

*Log-histogram of
all groups of order
°G=1 to 64
Abelian shown in Black
Non-Abelian in White*

Group "census"

C_6 is product $C_3 \times C_2$ (but C_4 is NOT $C_2 \times C_2$)

C_3	1	r	r²	×	C_2	1	R	=	$C_3 \times C_2$	1	r	r²	1 · R	r · R	r² · R
$(0)_3$	1	1	1		$(0)_2$	1	1		$(0)_3 \cdot (0)_2$	1 · 1	1 · 1	1 · 1	1 · 1	1 · 1	1 · 1
$(1)_3$	1	$e^{2\pi i/3}$	$e^{-2\pi i/3}$		$(1)_2$	1	-1		$(1)_3 \cdot (0)_2$	1 · 1	$e^{2\pi i/3} \cdot 1$	$e^{-2\pi i/3} \cdot 1$	1 · 1	$e^{2\pi i/3} \cdot 1$	$e^{-2\pi i/3} \cdot 1$
$(2)_3$	1	$e^{-2\pi i/3}$	$e^{2\pi i/3}$						$(2)_3 \cdot (0)_2$	1 · 1	$e^{-2\pi i/3} \cdot 1$	$e^{2\pi i/3} \cdot 1$	1 · 1	$e^{-2\pi i/3} \cdot 1$	$e^{2\pi i/3} \cdot 1$
							$(0)_3 \cdot (1)_2$	1 · 1	1 · 1	1 · 1	1 · (-1)	1 · (-1)	1 · (-1)		
							$(1)_3 \cdot (1)_2$	1 · 1	1 · 1	$e^{-2\pi i/3} \cdot 1$	1 · (-1)	$e^{2\pi i/3} \cdot (-1)$	$e^{-2\pi i/3} \cdot (-1)$		
							$(2)_3 \cdot (1)_2$	1 · 1	$e^{-2\pi i/3} \cdot 1$	1 · 1	1 · (-1)	$e^{-2\pi i/3} \cdot (-1)$	$e^{2\pi i/3} \cdot (-1)$		

C_6 is product $C_3 \times C_2$ (but C_4 is NOT $C_2 \times C_2$)

C_3	1	r	r²	×	C_2	1	R	=	$C_3 \times C_2$	1	r	r²	1 · R	r · R	r² · R	
$(0)_3$	1	1	1		$(0)_2$	1	1		$(0)_3 \cdot (0)_2$	1 · 1	1 · 1	1 · 1	1 · 1	1 · 1	1 · 1	1 · 1
$(1)_3$	1	$e^{2\pi i/3}$	$e^{-2\pi i/3}$		$(1)_2$	1	-1		$(1)_3 \cdot (0)_2$	1 · 1	$e^{2\pi i/3} \cdot 1$	$e^{-2\pi i/3} \cdot 1$	$e^{2\pi i/3} \cdot 1$	$e^{-2\pi i/3} \cdot 1$	$e^{2\pi i/3} \cdot 1$	$e^{-2\pi i/3} \cdot 1$
$(2)_3$	1	$e^{-2\pi i/3}$	$e^{2\pi i/3}$		$(1)_2$	1	-1		$(2)_3 \cdot (0)_2$	1 · 1	$e^{-2\pi i/3} \cdot 1$	$e^{2\pi i/3} \cdot 1$	$e^{-2\pi i/3} \cdot 1$	$e^{2\pi i/3} \cdot 1$	1 · (-1)	1 · (-1)
							$(0)_3 \cdot (1)_2$	1 · 1	1 · 1	1 · 1	1 · (-1)	1 · (-1)	1 · (-1)	1 · (-1)	1 · (-1)	
							$(1)_3 \cdot (1)_2$	1 · 1	1 · 1	$e^{-2\pi i/3} \cdot 1$	1 · (-1)	$e^{2\pi i/3} \cdot (-1)$	$e^{-2\pi i/3} \cdot (-1)$	$e^{2\pi i/3} \cdot (-1)$	$e^{-2\pi i/3} \cdot (-1)$	
							$(2)_3 \cdot (1)_2$	1 · 1	$e^{-2\pi i/3} \cdot 1$	1 · 1	1 · (-1)	$e^{-2\pi i/3} \cdot (-1)$	$e^{2\pi i/3} \cdot (-1)$	$e^{2\pi i/3} \cdot (-1)$	$e^{2\pi i/3} \cdot (-1)$	

$C_3 \times C_2 = C_6$	1	r = h²	r² = h⁴	R = h³	r · R = h	r² · R = h⁵
$(0)_3 \cdot (0)_2 = (0)_6$	1	1	1	1	1	1
$(1)_3 \cdot (0)_2 = (2)_6$	1	$e^{2\pi i/3}$	$e^{-2\pi i/3}$	1	$e^{2\pi i/3}$	$e^{-2\pi i/3}$
$(2)_3 \cdot (0)_2 = (4)_6$	1	$e^{-2\pi i/3}$	$e^{2\pi i/3}$	1	$e^{-2\pi i/3}$	$e^{2\pi i/3}$
$(0)_3 \cdot (1)_2 = (3)_6$	1	1	1	-1	-1	-1
$(1)_3 \cdot (1)_2 = (5)_6$	1	$e^{2\pi i/3}$	$e^{-2\pi i/3}$	-1	$-e^{2\pi i/3}$	$-e^{-2\pi i/3}$
$(2)_3 \cdot (1)_2 = (1)_6$	1	$e^{-2\pi i/3}$	$e^{2\pi i/3}$	-1	$-e^{-2\pi i/3}$	$-e^{2\pi i/3}$

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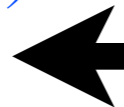
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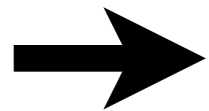
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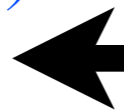
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Subtracting gives:

$$\chi^j(\Theta)(1 - e^{-i\Theta}) = -e^{-i\Theta(j+1)} + e^{+i\Theta j}$$

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For C_n angle $\Theta=2\pi/n$ this χ^j has a lot of geometric significance.

$$\chi^j\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{\pi}{n}(2j+1)}{\sin\frac{\pi}{n}} = \frac{\sin\frac{\pi\ell^j}{n}}{\sin\frac{\pi}{n}}$$

Character Spectral Function
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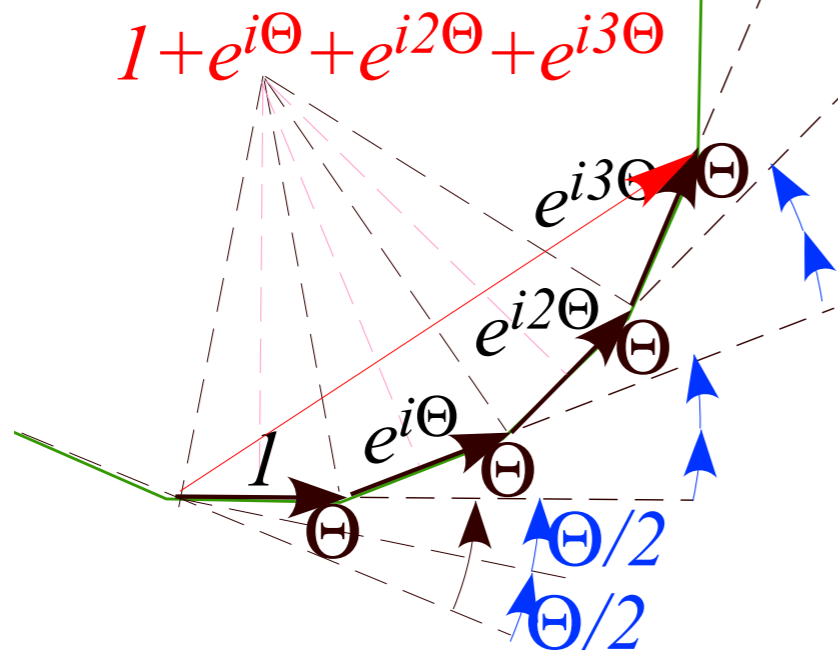
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Algebra



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$$\chi^j\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{\pi}{n}(2j+1)}{\sin\frac{\pi}{n}} = \frac{\sin\frac{\pi\ell^j}{n}}{\sin\frac{\pi}{n}}$$

Character Spectral Function
where: $\ell^j = 2j+1$
is $U(2)$ irrep dimension

$(j)^{th}$ n -gon segments

$$\chi^j(2\pi/n) = \sin\left(\frac{\pi}{n}\ell^j\right) / \sin\frac{\pi}{n}$$

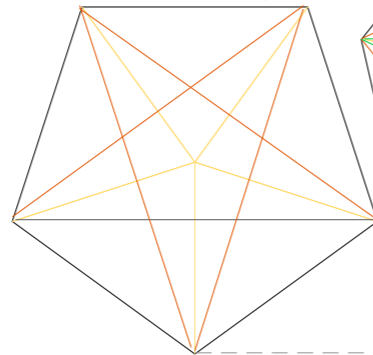
$$\ell^j = 2j+1$$

$$n = 7$$

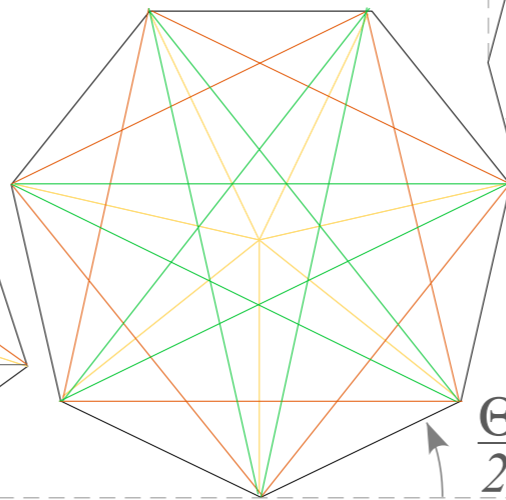
$$\ell^j = 1, 2, 3$$

$$n = 5$$

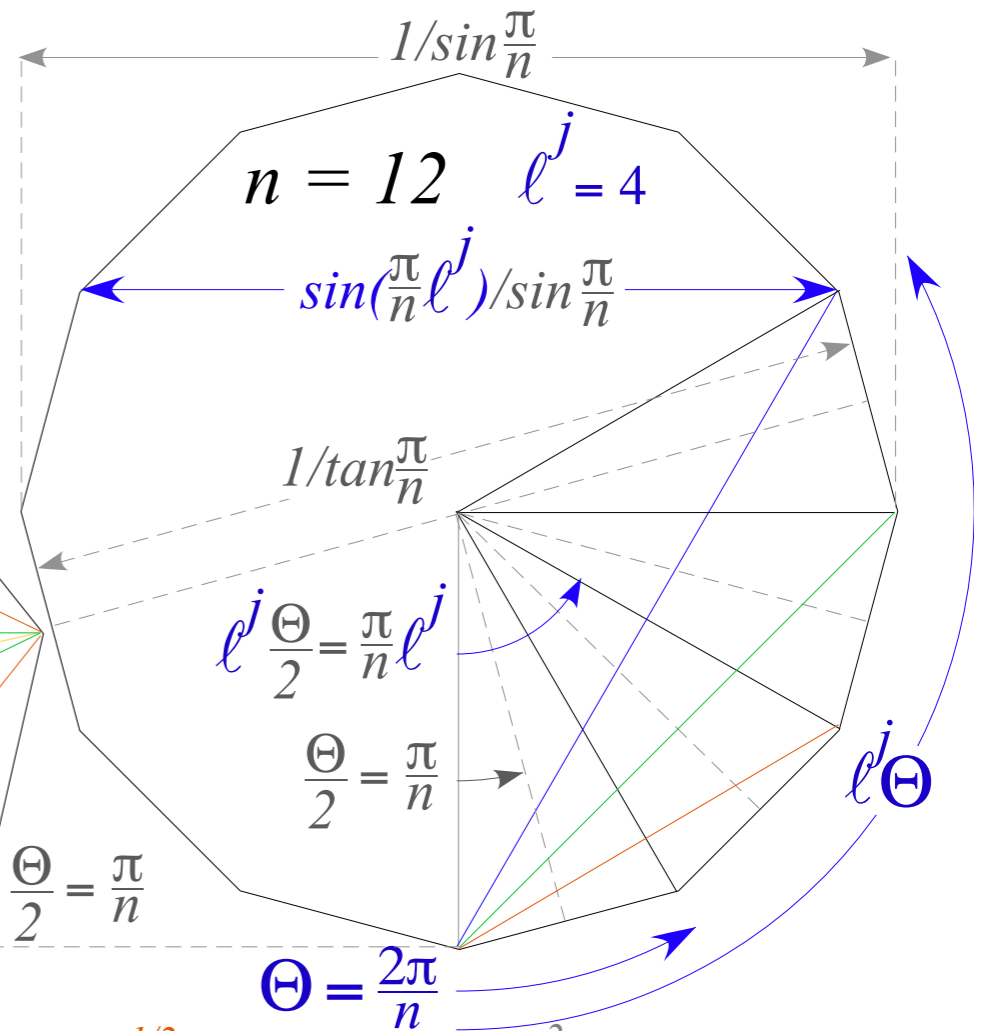
$$\ell^j = 1, 2$$



$$\begin{aligned} \chi^0(2\pi/5) &= 1 \\ \chi^{1/2}(2\pi/5) &= 1.618... \\ &= (1+\sqrt{5})/2 = \end{aligned}$$



$$\begin{aligned} \chi^0(2\pi/7) &= 1 \\ \chi^{1/2}(2\pi/7) &= 1.802... \\ \chi^1(2\pi/7) &= 2.247... \\ \chi^{3/2}(2\pi/7) &= 2.247... \end{aligned}$$

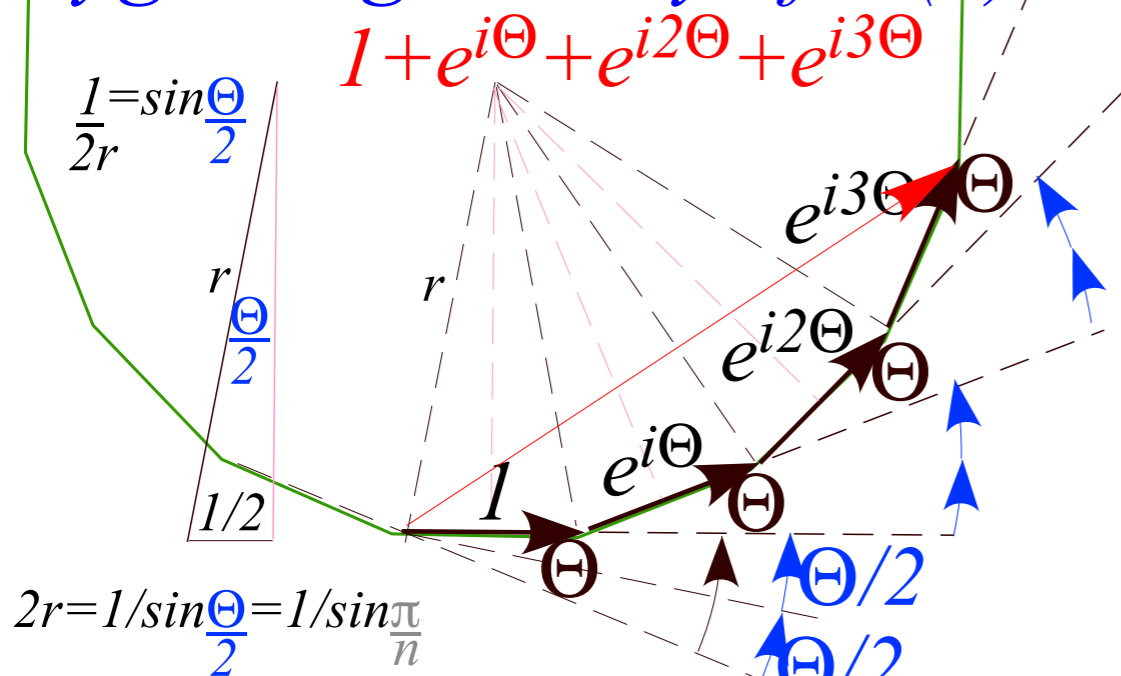


$$\begin{aligned} \chi^{1/2}(2\pi/12) &= 1.932... & \chi^2(2\pi/12) &= 3.732... \\ \chi^1(2\pi/12) &= 2.732... & \chi^{5/2}(2\pi/12) &= 3.864... \\ \chi^{3/2}(2\pi/12) &= 3.346... & \chi^3(2\pi/12) &= 3.732... \end{aligned}$$

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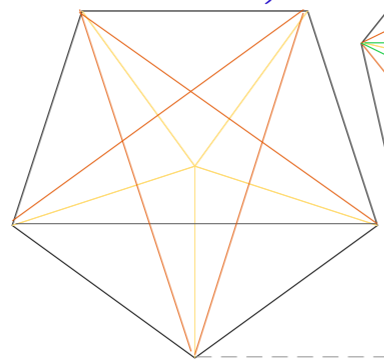
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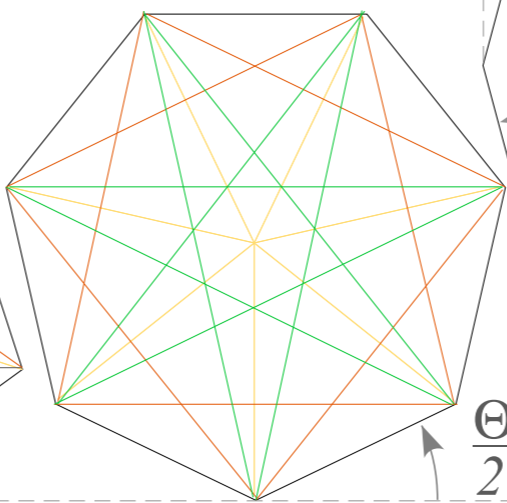
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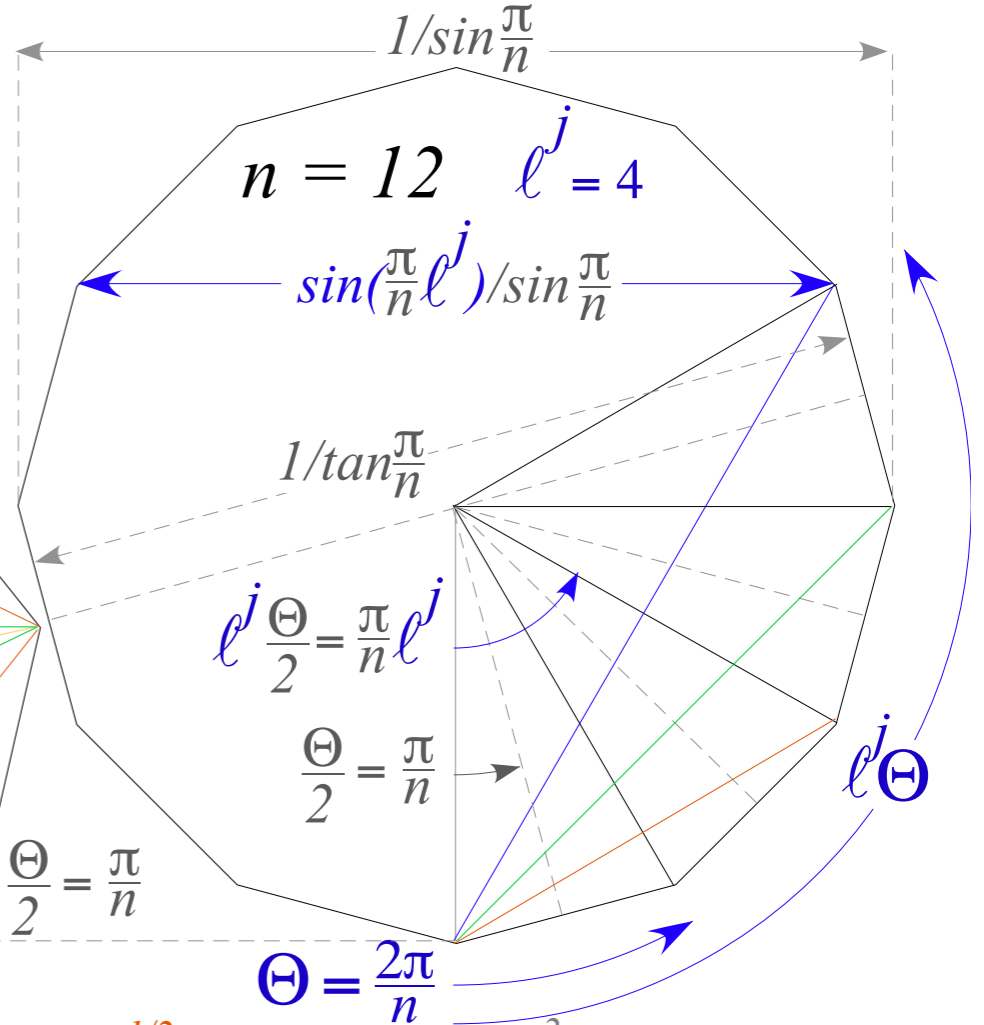


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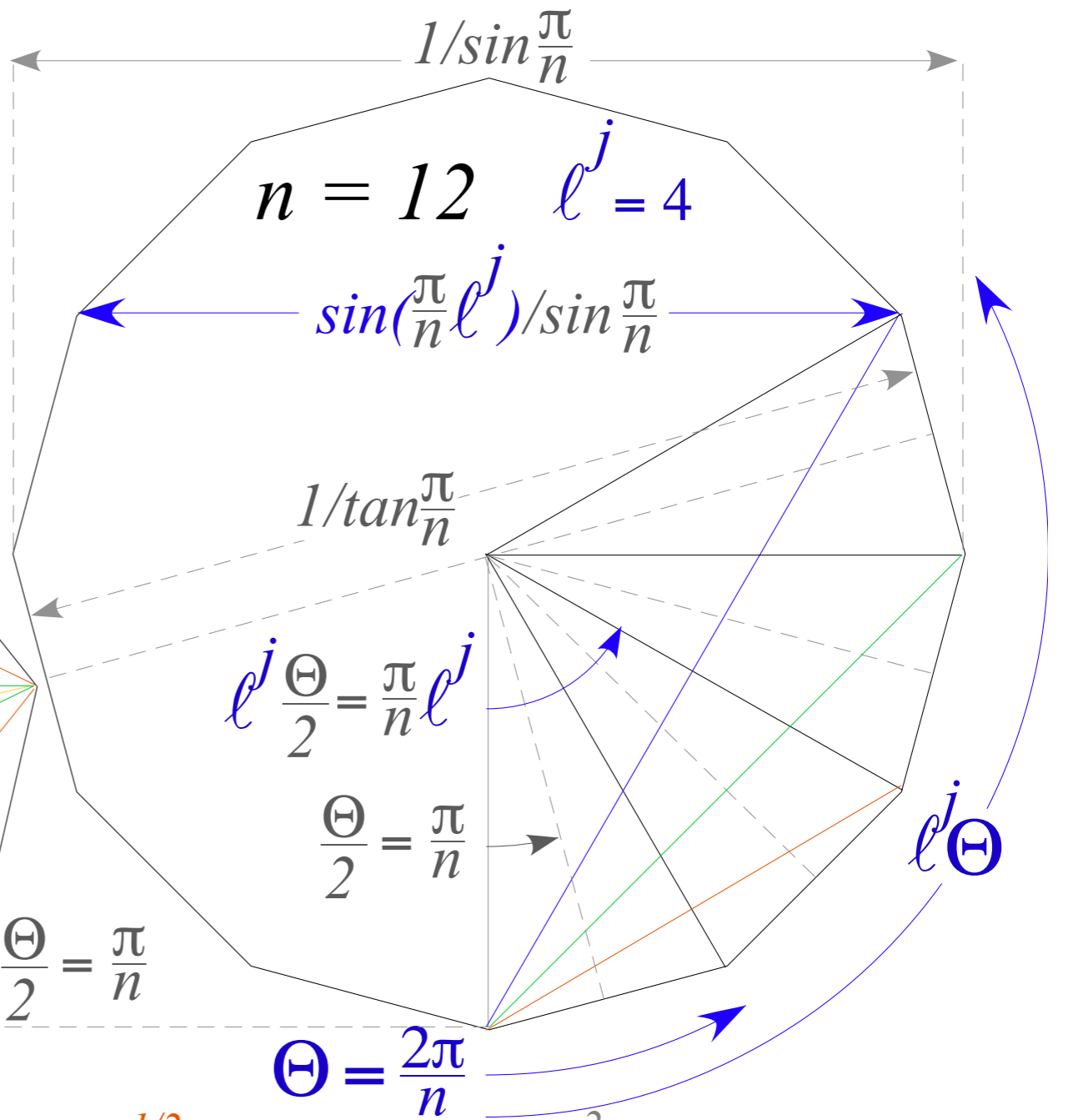
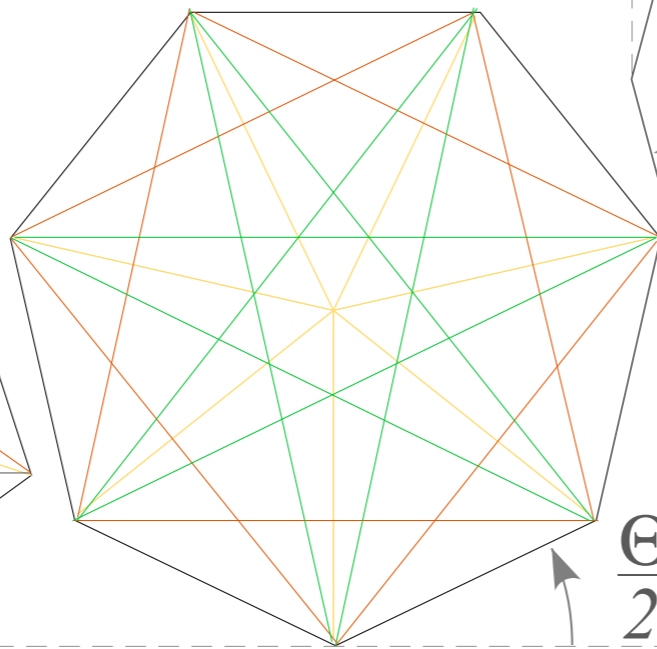
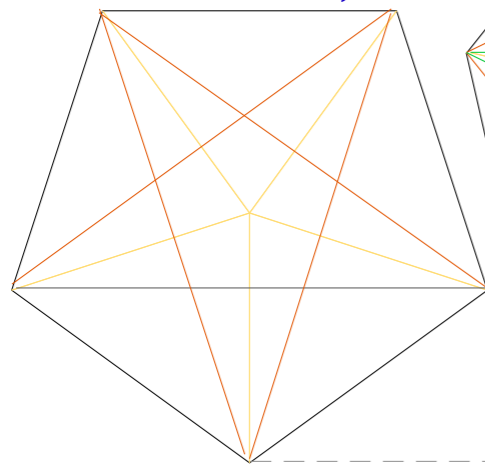
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$$\Theta = \frac{2\pi}{n}$$

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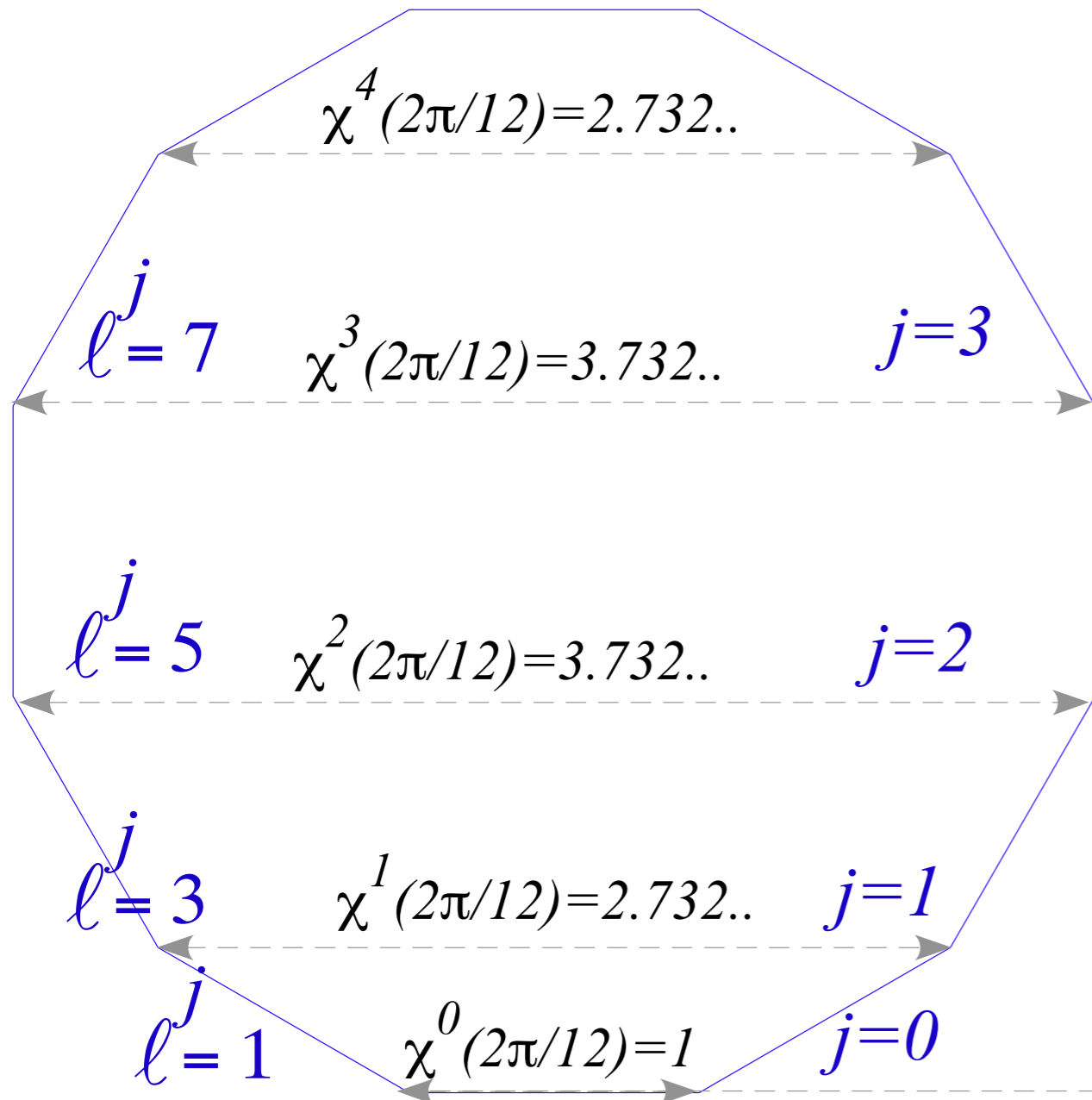
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Integer j for $n=12$

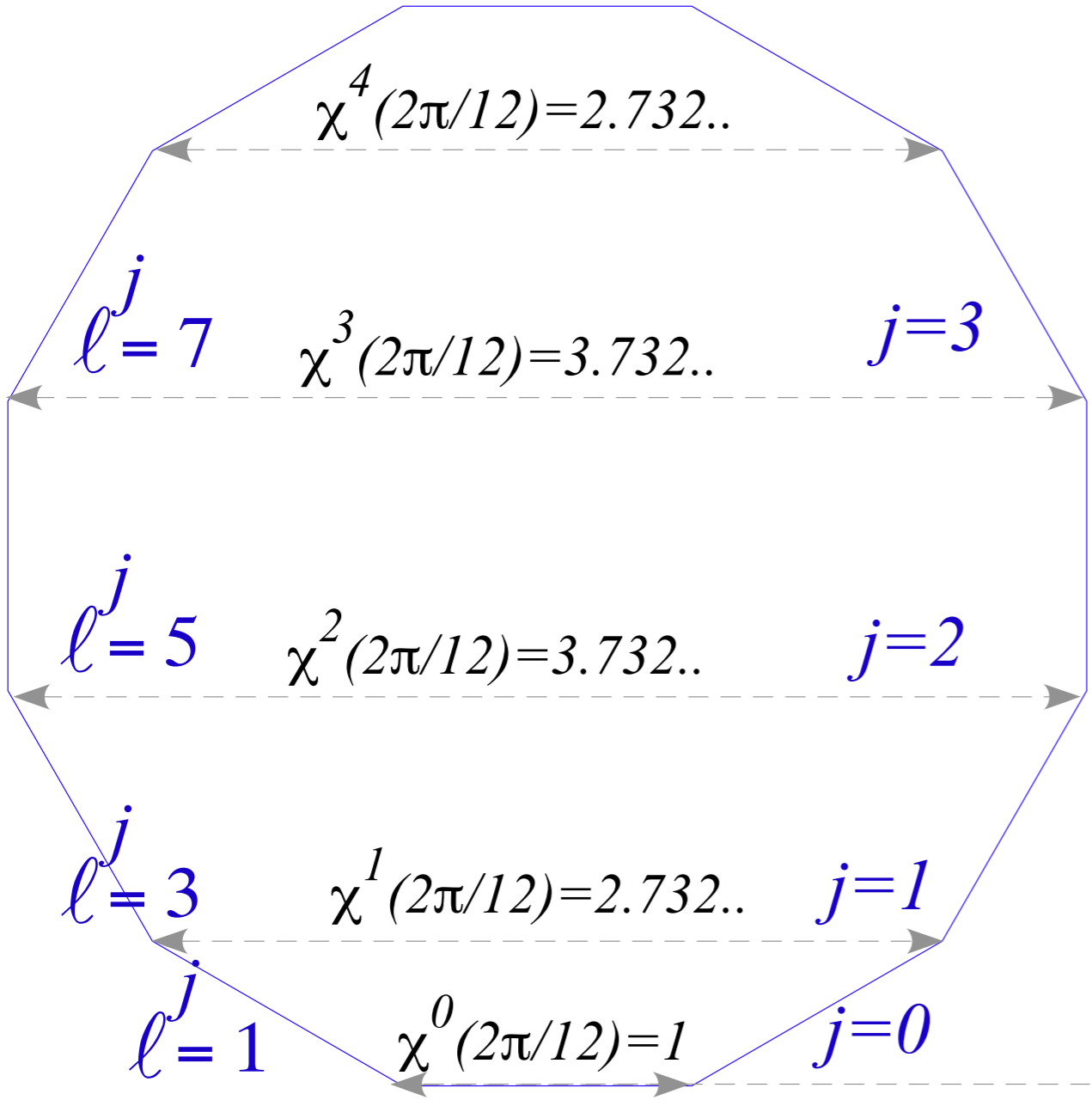


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1/2-Integer j for $n=12$

