Group Theory in Quantum Mechanics

Lecture 13 (3.05.15)

C_N symmetry systems coupled, uncoupled, and re-coupled

(Geometry of U(2) characters - Ch. 6-12 of Unit 3)

(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 (and review of revival)
  - ∞-Square well paths analyzed using Bohr rotor paths
- Breaking C_{2N+2} to approximate linear N-chain
  - Band-It simulation: Intro to scattering approach to quantum symmetry

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 "4-Group(s)" D_2 and C_{2v}
- Spectral decomposition of D_2
  - Some D_2 modes
- Outer product properties and the Crystal-Point Group Zoo

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Spectral decomposition of D_2

Some D_2 modes

Outer product properties and the Group Zoo

Review: ∞-*Square well PE & Bohr rotor*

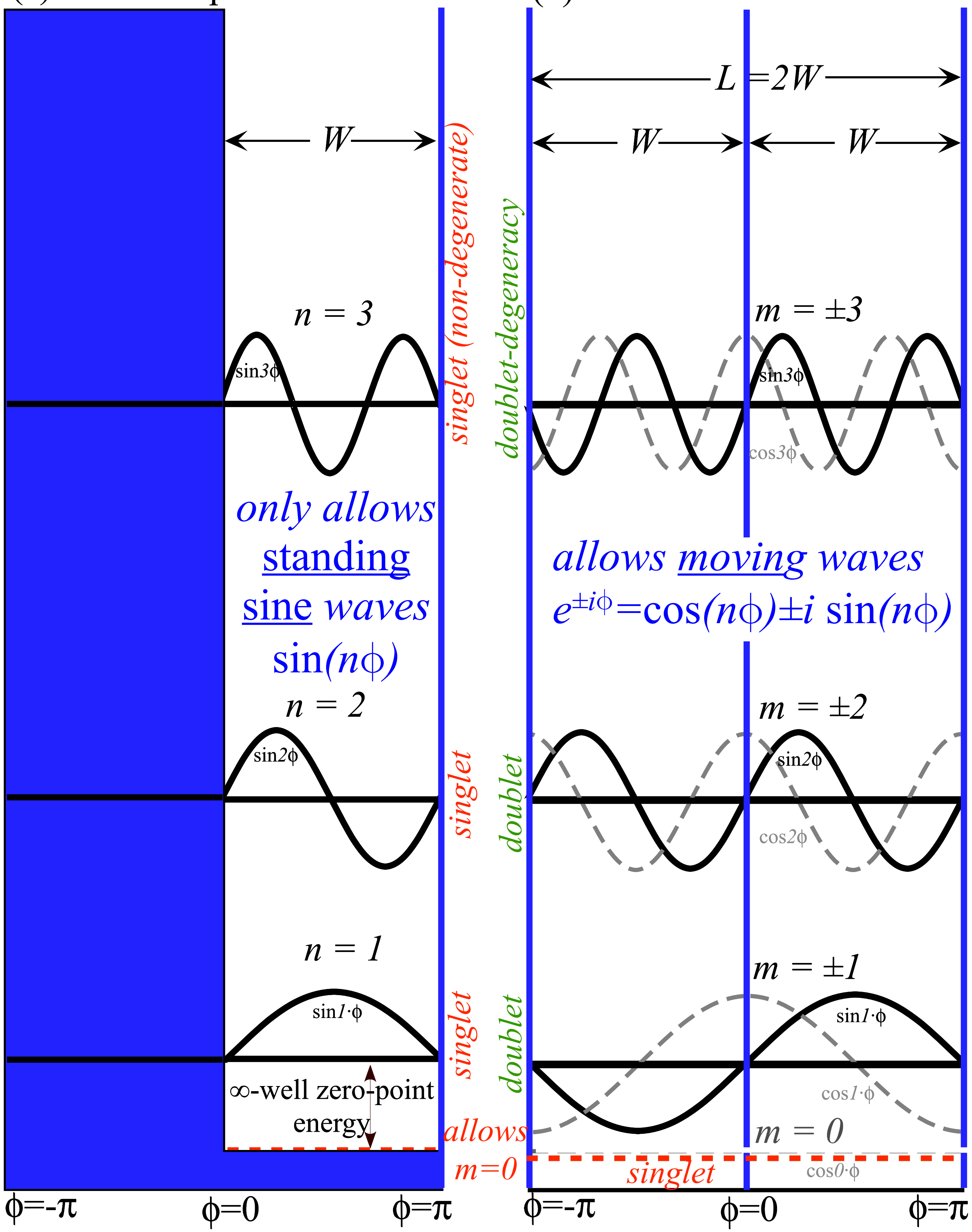
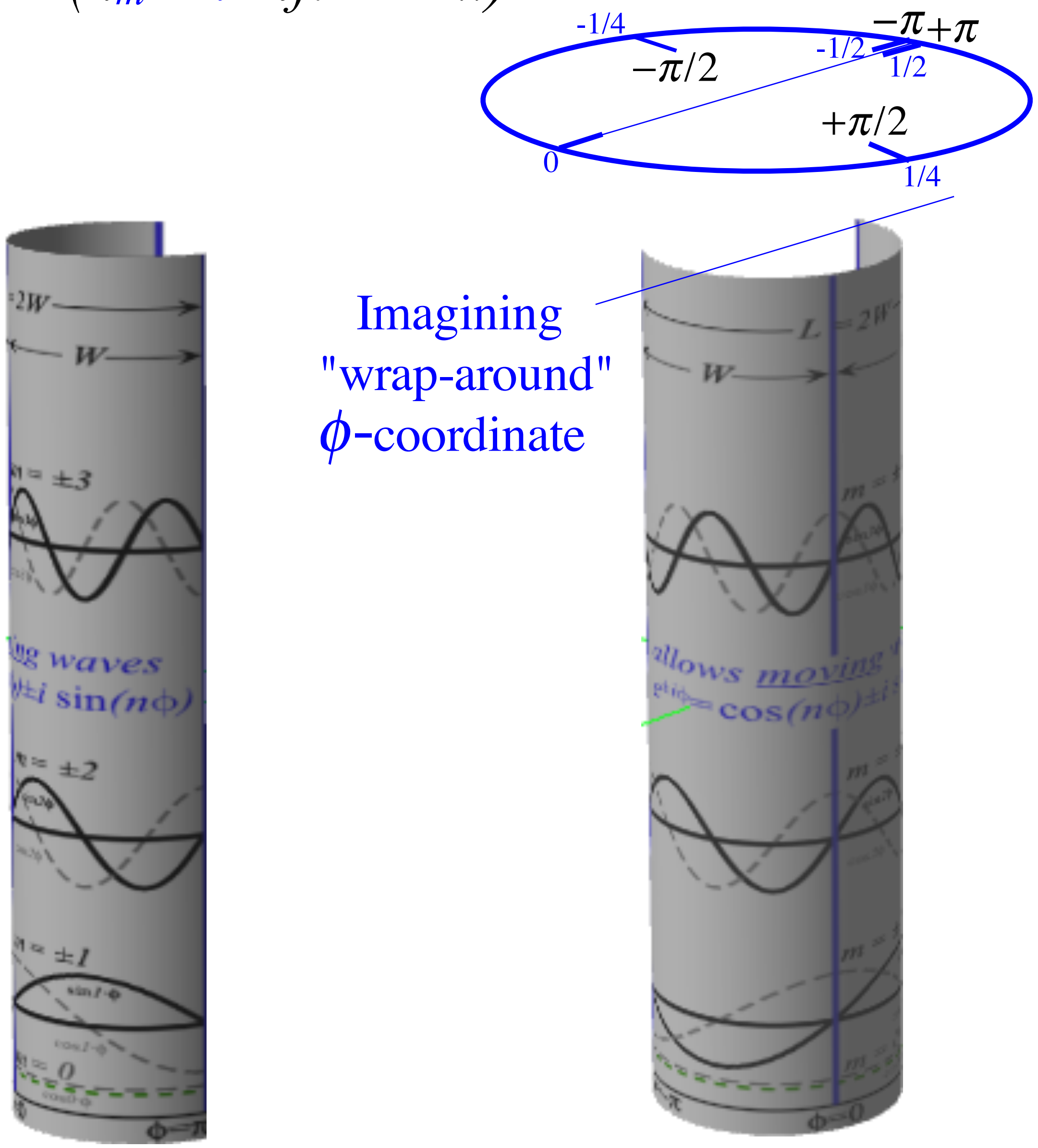


Fig. 12.2.6 Comparison of eigensolutions for (a) Infinite square well, and (b) Bohr rotor.

From QTCA Unit 5 Ch. 12

m=0, ±1, ±2, ±3,...are momentum quanta in wavevector formula: $k_m=2\pi m/L$

($k_m=m$ *if:* $L=2\pi$)



Review: ∞-Square well PE & Bohr rotor

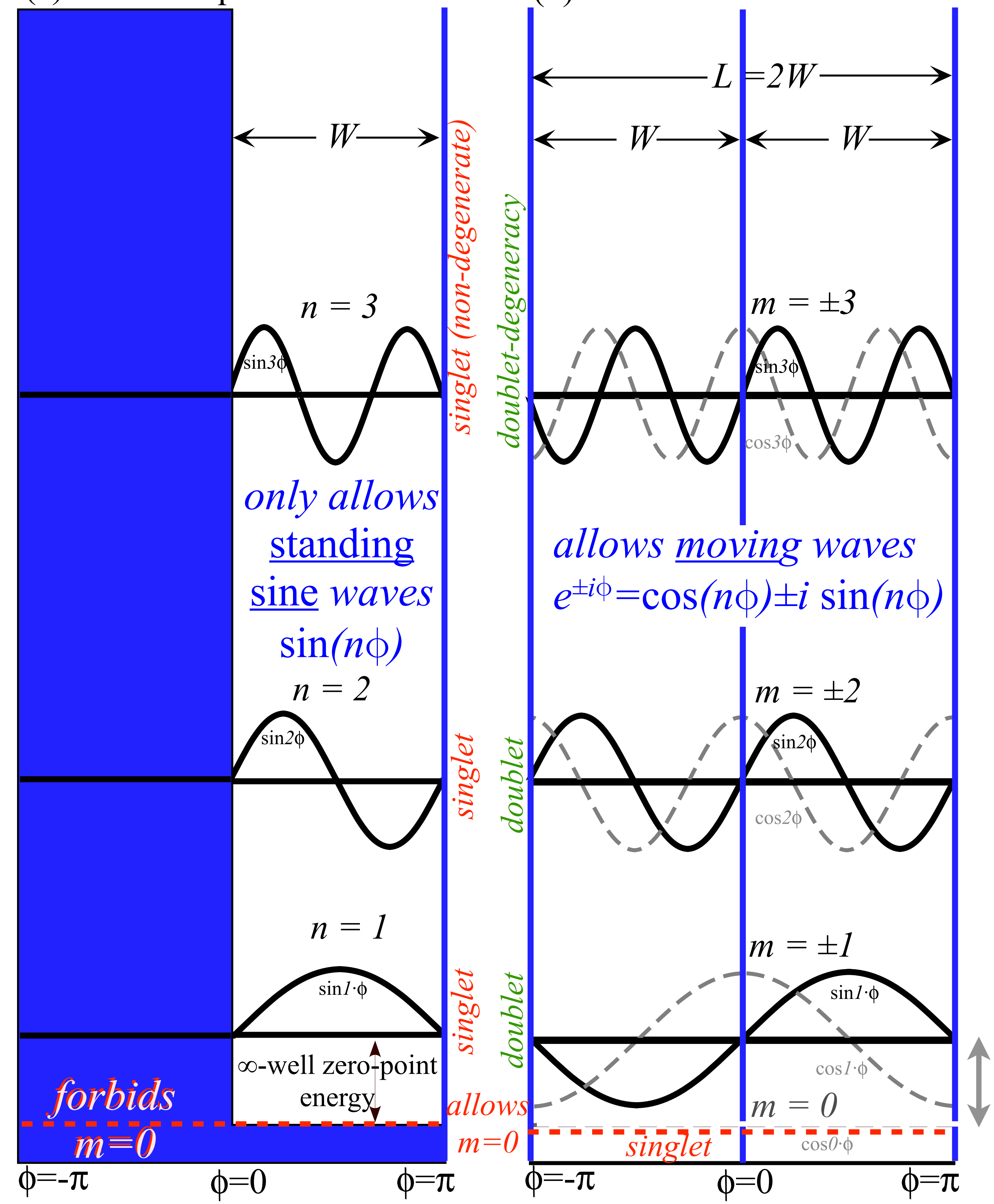


Fig. 12.2.6 Comparison of eigensolutions for (a) Infinite square well, and (b) Bohr rotor.

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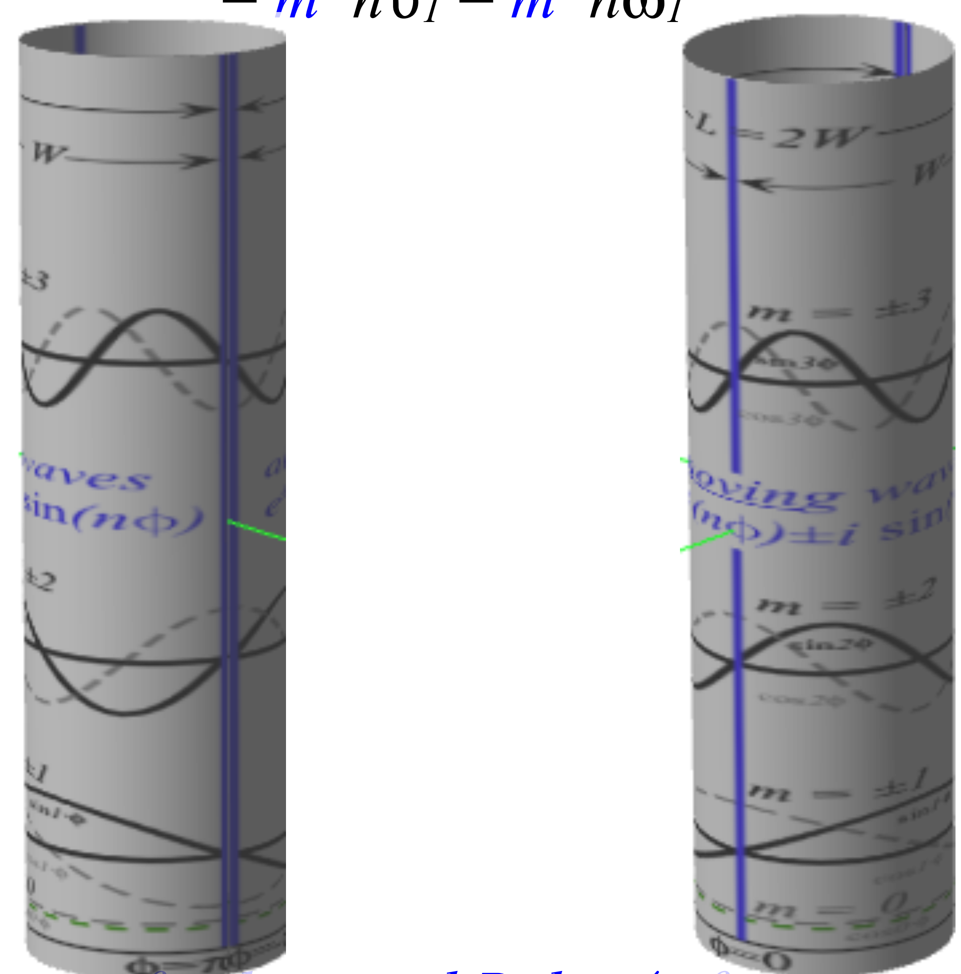
$m=0, \pm1, \pm2, \pm3$,...are momentum quanta in wavevector formula: $k_m=2\pi m/L$

($k_m=m$ if: $L=2\pi$)

$E_m= (\hbar k_m)^2/2M = m^2[h^2/2ML^2]$

$= m^2\, h\upsilon_1 = m^2\, \hbar\omega_1$



fundamental Bohr ∠−frequency

$\omega_1=2\pi\upsilon_1$

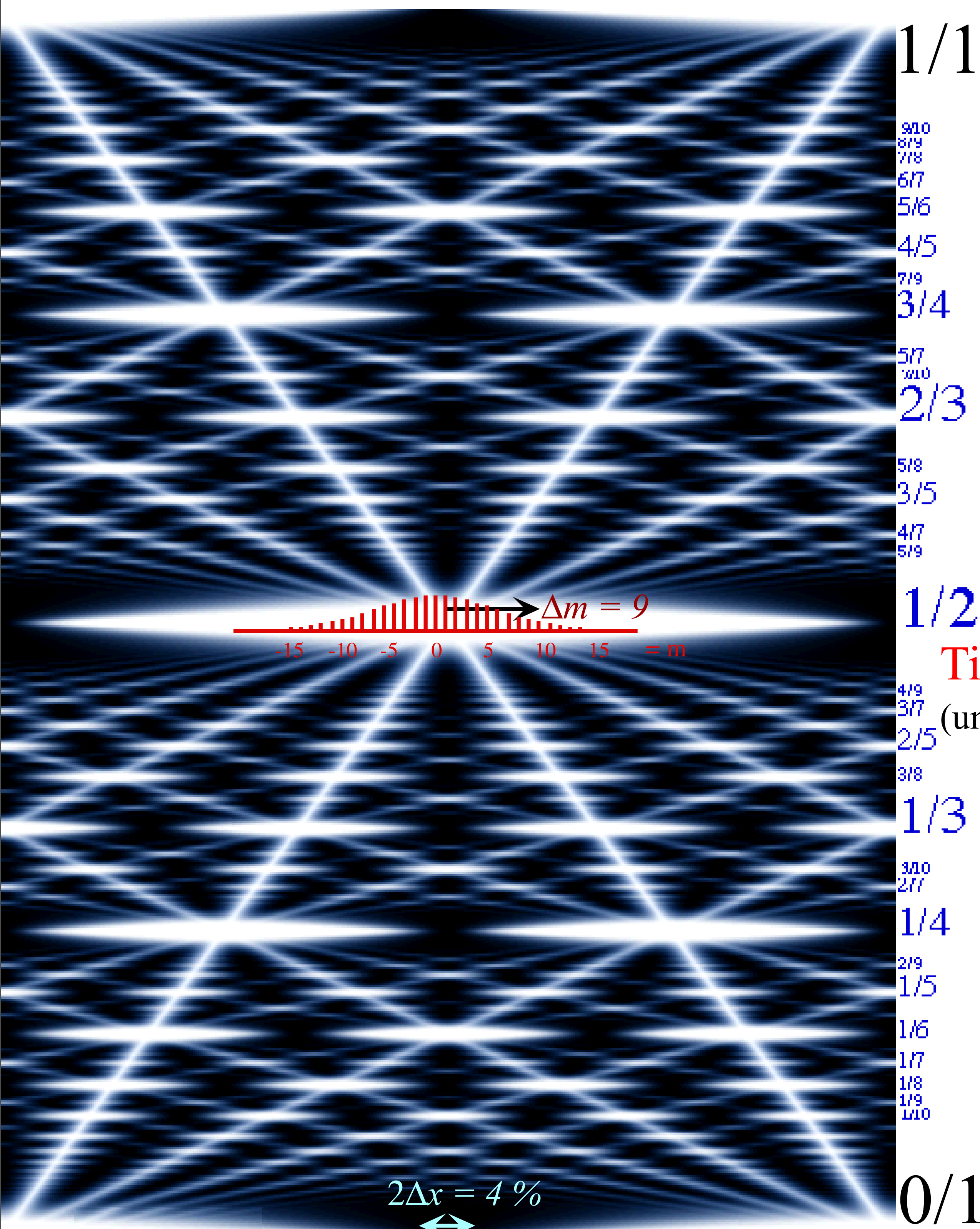
lowest *transition (beat) frequency*

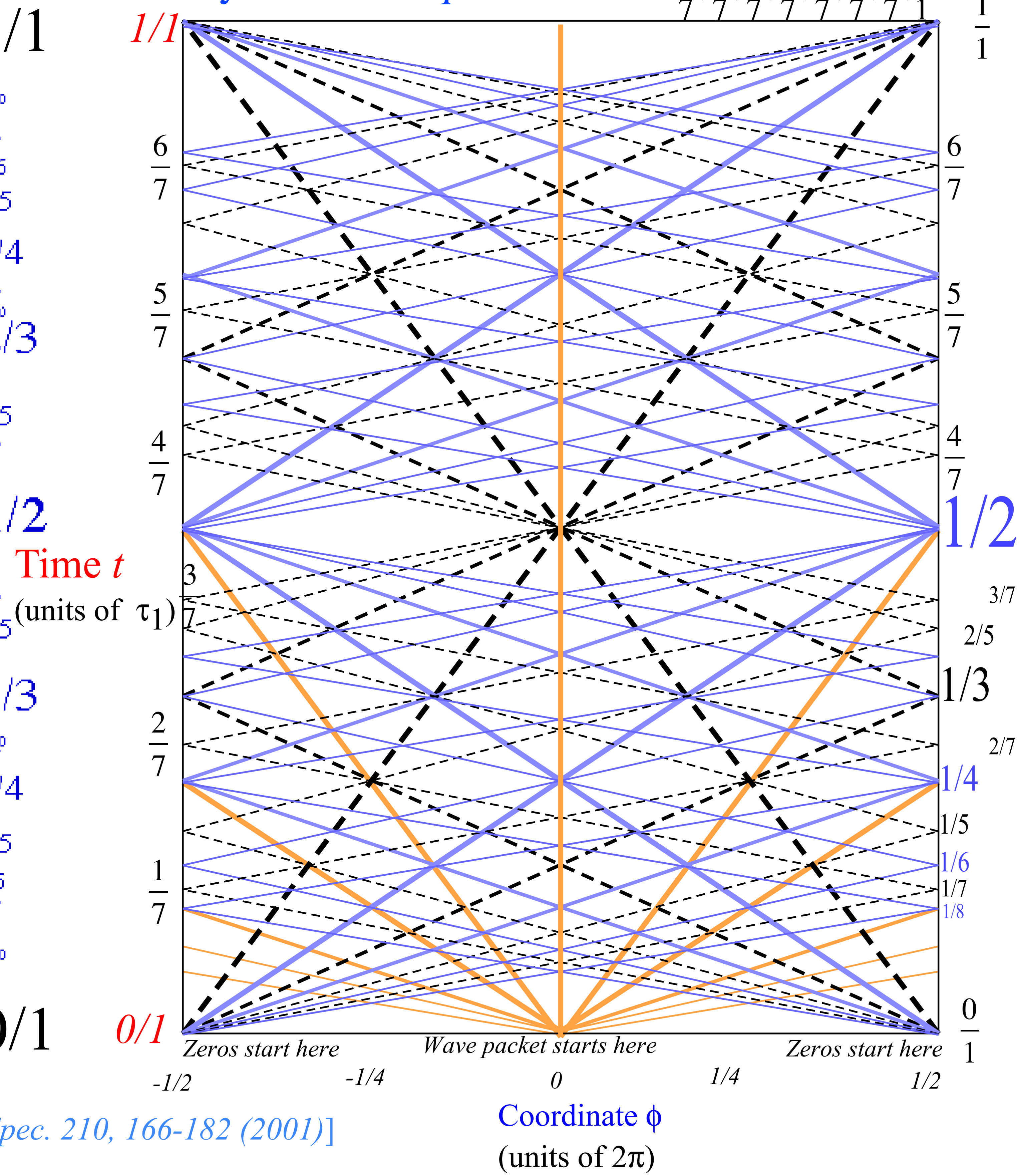
$\upsilon_1 =(E_1-E_0)/h$ (E_0 *is defined as zero*)

Review: ∞*-Square well PE* *paths analyzed using* *Bohr rotor* *paths*

(9 or10-levels (0, ±1, ±2, ±3, ±4,..., ±9, ±10, ±11...) excited)

Zeros (clearly) and "particle-packets" (faintly) have paths labeled by fraction sequences like: $\frac{0}{7},\frac{1}{7},\frac{2}{7},\frac{3}{7},\frac{4}{7},\frac{5}{7},\frac{6}{7},\frac{1}{1}$





[Harter, J. Mol. Spec. 210, 166-182 (2001)]

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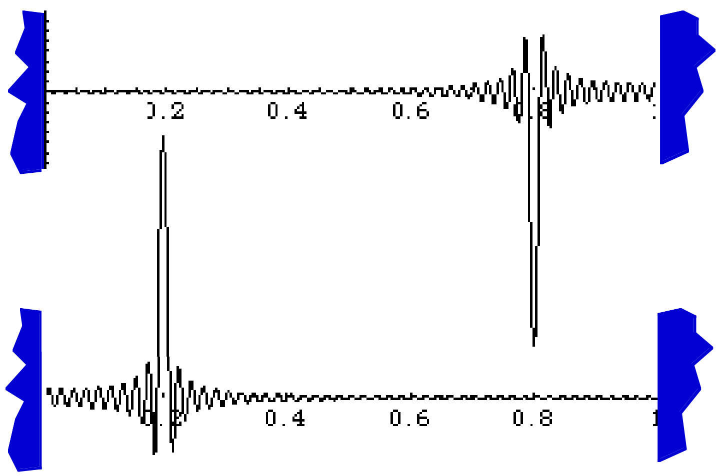
Review: ∞-Square well PE paths analyzed using Bohr rotor paths

All ∞-well peak must be made of sine wave components.

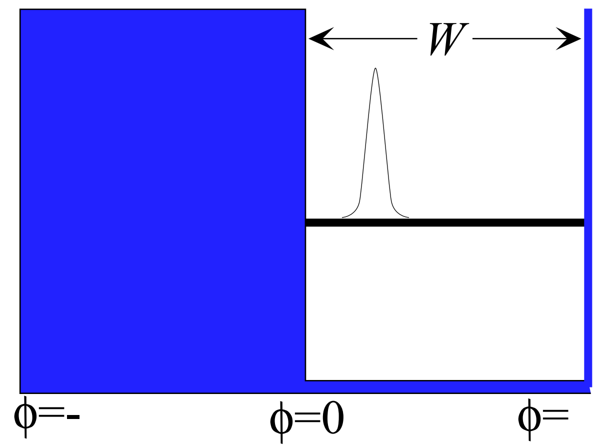
$t = 0.5000\tau_1$
$= 1.5\tau_{beat}$

$t = 1.0000\tau_1$
$= 3.0\tau_{beat}$

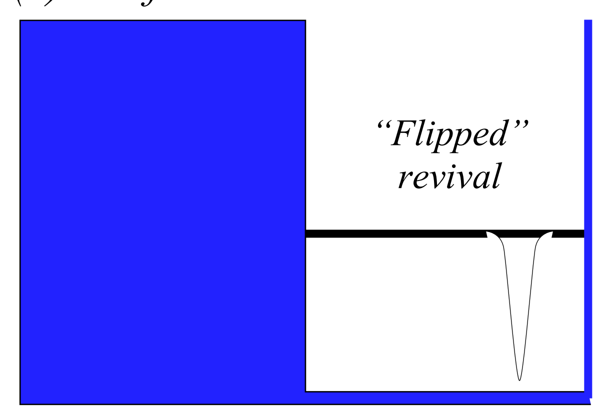


After only 50 round-trips
M's wave does a *partial revival*
as it makes an upside down-delta
function around *x=0.8W*.

(a) Infinite Square Well at t=0

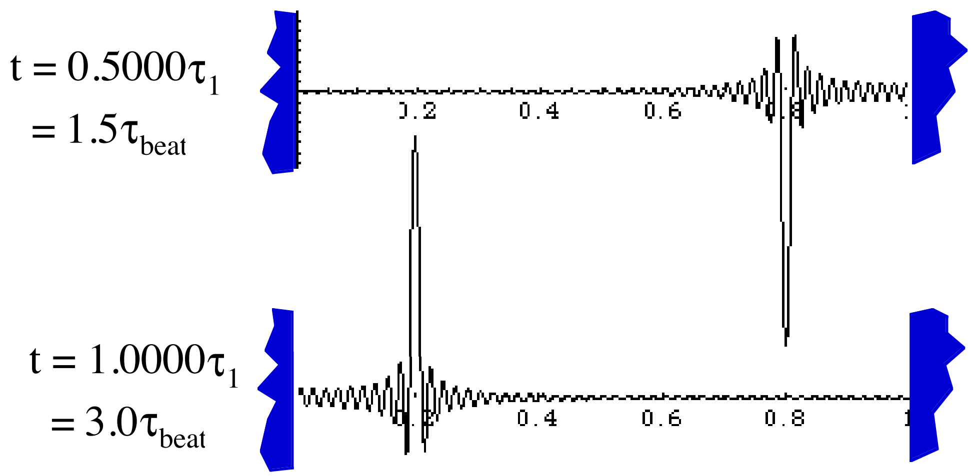


(c) Half-time revival at t=τ/2



So how is the ∞-well "flipped revival explained?

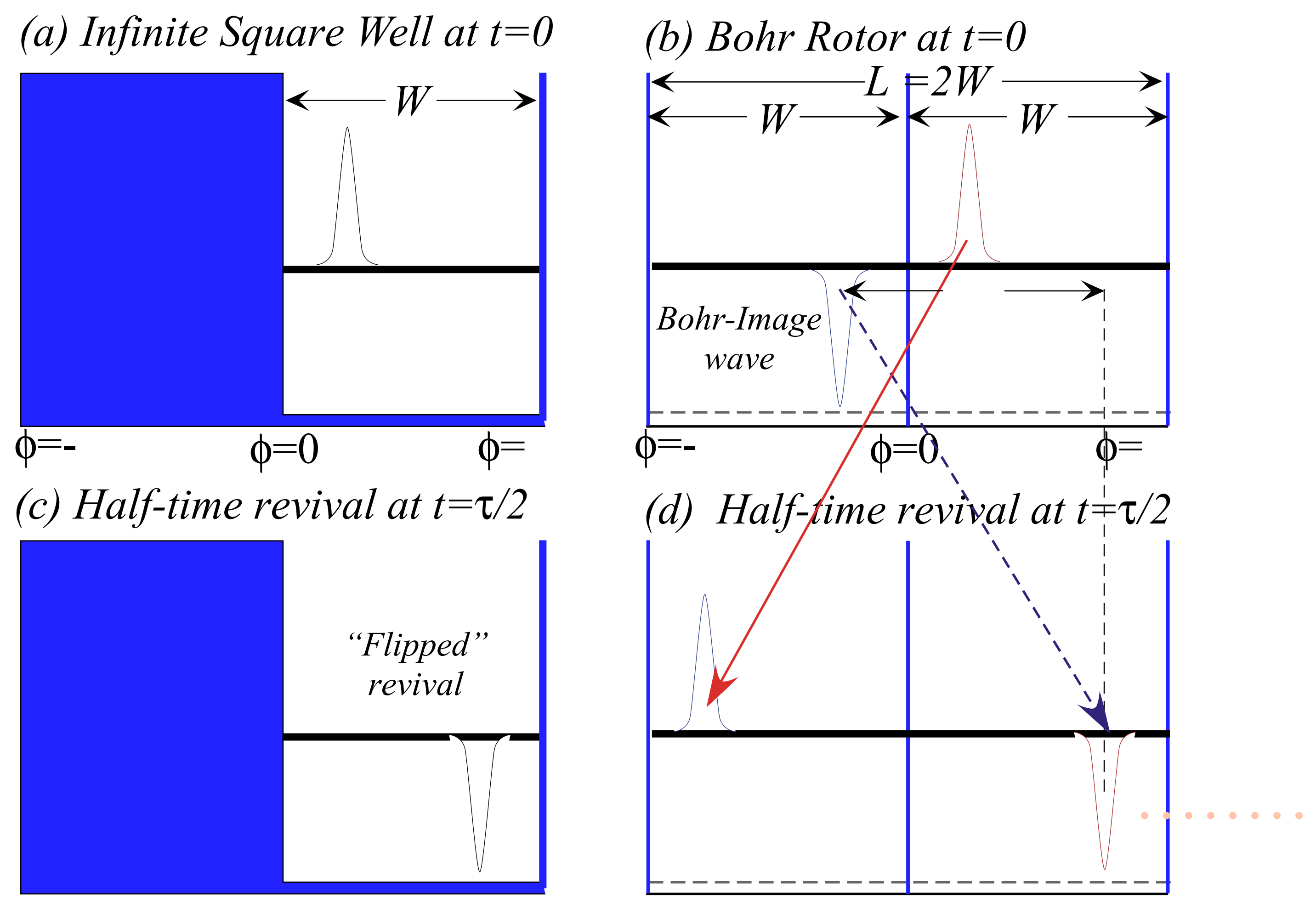
Review: ∞-*Square well PE* *paths analyzed using* **Bohr rotor** *paths*



After only 50 round-trips *M*'s wave does a *partial revival* as it makes an upside down-delta function around *x=0.8W*.

1.
All ∞-well peak must be made of sine wave components.

2. Bohr rotor peak made of *sine* wave components is *anti*-symmetric, so an *upside-down mirror* image peak must accompany any peak.



3. So how is the ∞-well "flipped revival explained?

4. Bohr rotor half-time revival is *same*-side-up copy of initial peak on *opposite* side of ring. So that upside-down Bohr-image will appear upside-down on the other side at half-time revival.

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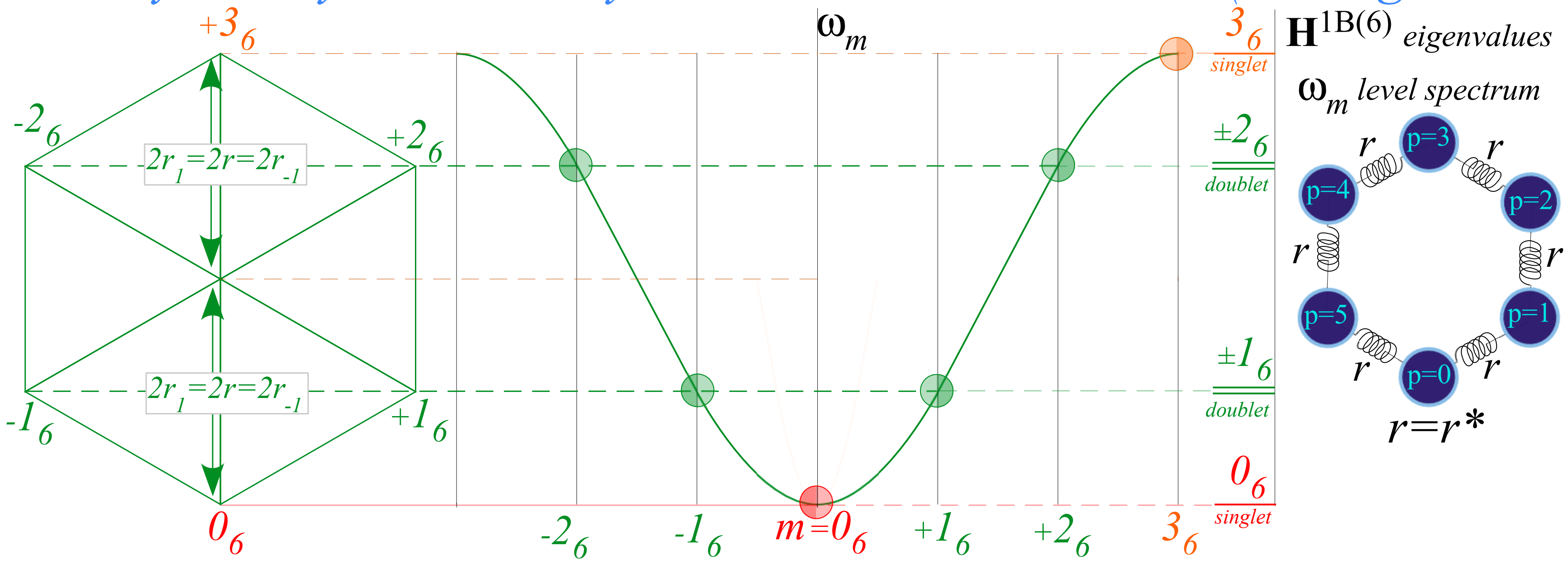
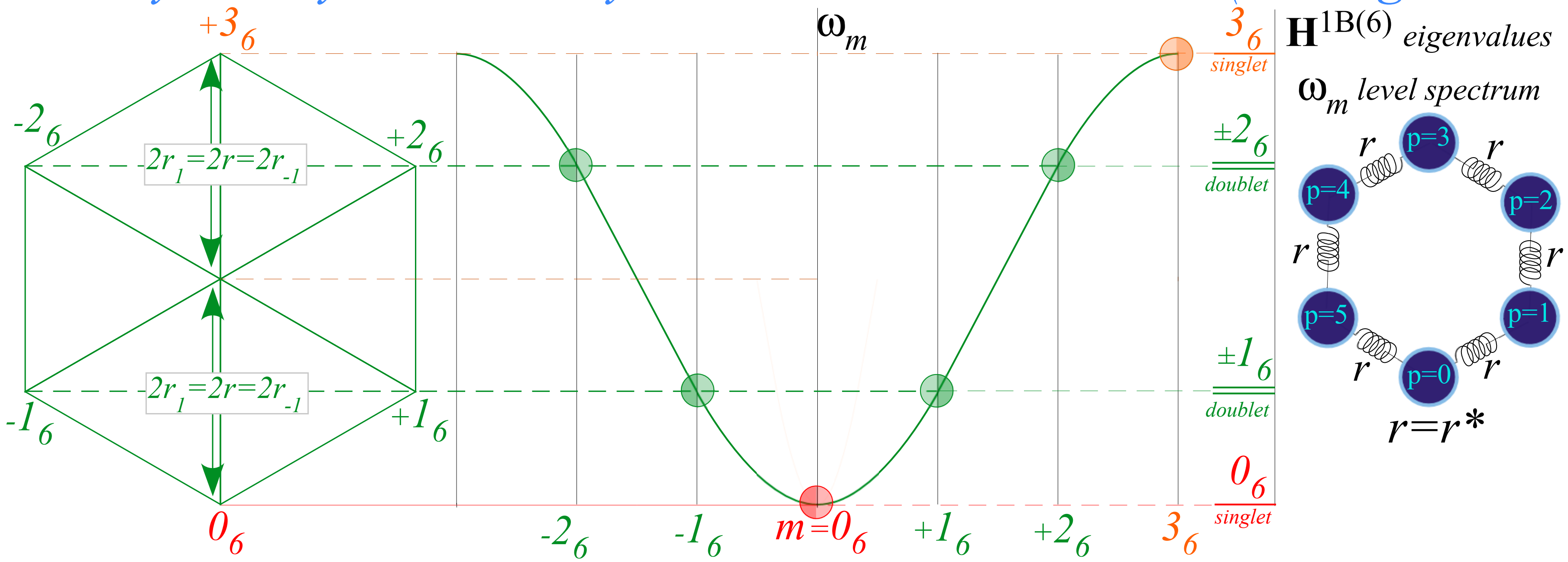
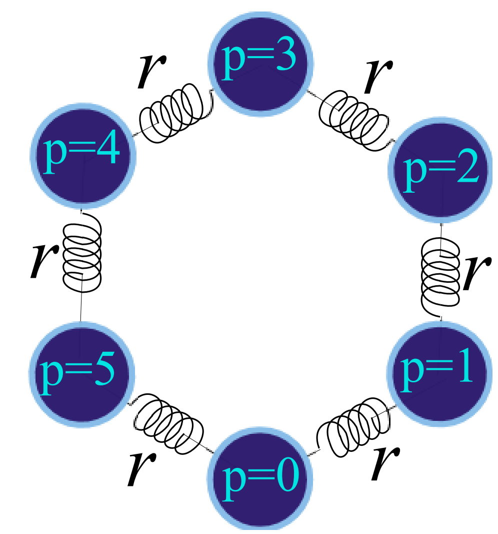
C_6 symmetry: Elementary Bloch Hamiltonian $\mathbf{H}^{1B(6)}$ (1^{st} neighbor coupling)



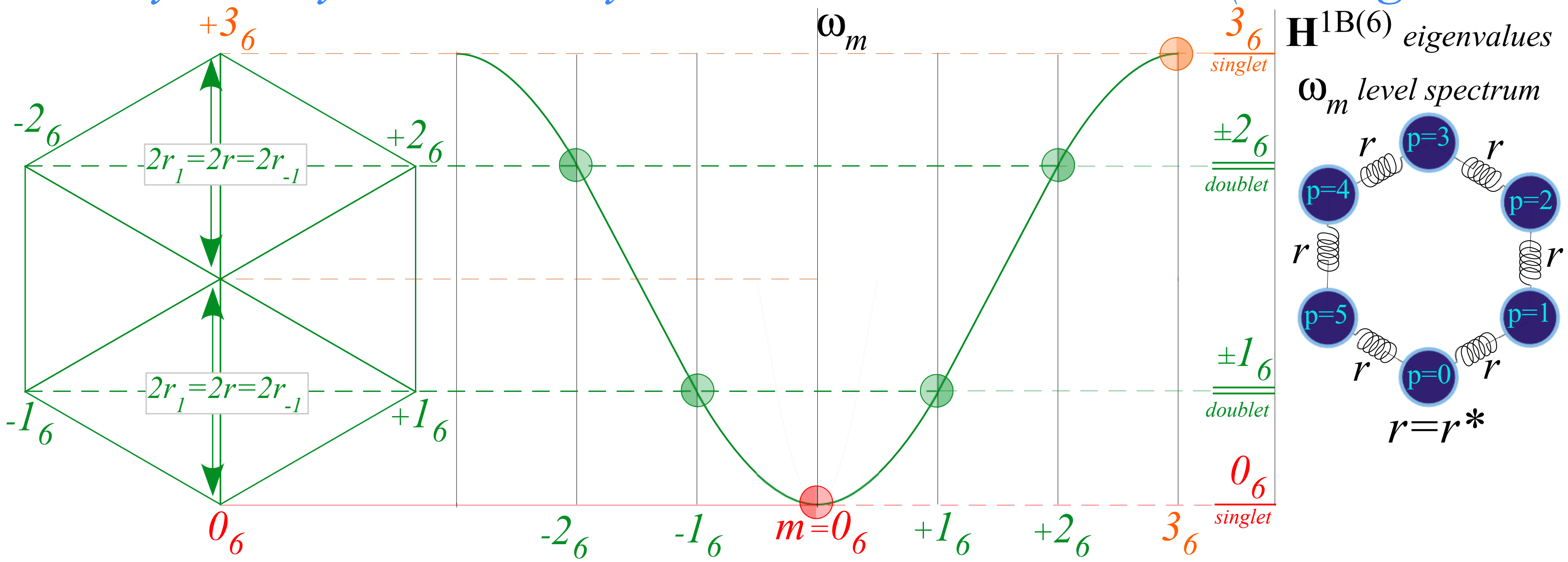
C_6 symmetry: Elementary Bloch Hamiltonian $\mathbf{H}^{1B(6)}$ (1^{st} neighbor coupling)



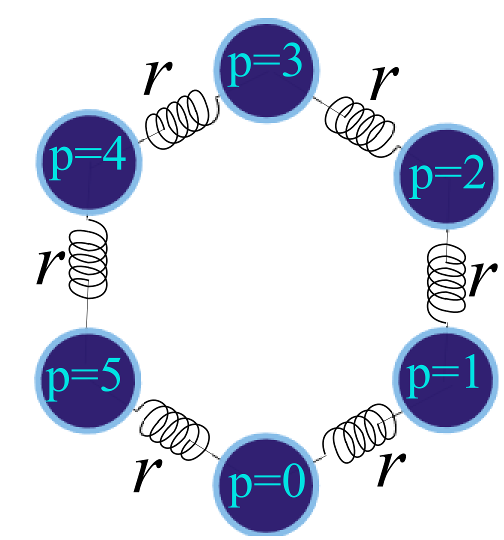
$$\mathbf{H}^{1B(6)}\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}=\begin{array}{cccccc} p=0 & 1 & 2 & 3 & 4 & 5\\ \end{array}\begin{pmatrix}2r & -r & \cdot & \cdot & \cdot & -r\\ -r & 2r & -r & \cdot & \cdot & \cdot\\ \cdot & -r & 2r & -r & \cdot & \cdot\\ \cdot & \cdot & -r & 2r & -r & \cdot\\ \cdot & \cdot & \cdot & -r & 2r & -r\\ -r & \cdot & \cdot & \cdot & -r & 2r\end{pmatrix}\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}=2r\left(1-\cos\frac{2\pi m}{6}\right)\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}$$



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



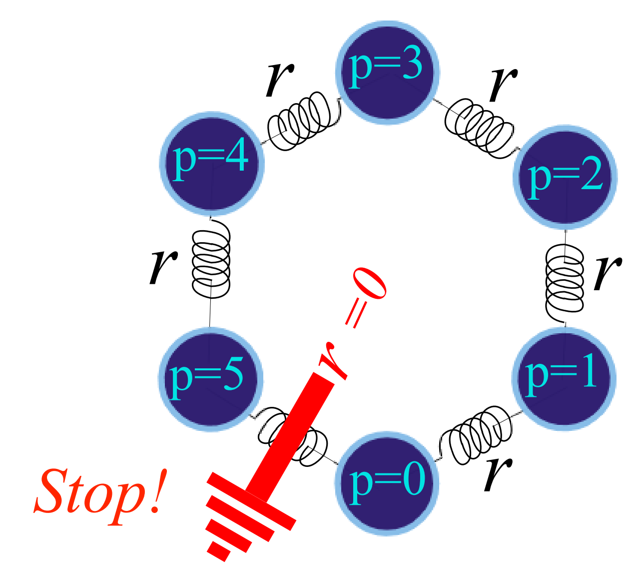
$$
\mathbf{H}^{1B(6)}\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}=
\begin{array}{c}
\begin{array}{cccccc} p=0 & 1 & 2 & 3 & 4 & 5\end{array}\\
\begin{pmatrix}
2r & -r & \cdot & \cdot & \cdot & -r\\
-r & 2r & -r & \cdot & \cdot & \cdot\\
\cdot & -r & 2r & -r & \cdot & \cdot\\
\cdot & \cdot & -r & 2r & -r & \cdot\\
\cdot & \cdot & \cdot & -r & 2r & -r\\
-r & \cdot & \cdot & \cdot & -r & 2r
\end{pmatrix}
\end{array}
\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}
=2r\left(1-\cos\frac{2\pi m}{6}\right)\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}
$$



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

$$
\mathbf{H}^{1B(6)}\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}=
\begin{array}{c}
\begin{array}{cccccc} p=0 & 1 & 2 & 3 & 4 & 5\end{array}\\
\begin{pmatrix}
2r & -r & \cdot & \cdot & \cdot & 0\\
-r & 2r & -r & \cdot & \cdot & \cdot\\
\cdot & -r & 2r & -r & \cdot & \cdot\\
\cdot & \cdot & -r & 2r & -r & \cdot\\
\cdot & \cdot & \cdot & -r & 2r & -r\\
0 & \cdot & \cdot & \cdot & -r & 2r
\end{pmatrix}
\end{array}
\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}
=?\begin{pmatrix}?\\ ?\\ ?\\ ?\\ ?\\ ?\end{pmatrix}
$$

(Not eigenvectors)



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

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

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

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

$$\begin{array}{c|c|cccccc|c|cccccc}
p \diagup p' & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & -6 & -5 & -4 & -3 & -2 & -1 \\ \hline
0 & 2r & -r & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -r \\ \hline
1 & -r & 2r & -r & \cdot & \cdot & \cdot & \cdot & & & & & & & \\
2 & \cdot & -r & 2r & -r & \cdot & \cdot & \cdot & & & & & & & \\
3 & \cdot & \cdot & -r & 2r & -r & \cdot & \cdot & & & & & & & \\
4 & \cdot & \cdot & \cdot & -r & 2r & -r & \cdot & & & & & & & \\
5 & \cdot & \cdot & \cdot & \cdot & -r & 2r & -r & & & & & & & \\
6 & \cdot & \cdot & \cdot & \cdot & \cdot & -r & 2r & -r & & & & & & \\ \hline
7 & \cdot & & & & & & -r & 2r & -r & & & & & \\ \hline
-6 & \cdot & & & & & & & -r & 2r & -r & \cdot & \cdot & \cdot & \cdot \\
-5 & \cdot & & & & & & & & -r & 2r & -r & \cdot & \cdot & \cdot \\
-4 & \cdot & & & & & & & & \cdot & -r & 2r & -r & \cdot & \cdot \\
-3 & \cdot & & & & & & & & \cdot & \cdot & -r & 2r & -r & \cdot \\
-2 & \cdot & & & & & & & & \cdot & \cdot & \cdot & -r & 2r & -r \\
-1 & -r & & & & & & & & \cdot & \cdot & \cdot & \cdot & -r & 2r
\end{array}
\left(\begin{array}{c} \vdots \\ \hline 0 \\ \hline s_1^m \\ s_2^m \\ s_3^m \\ s_4^m \\ s_5^m \\ s_6^m \\ \hline 0 \\ \hline s_{-6}^m \\ s_{-5}^m \\ s_{-4}^m \\ s_{-3}^m \\ s_{-2}^m \\ s_{-1}^m \end{array}\right)
= \omega^{m(14)}
\left(\begin{array}{c} \vdots \\ \hline 0 \\ \hline s_1^m \\ s_2^m \\ s_3^m \\ s_4^m \\ s_5^m \\ s_6^m \\ \hline 0 \\ \hline s_{-6}^m \\ s_{-5}^m \\ s_{-4}^m \\ s_{-3}^m \\ s_{-2}^m \\ s_{-1}^m \end{array}\right)$$

where:

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

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

$$\langle cos^m| = \left(c_0^m=1 \;\middle|\; c_1^m \;\; c_2^m \;\; c_3^m \;\; c_4^m \;\; c_5^m \;\; c_6^m \;\middle|\; c_7^m=1 \;\middle|\; c_{-6}^m \;\; c_{-5}^m \;\; c_{-4}^m \;\; c_{-3}^m \;\; c_{-2}^m \;\; c_{-1}^m \right)$$

$$\langle sin^m| = \left(s_0^m=0 \;\middle|\; s_1^m \;\; s_2^m \;\; s_3^m \;\; s_4^m \;\; s_5^m \;\; s_6^m \;\middle|\; s_7^m=0 \;\middle|\; s_{-6}^m \;\; s_{-5}^m \;\; s_{-4}^m \;\; s_{-3}^m \;\; s_{-2}^m \;\; s_{-1}^m \right)$$

$$c_p^m = \cos\left(m \cdot p \frac{\pi}{7}\right) = c_{-p}^m$$

$$s_p^m = \sin\left(m \cdot p \frac{\pi}{7}\right) = -s_{-p}^m$$

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

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

$$\begin{array}{c|c|cccccc|c|cccccc|}
p \diagup p' & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & -6 & -5 & -4 & -3 & -2 & -1 \\ \hline
0 & 2r & -r & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -r \\
1 & -r & 2r & -r & \cdot & \cdot & \cdot & \cdot\;0 & & & & & & & \\
2 & \cdot & -r & 2r & -r & \cdot & \cdot & \cdot & & & & & & & \\
3 & \cdot & \cdot & -r & 2r & -r & \cdot & \cdot & & & & & & & \\
4 & \cdot & \cdot & \cdot & -r & 2r & -r & \cdot & & & & & & & \\
5 & \cdot & \cdot & \cdot & \cdot & -r & 2r & -r & & & & & & & \\
6 & \cdot & \cdot\;0 & \cdot & \cdot & \cdot & -r & 2r & -r & & & & & & \\
7 & \cdot & & & & & & -r & 2r & -r & & & & & \\
-6 & \cdot & & & & & & & -r & 2r & -r & \cdot & \cdot & \cdot & \cdot \\
-5 & \cdot & & & & & & & & -r & 2r & -r & \cdot & \cdot & \cdot \\
-4 & \cdot & & & & & & & & \cdot & -r & 2r & -r & \cdot & \cdot \\
-3 & \cdot & & & & & & & & \cdot & \cdot & -r & 2r & -r & \cdot \\
-2 & \cdot & & & & & & & & \cdot & \cdot & \cdot & -r & 2r & -r \\
-1 & -r & & & & & & & & \cdot & \cdot & \cdot & \cdot & -r & 2r
\end{array}
\begin{pmatrix} 0 \\ s_1^m \\ s_2^m \\ s_3^m \\ s_4^m \\ s_5^m \\ s_6^m \\ 0 \\ s_{-6}^m \\ s_{-5}^m \\ s_{-4}^m \\ s_{-3}^m \\ s_{-2}^m \\ s_{-1}^m \end{pmatrix}
= \omega^{m(14)}
\begin{pmatrix} 0 \\ s_1^m \\ s_2^m \\ s_3^m \\ s_4^m \\ s_5^m \\ s_6^m \\ 0 \\ s_{-6}^m \\ s_{-5}^m \\ s_{-4}^m \\ s_{-3}^m \\ s_{-2}^m \\ s_{-1}^m \end{pmatrix}$$

where :

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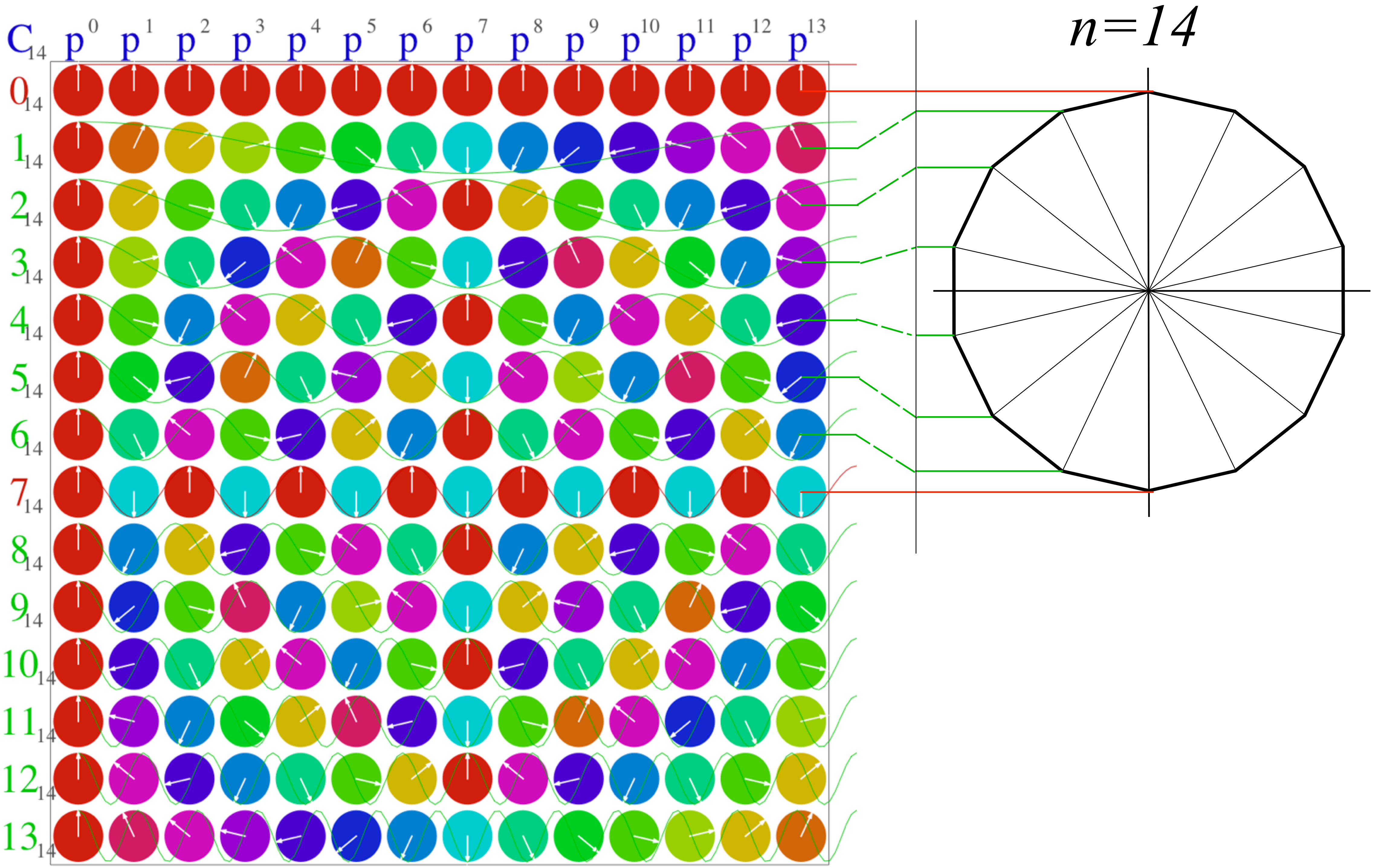
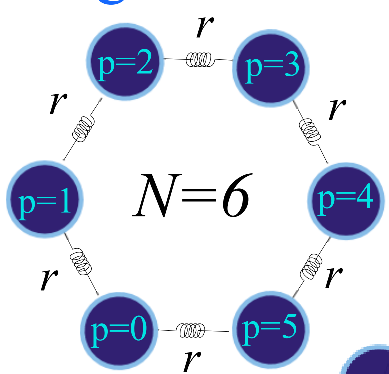
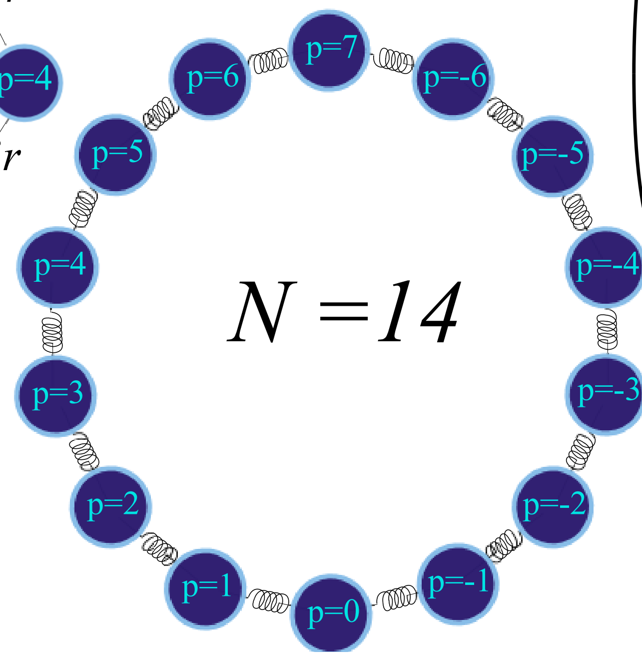
$\mathbf{H}^{EB(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{CM(6)}$ using its sine-waves only



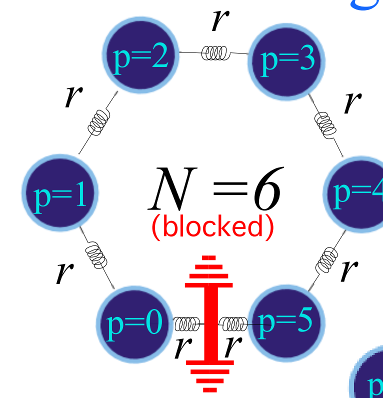
$\mathbf{H}^{EB(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{CM(6)}$ using its sine-waves only

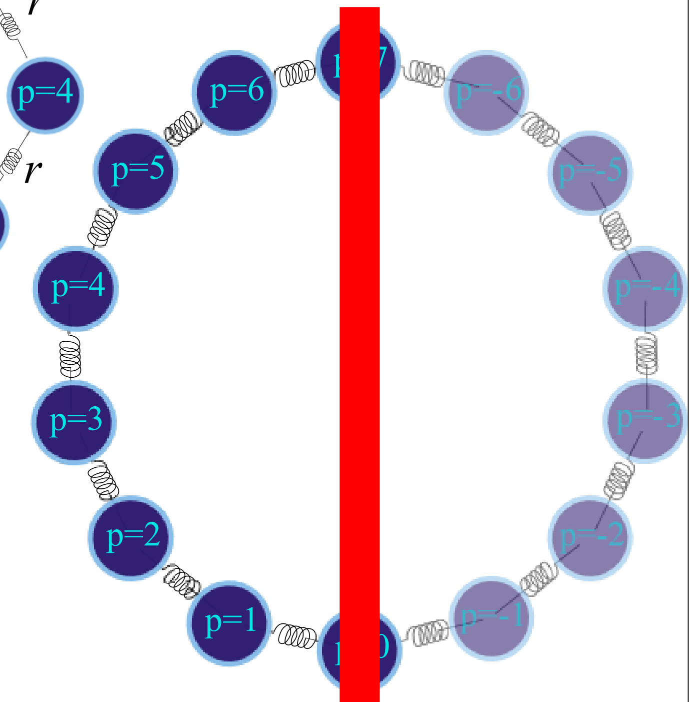
$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & -r \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ -r & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$





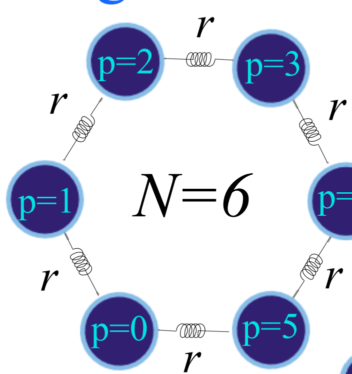
$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & 0 \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ 0 & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$

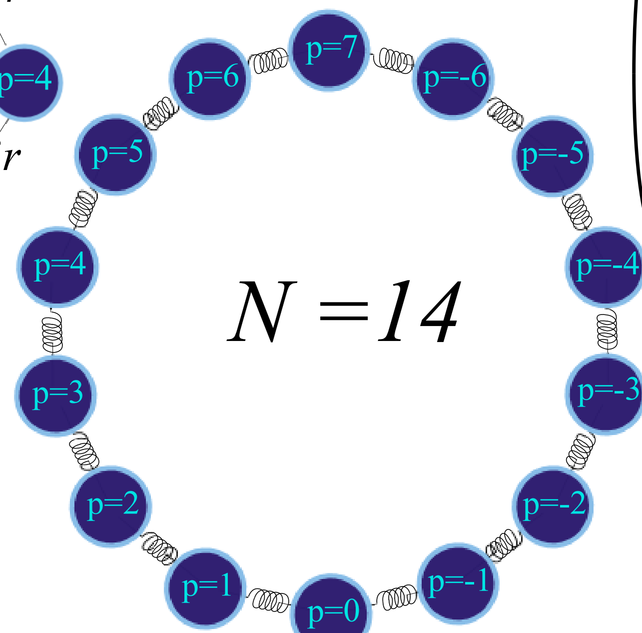




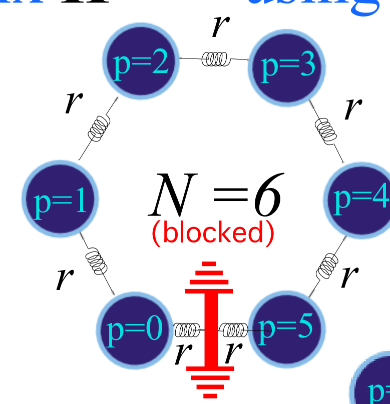
$\mathbf{H}^{EB(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{CM(6)}$ using its sine-waves only

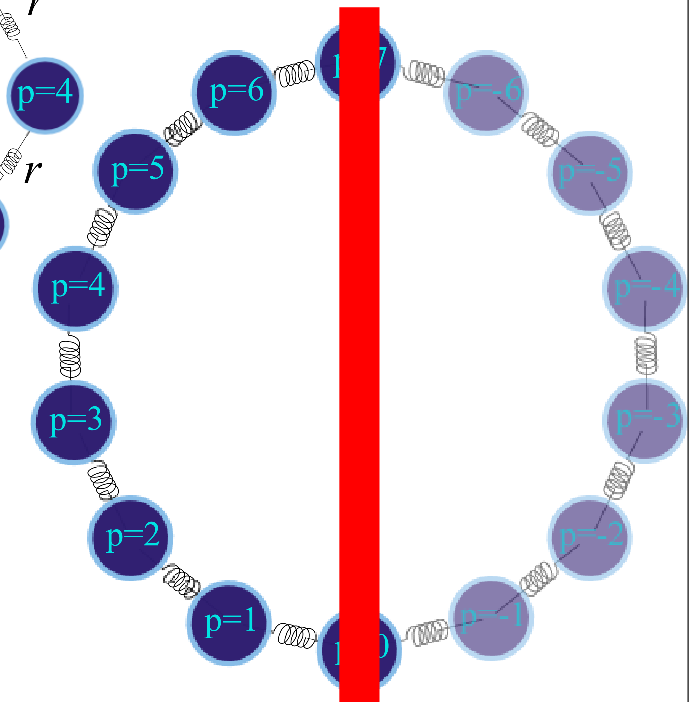
$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & -r \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ -r & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$



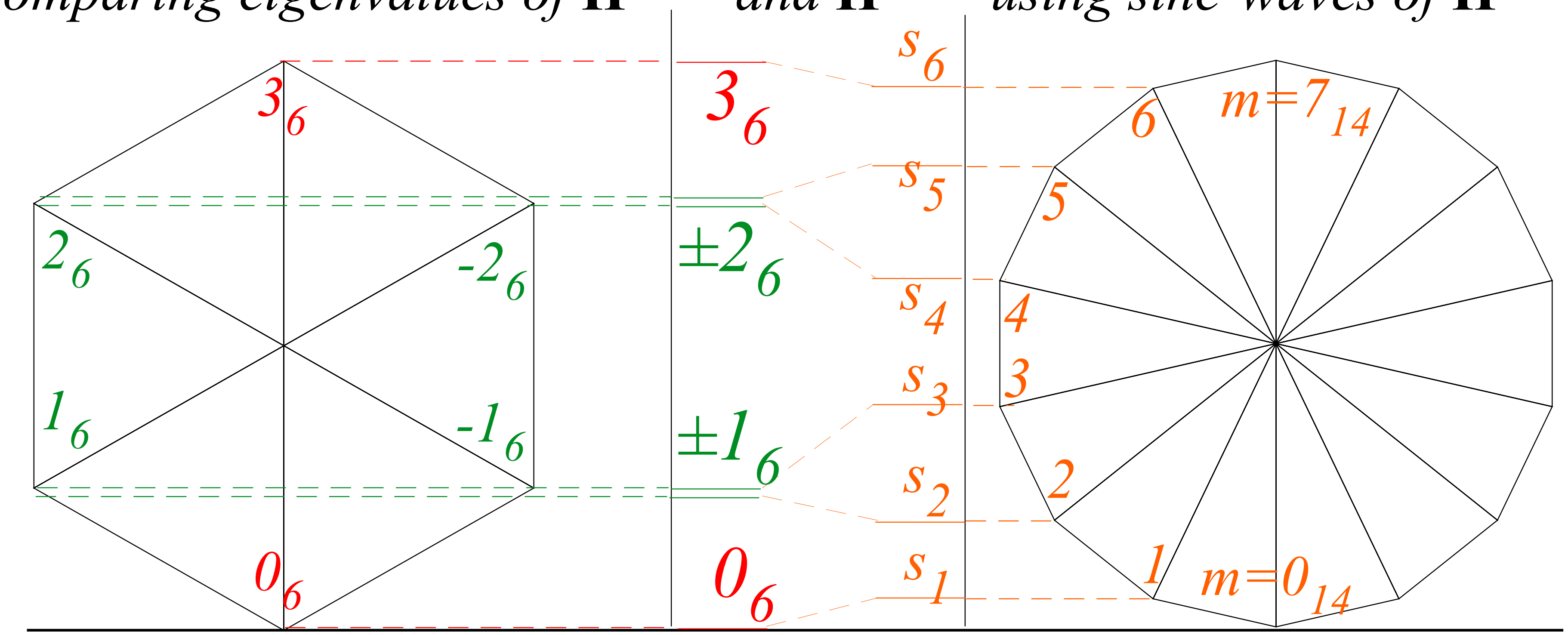


$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & 0 \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ 0 & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$



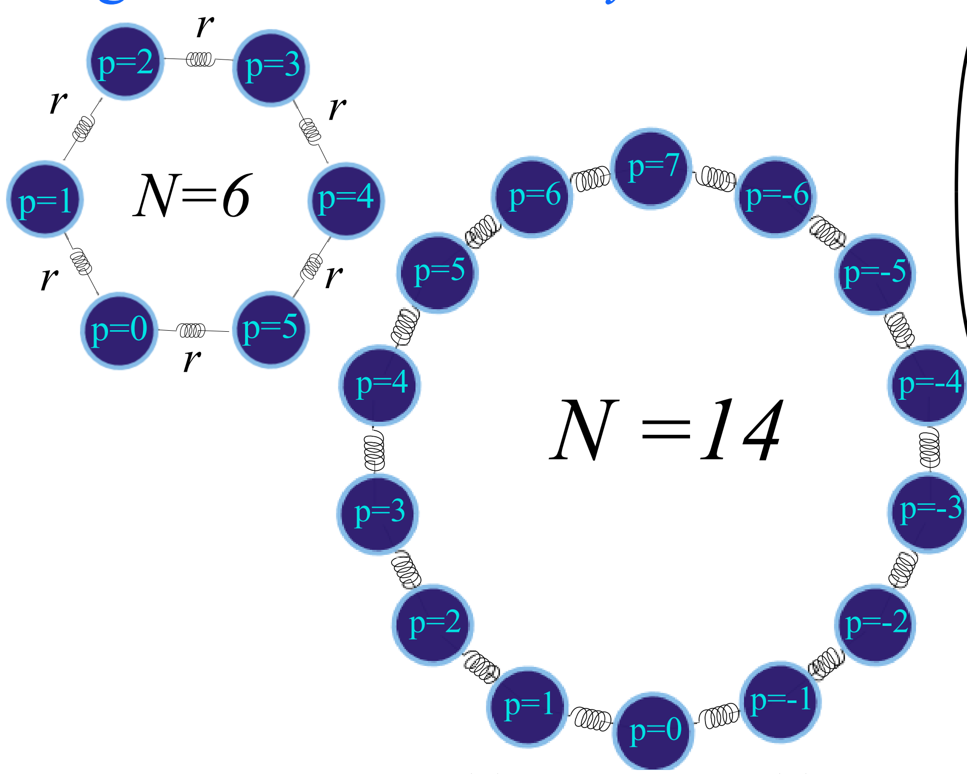


Comparing eigenvalues of $\mathbf{H}^{EB(6)}$ *and* $\mathbf{H}^{CM(6)}$ *using sine-waves of* $\mathbf{H}^{EB(14)}$



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

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



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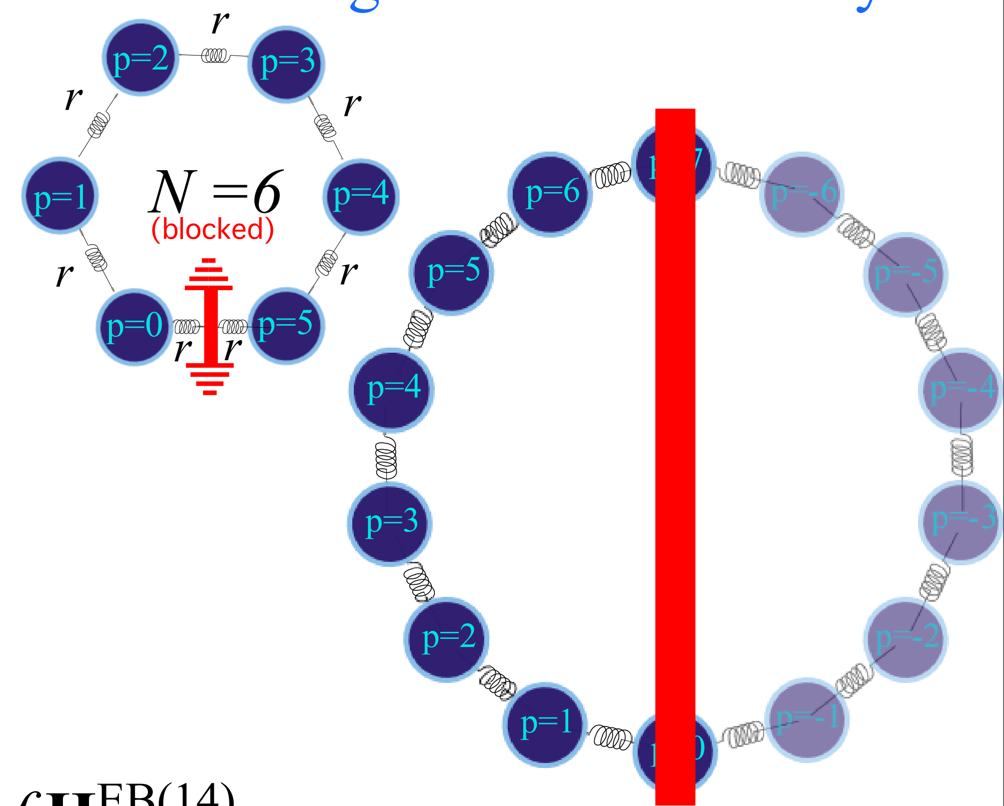

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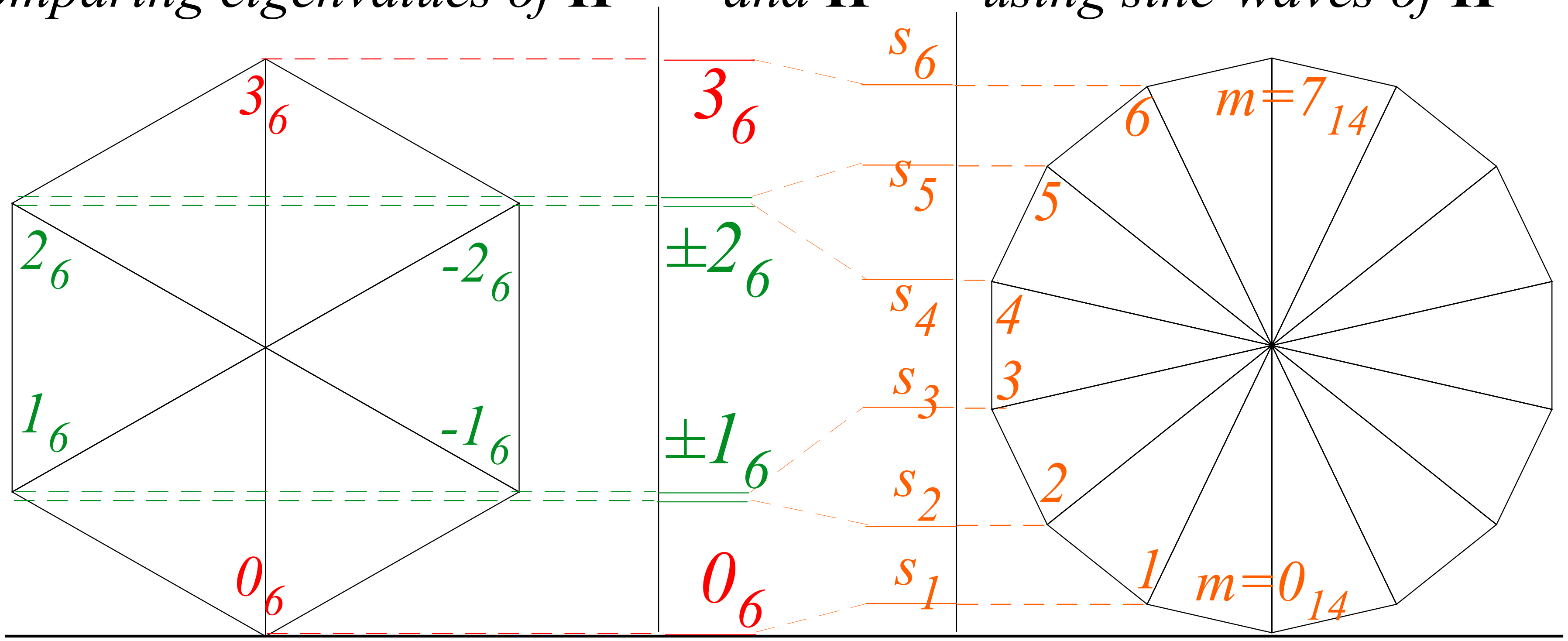

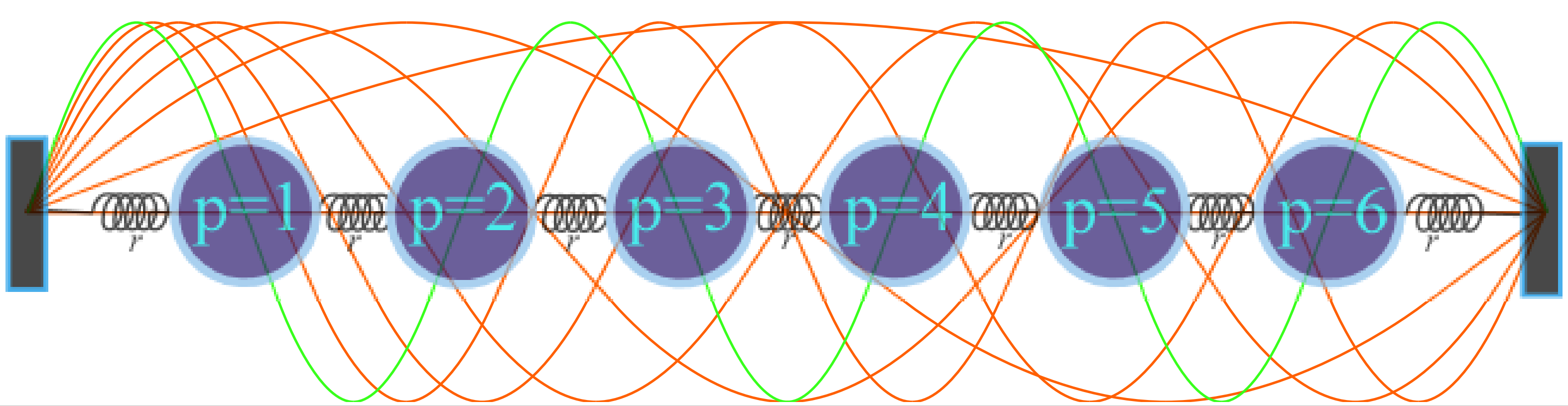

Breaking C_N cyclic coupling into linear chains

Review of 1D-Bohr-ring related to infinite square well (and review of revival)

∞-Square well paths analyzed using Bohr rotor paths

Breaking C_{2N+2} to approximate linear N-chain

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

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Acoustical modes vs. Optical modes

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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 Group Zoo

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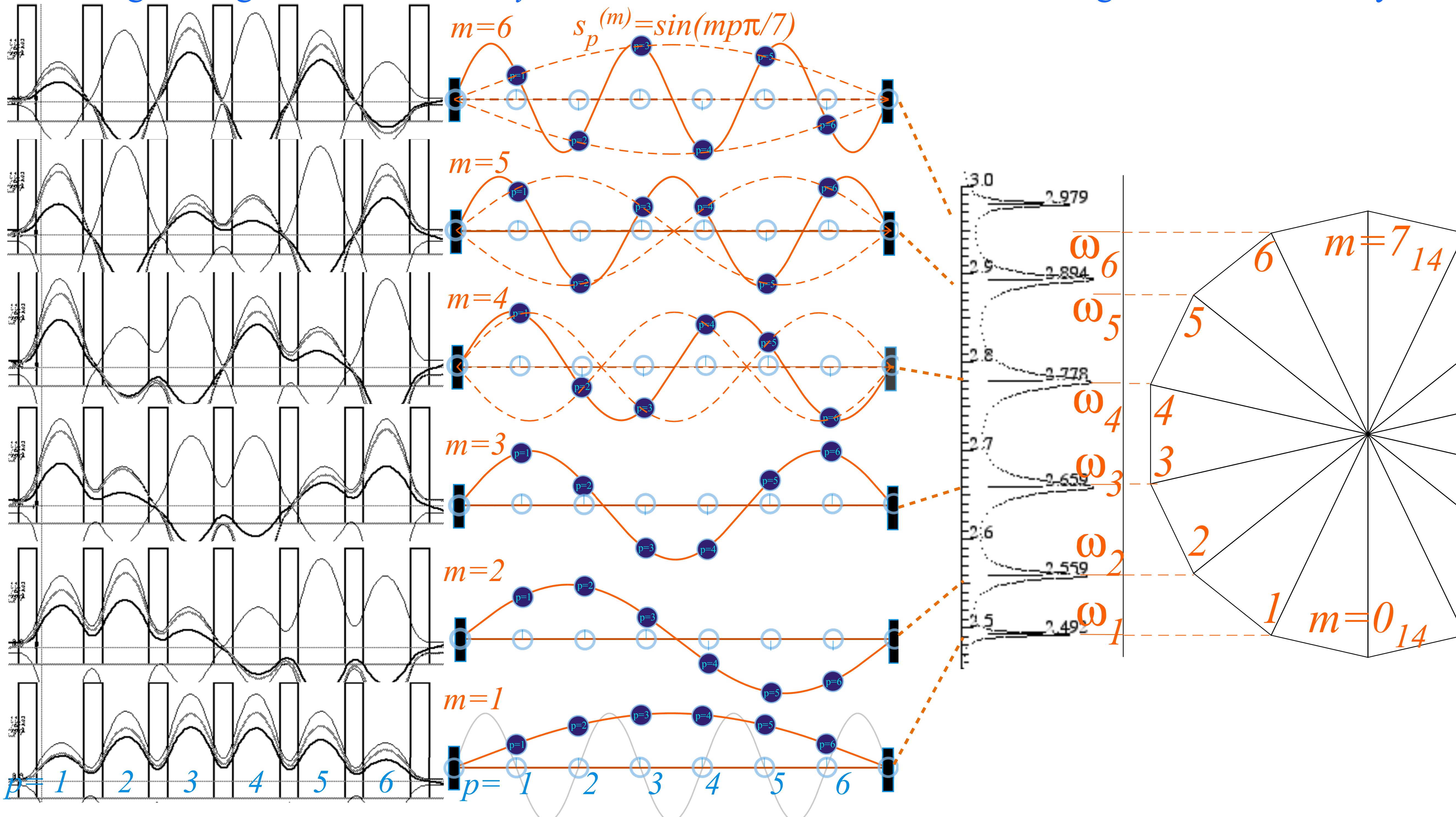

Band-It simulation is
Mac OS 9 application
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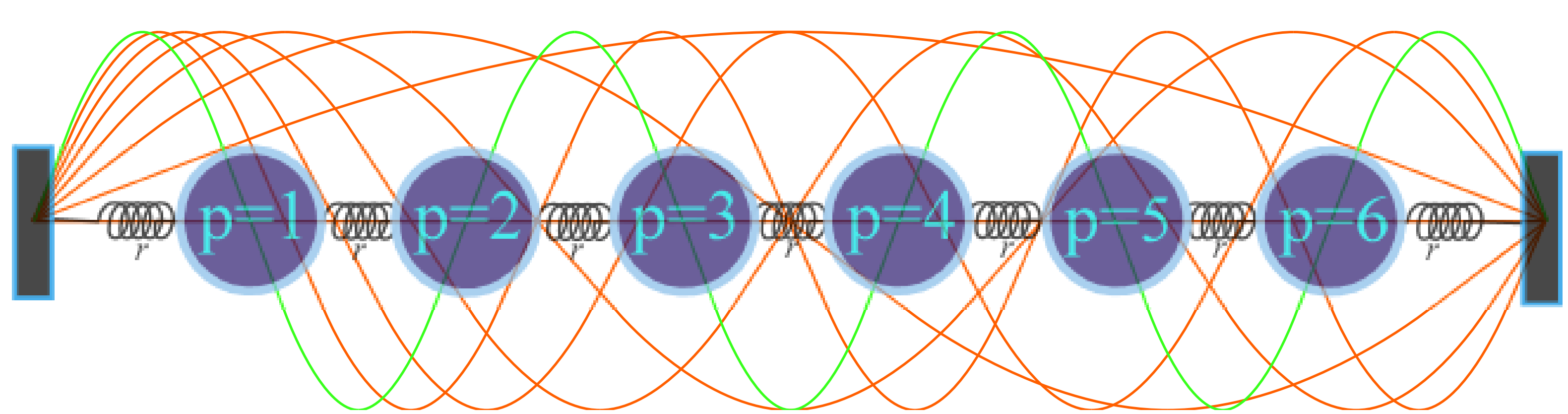

How Band-It simulation works (from QTfCA Unit 4 Chapter 13)

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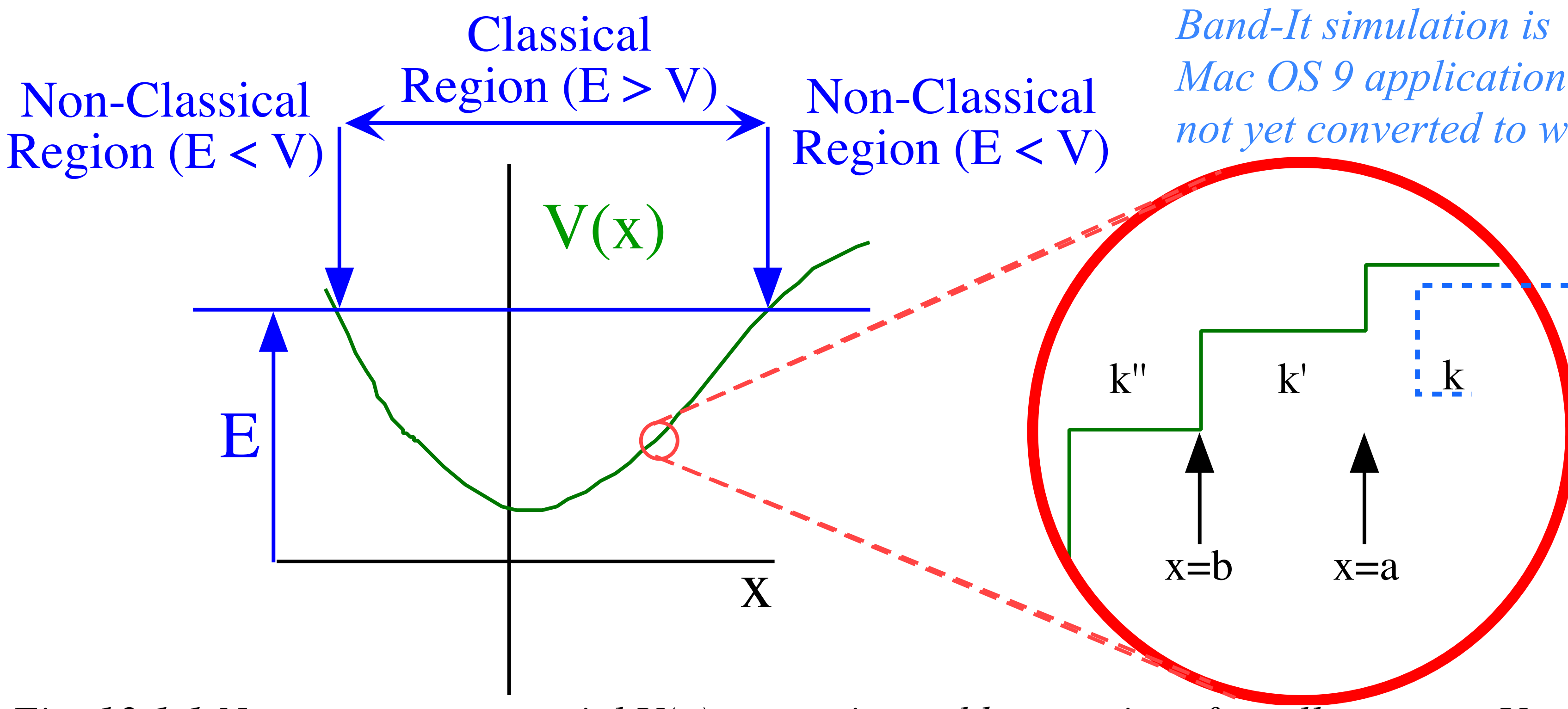

Fig. 13.1.1 Non-constant potential V(x) approximated by a series of small constant-V steps.

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

$$\Psi_E(x,0) = Re^{ikx} + Le^{-ikx}$$

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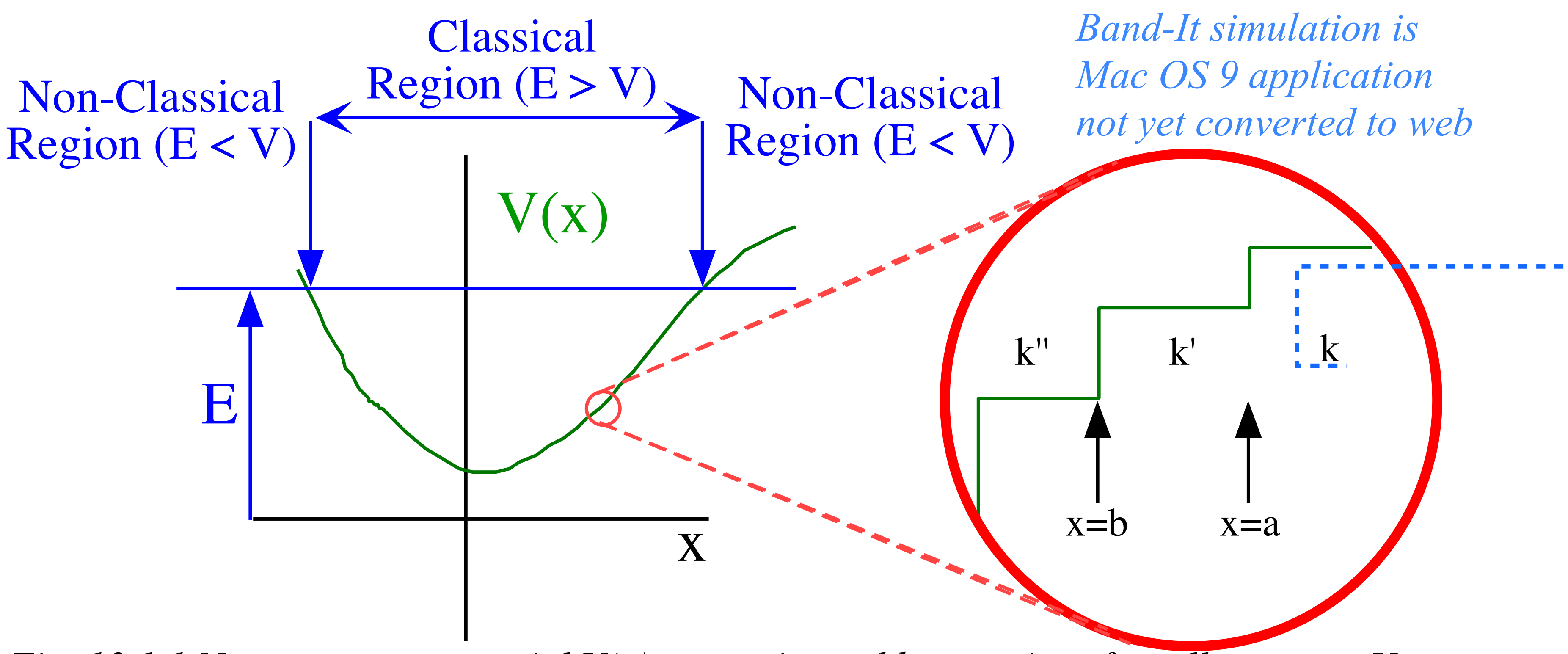

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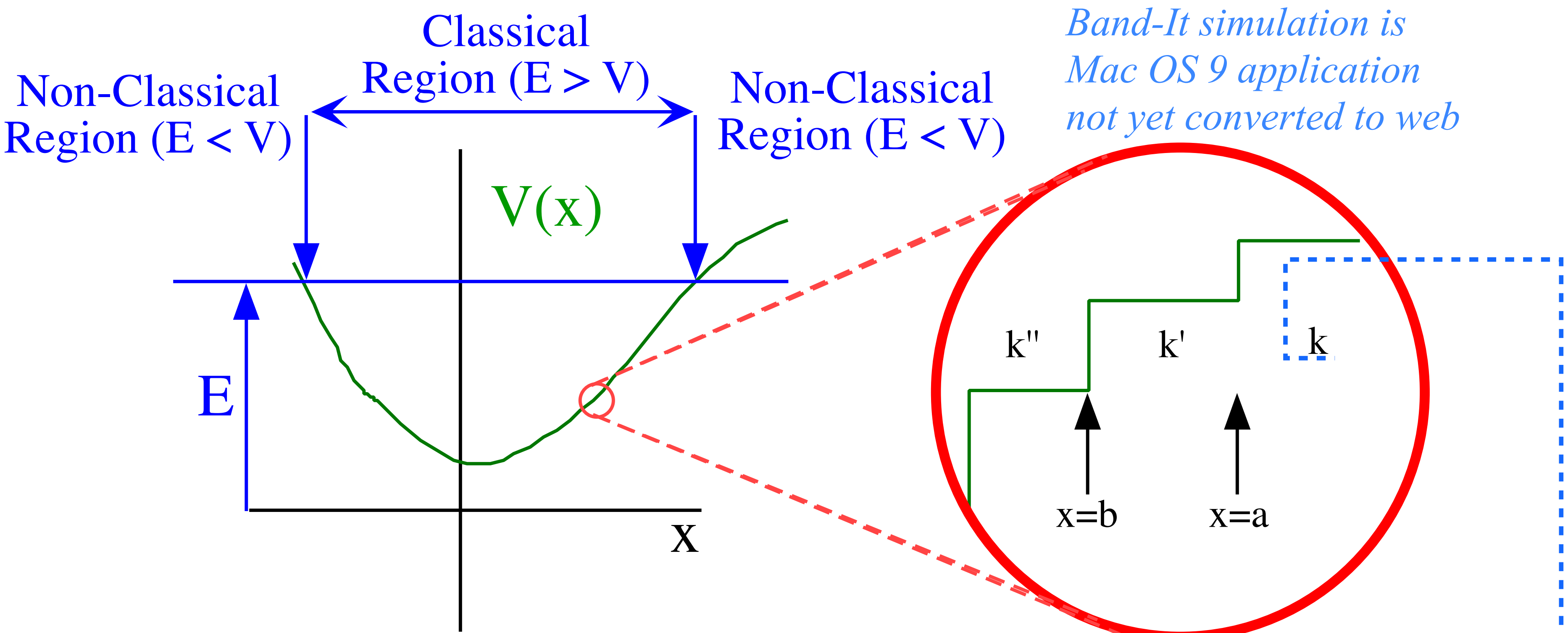

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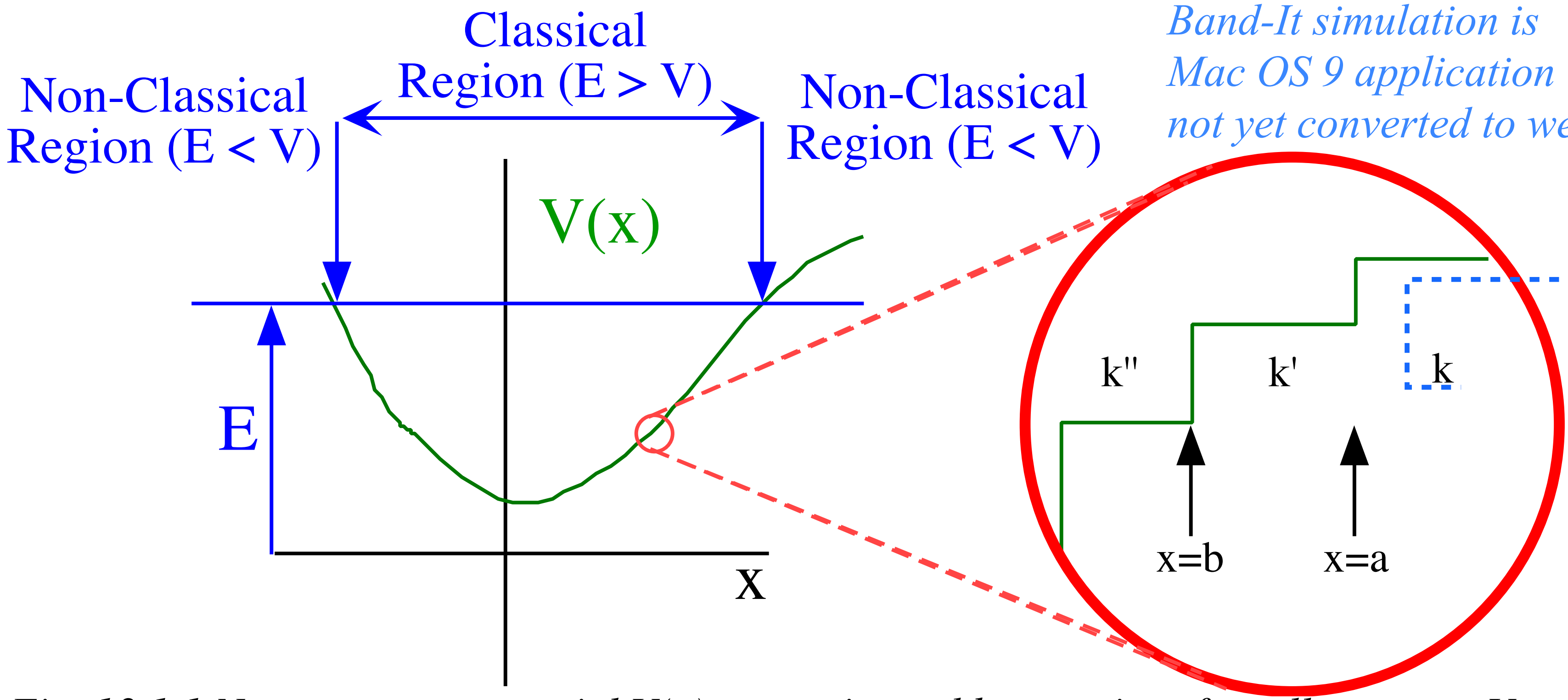

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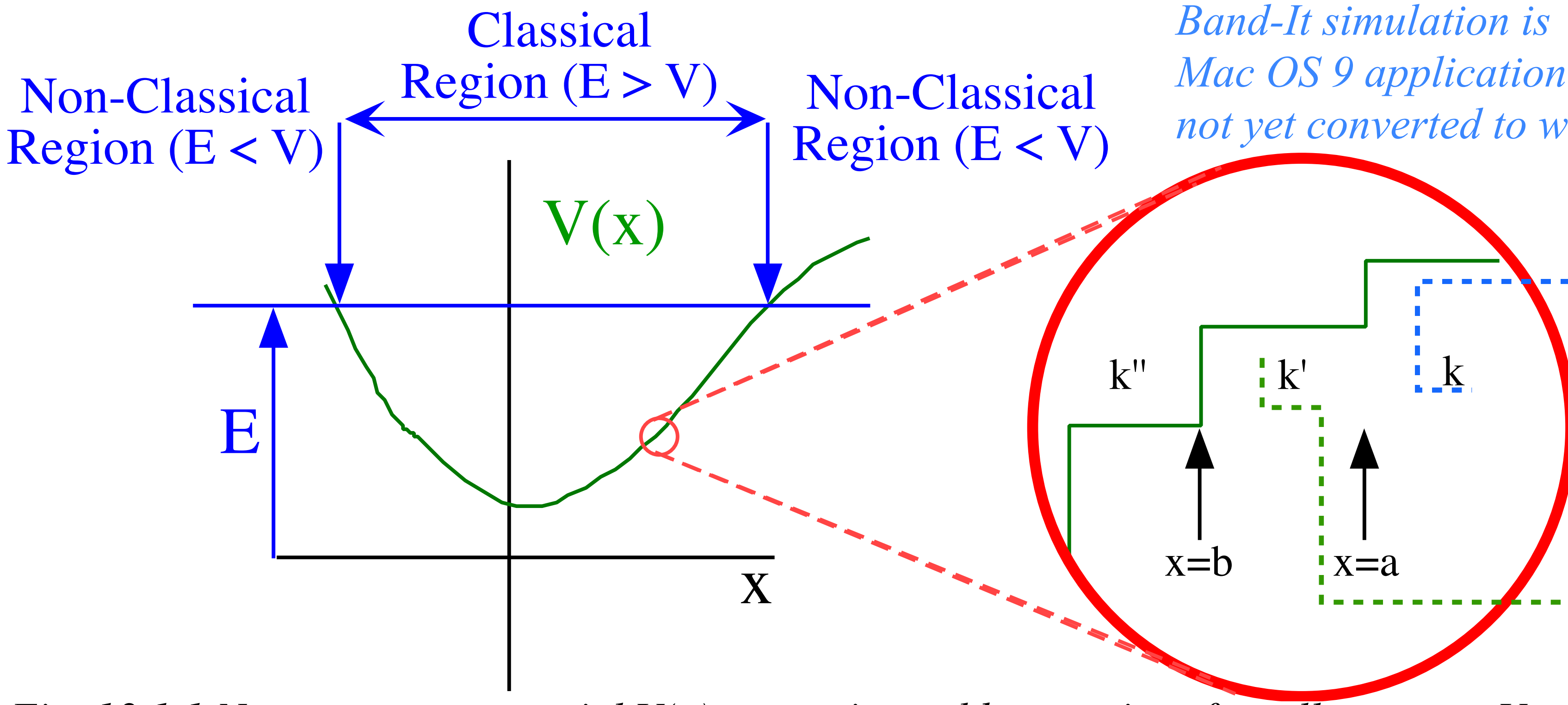

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Relations on the other side of the step boundary just below $x=a$. *(Inverted)*

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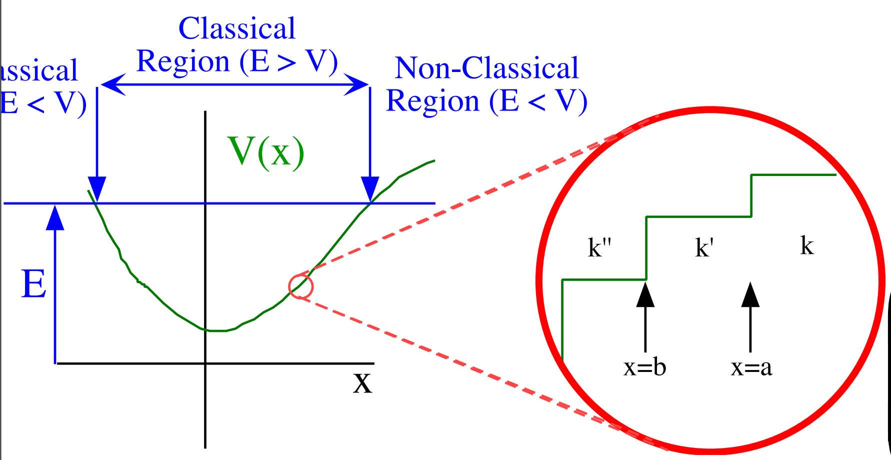

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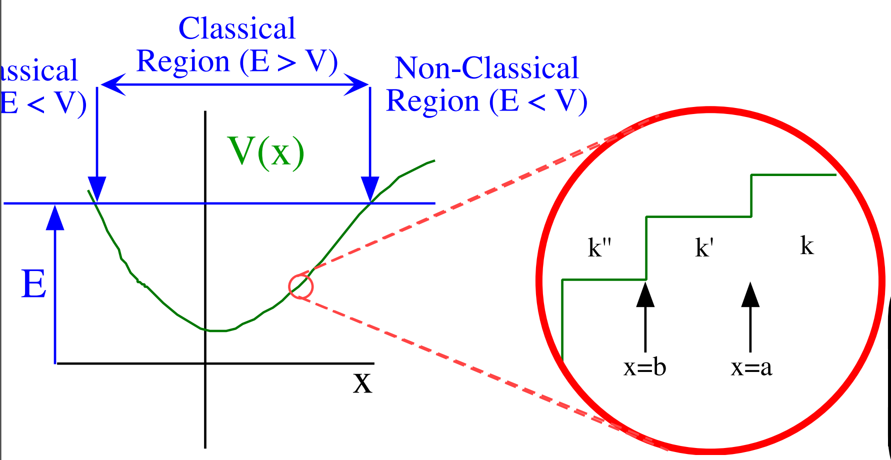

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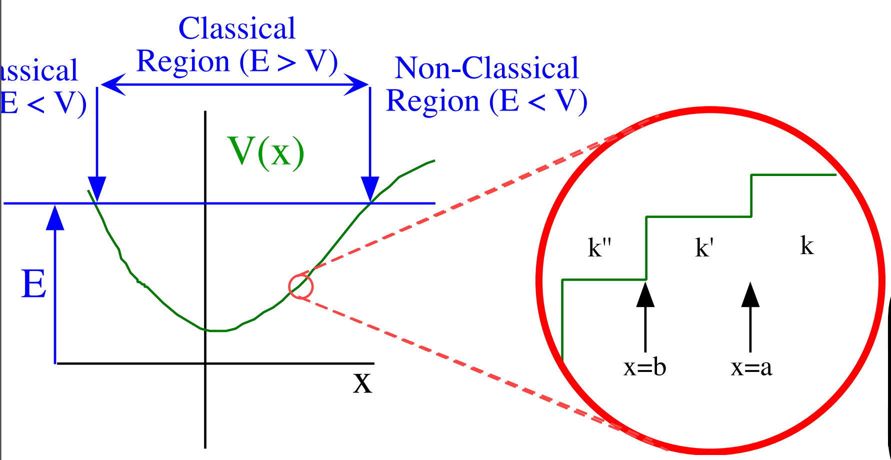

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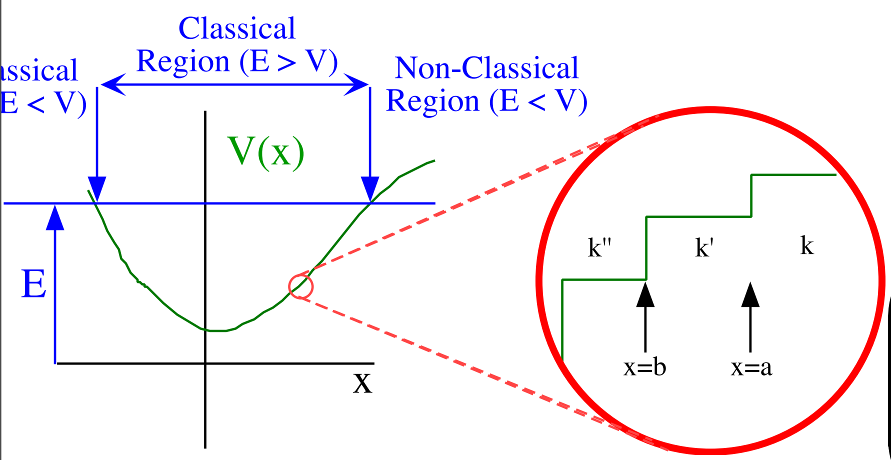

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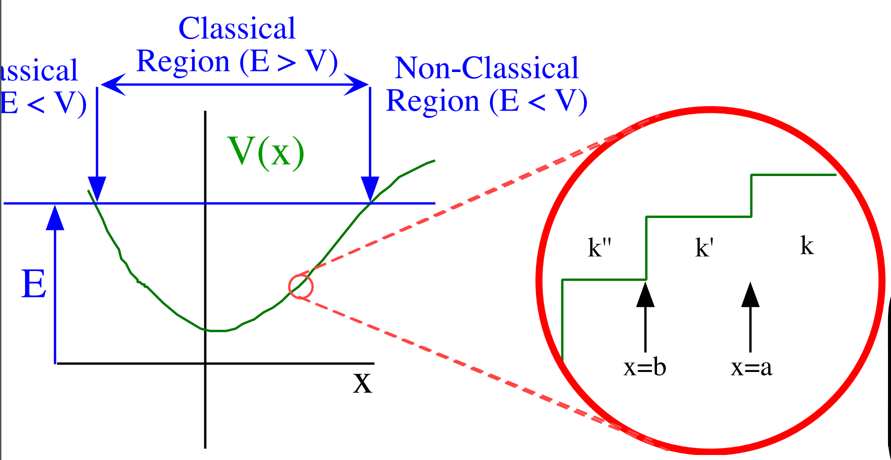

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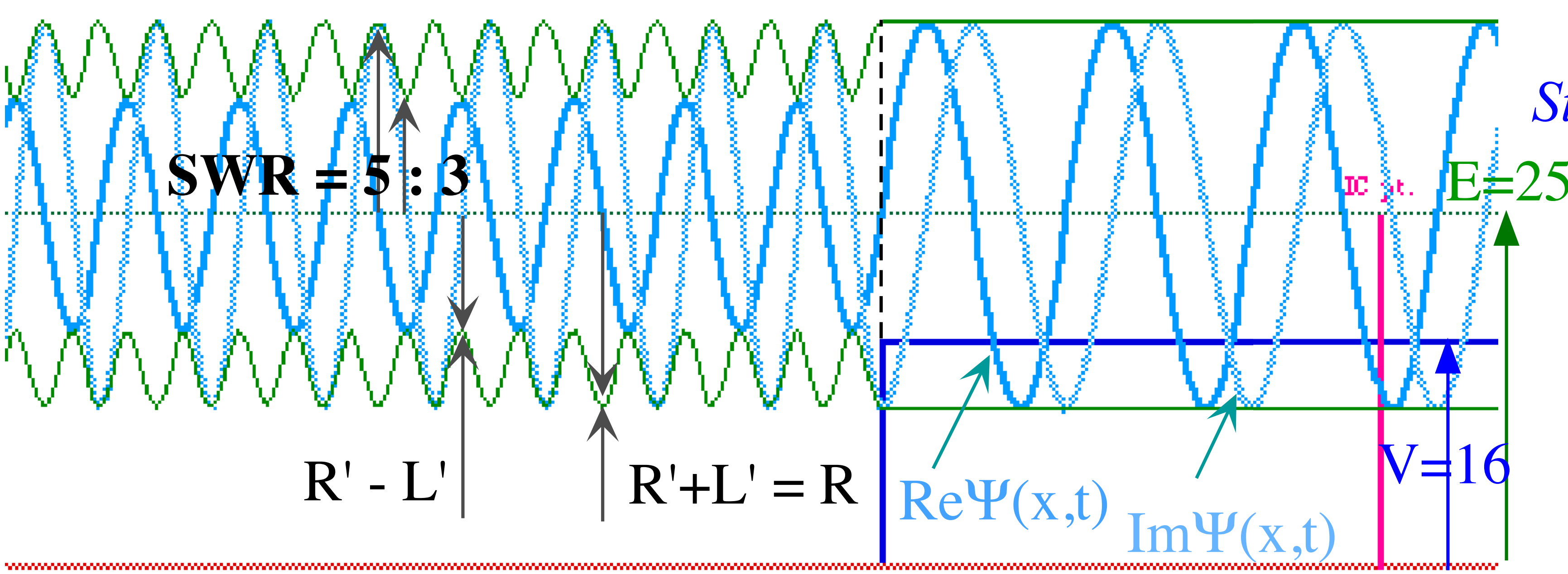
This gives *transmitted or output amplitude R* and *reflected amplitude L'* given an *input amplitude R'*.

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

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

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



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

Fig. 2.7.6 PSDS

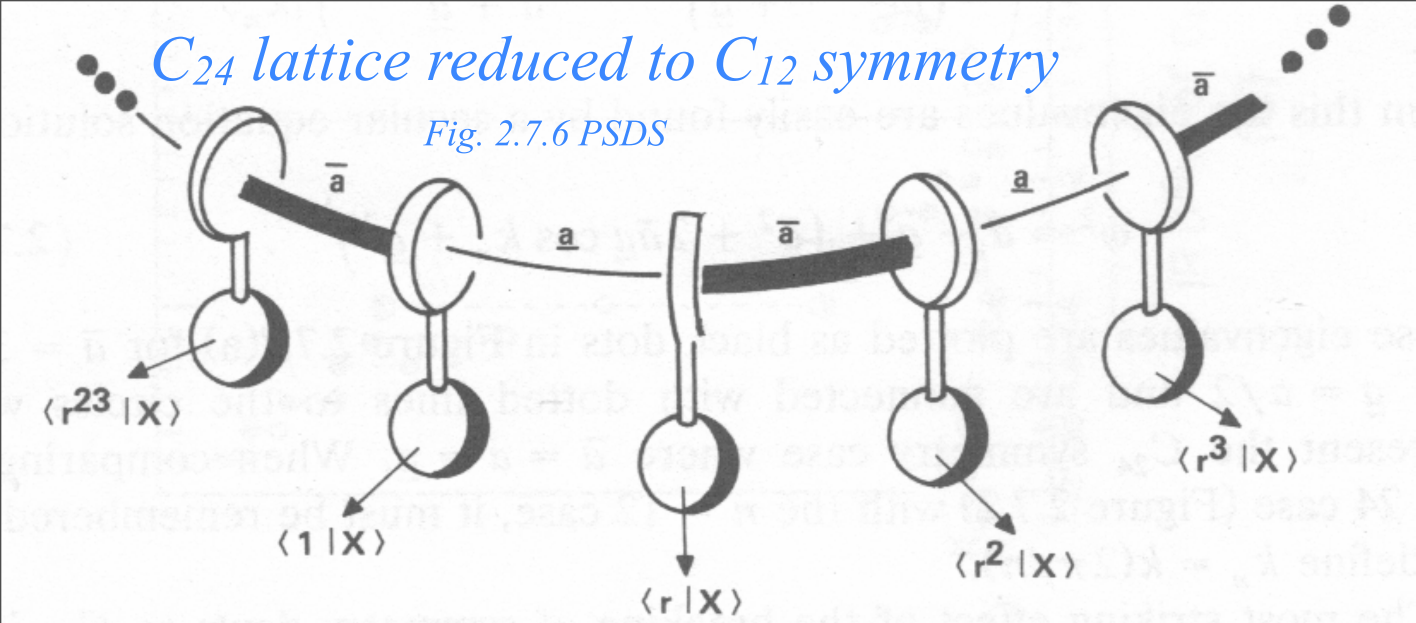

Fig. 2.7.6 PrinciplesSymmetryDynamics&Spectroscopy

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

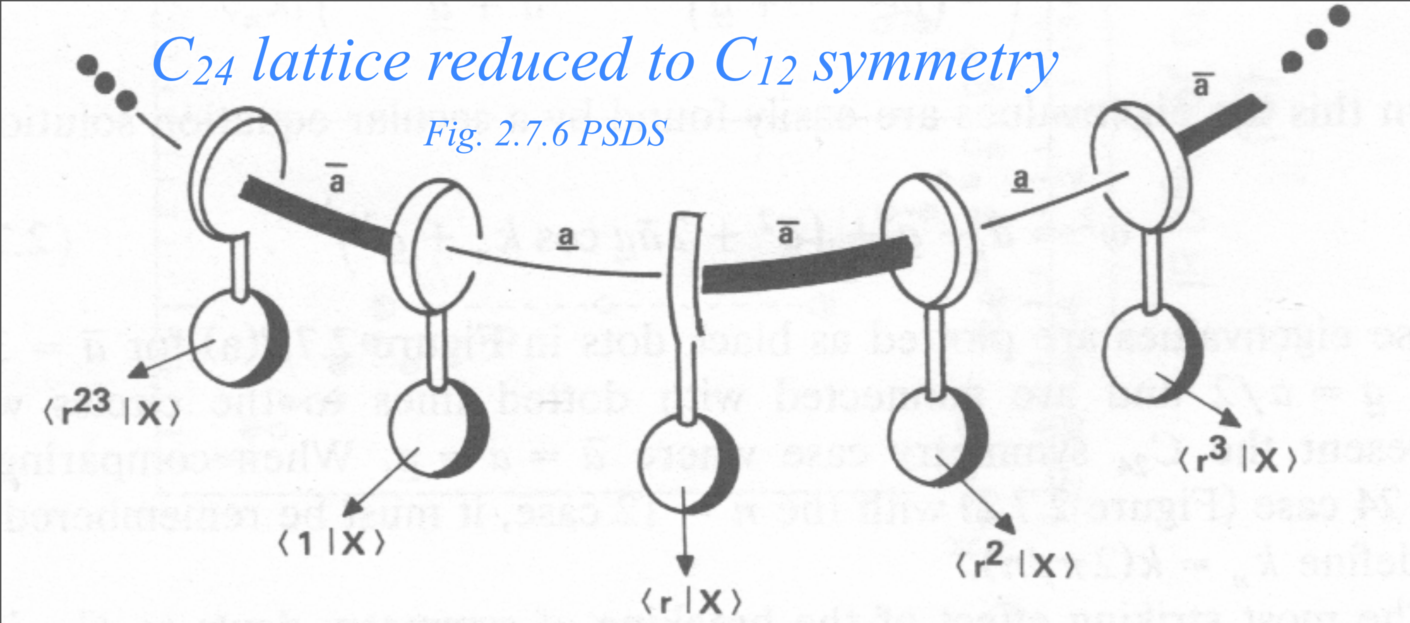

Fig. 2.7.6 PrinciplesSymmetryDynamics&Spectroscopy

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

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

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

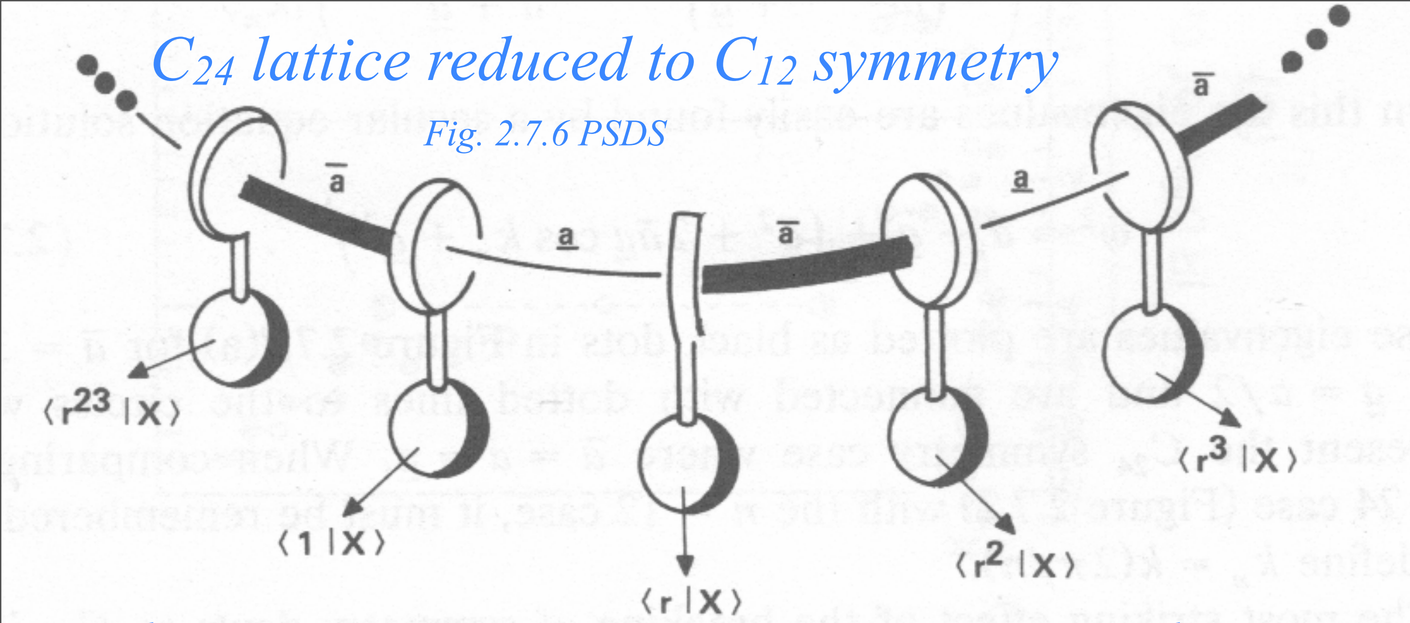

Fig. 2.7.6 PSDS

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

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

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

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

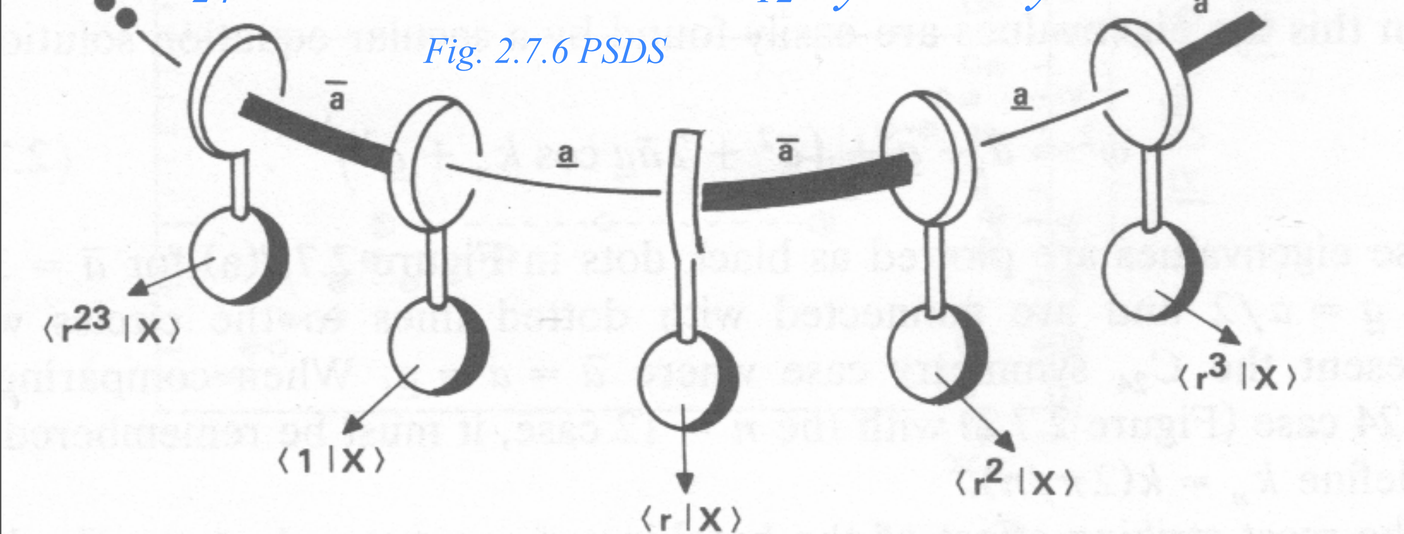

Fig. 2.7.6 PSDS

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

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

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

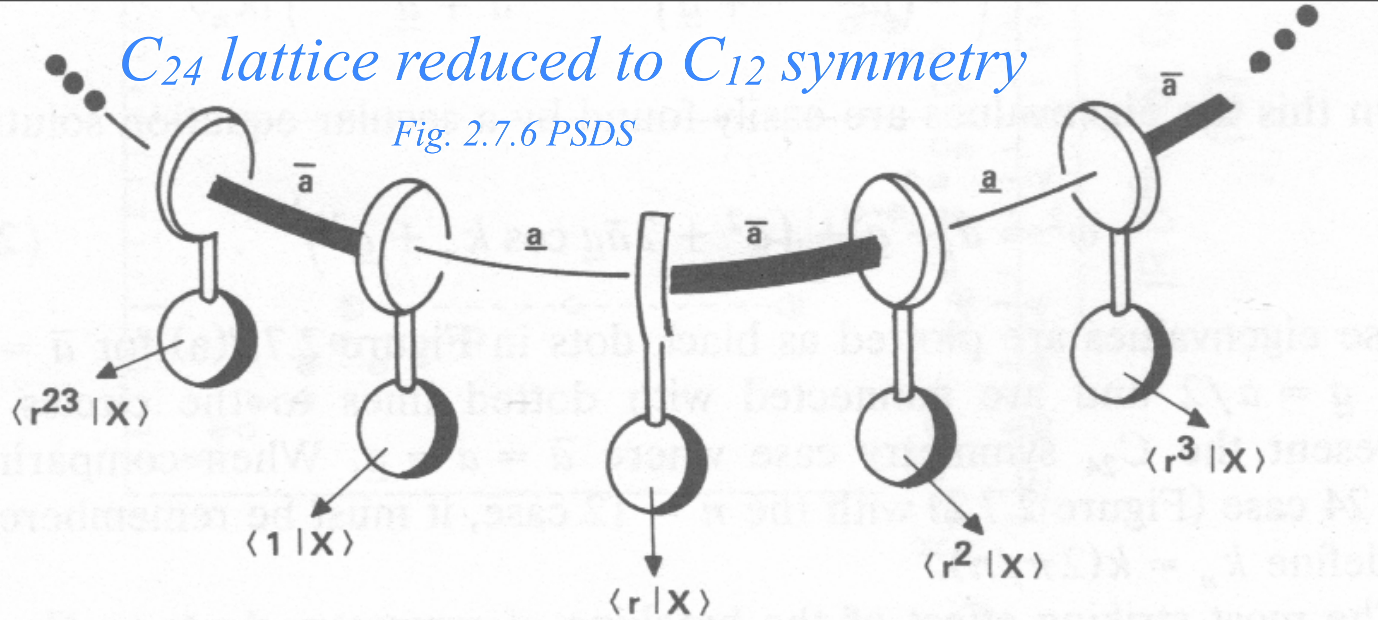

Fig. 2.7.6 PSDS

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

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

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Two kinds of C_{12} symmetry ***m****-states are coupled by* **K**-*matrix.*

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

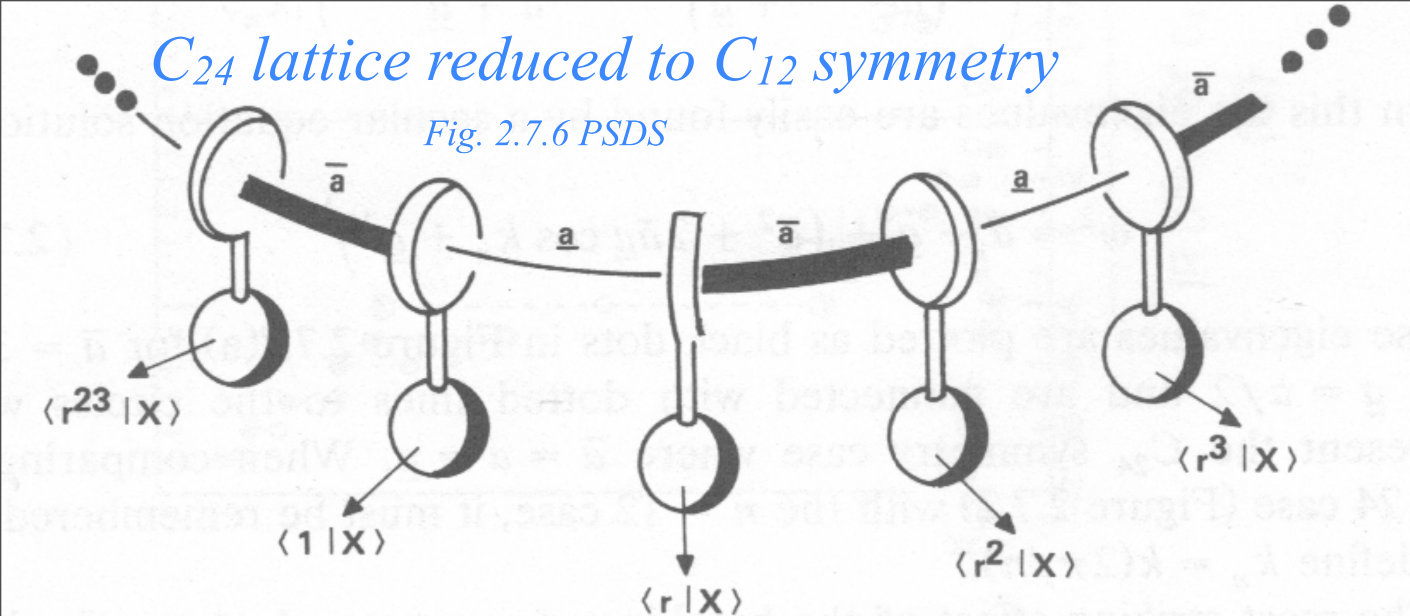


Fig. 2.7.6 PSDS

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

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

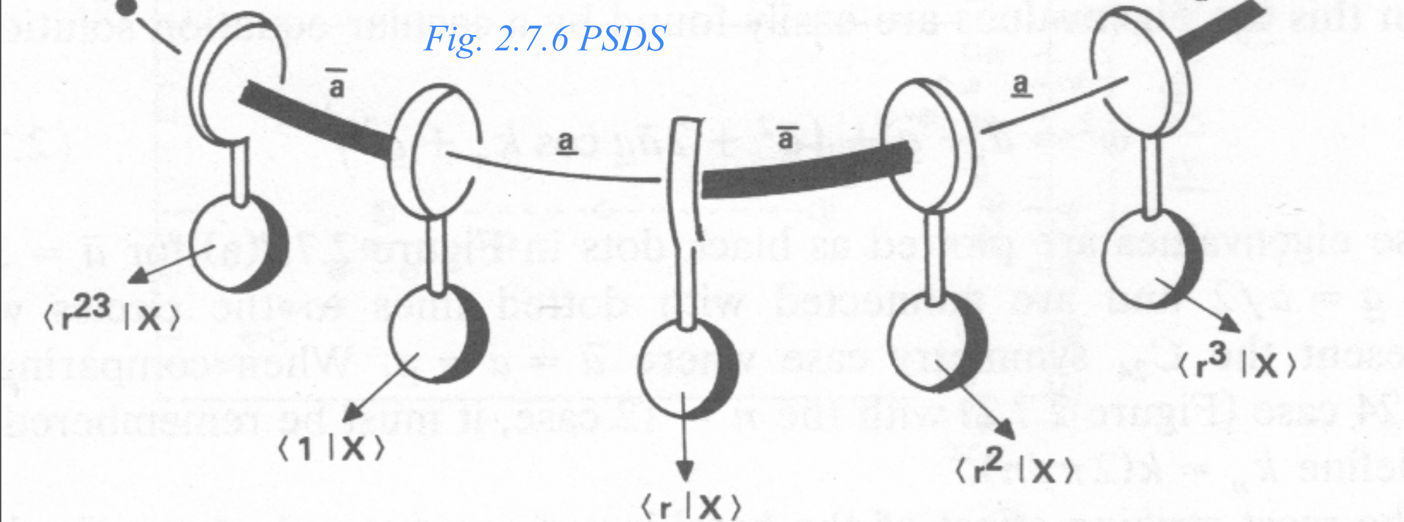
$$
\mathbf{P}^{(m)} = \frac{1}{12}\left(\mathbf{1} + e^{-ik_m}\mathbf{r}^2 + e^{-2ik_m}\mathbf{r}^4 + e^{-3ik_m}\mathbf{r}^6 + \ldots + e^{+2ik_m}\mathbf{r}^{-4} + e^{+ik_m}\mathbf{r}^{-2}\right) \quad \text{where:} \quad k_m = \frac{2\pi m}{12}
$$

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

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

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

Fig. 2.7.6 PSDS



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

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

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

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$$\begin{aligned} \langle k_m|\mathbf{K}|k_m\rangle &= \langle r^0|\mathbf{P}^{(m)}\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle\cdot 12 = \langle r^0|\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle\cdot 12 \\ &= \langle r^0|\mathbf{K}|r^0\rangle + e^{-ik_m}\langle r^0|\mathbf{K}|r^2\rangle + e^{-2ik_m}\langle r^0|\mathbf{K}|r^4\rangle|r^5\rangle + \dots \\ &= \underline{a}+\bar{a} \quad + \quad 0 \quad + \quad 0 \quad + \dots \end{aligned}$$

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

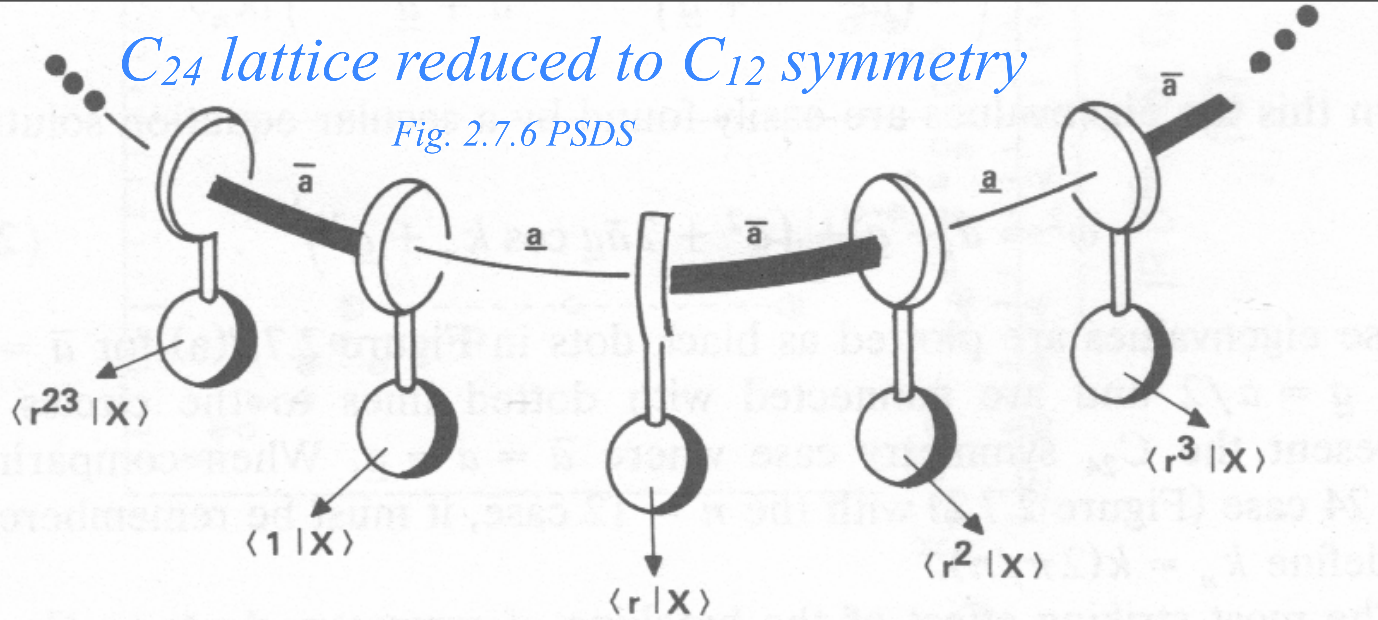

Fig. 2.7.6 PSDS

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

Only C_{12} symmetry projectors commute with **K**-*matrix if* $\underline{a} \neq \bar{a}$. *Then C_{24}-symmetry is b r o k e n !*

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

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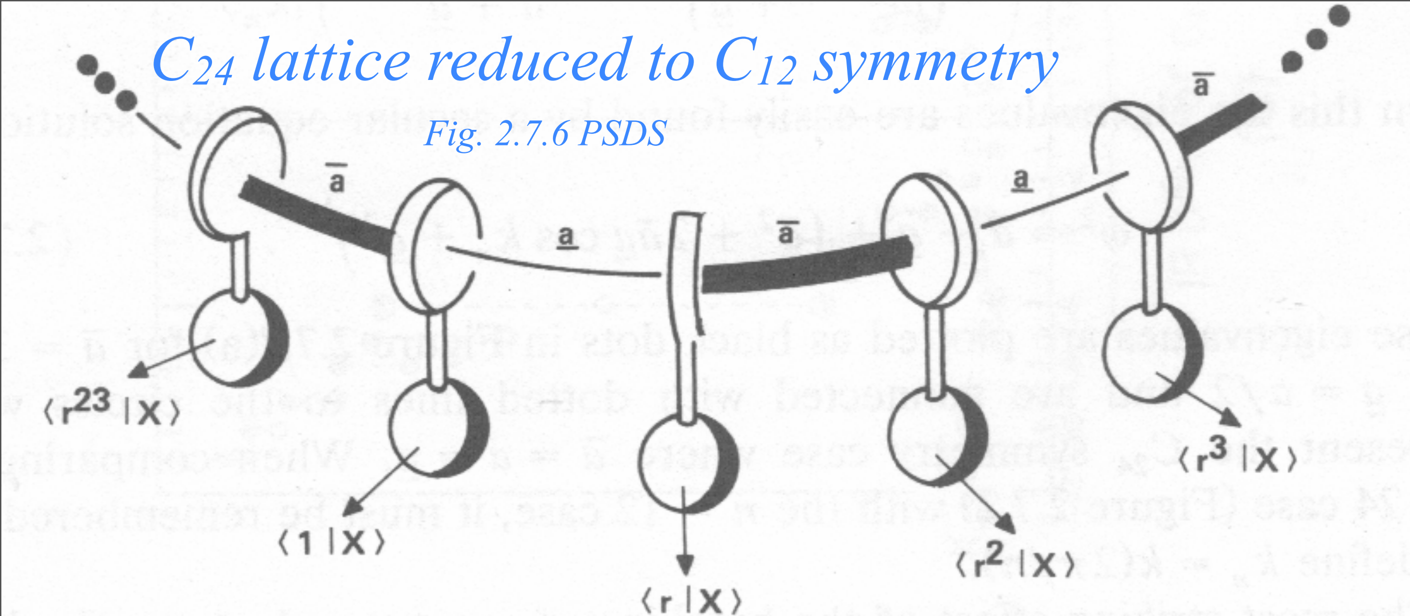
$$\begin{aligned} \langle k'_m|\mathbf{K}|k_m\rangle &= \langle r^1|\mathbf{P}^{(m)}\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle \cdot 12 = \langle r^1|\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle \cdot 12 \\ &= \langle r^1|\mathbf{K}|r^0\rangle + e^{-ik_m}\langle r^1|\mathbf{K}|r^2\rangle + e^{-2ik_m}\langle r^1|\mathbf{K}|r^4\rangle|r^5\rangle + \dots \\ &= \quad -\underline{a} \quad + \ e^{-ik_m}\ (-\bar{a}) \quad + \quad 0 \quad + \dots \\ &= \quad -(\underline{a} \quad + \ e^{-ik_m}\bar{a}) \ = \ \langle k_m|\mathbf{K}|k'_m\rangle^* \end{aligned}$$

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

$$\begin{aligned}\langle k'_m|\mathbf{K}|k_m\rangle &= \langle r^1|\mathbf{P}^{(m)}\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle\cdot 12 = \langle r^1|\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle\cdot 12 \\ &= \langle r^1|\mathbf{K}|r^0\rangle + e^{-ik_m}\langle r^1|\mathbf{K}|r^2\rangle + e^{-2ik_m}\langle r^1|\mathbf{K}|r^4\rangle|r^5\rangle + \dots \\ &= -\underline{a} \quad + e^{-ik_m}\ (-\bar{a}) \quad + \quad 0 \quad + \dots \\ &= -(\underline{a} \quad + e^{-ik_m}\bar{a}) \quad = \langle k_m|\mathbf{K}|k'_m\rangle^*\end{aligned}$$

Breaking C_N cyclic coupling into linear chains

Review of 1D-Bohr-ring related to infinite square well (and review of revival)

Breaking C_{2N+2} to approximate linear N-chain

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

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

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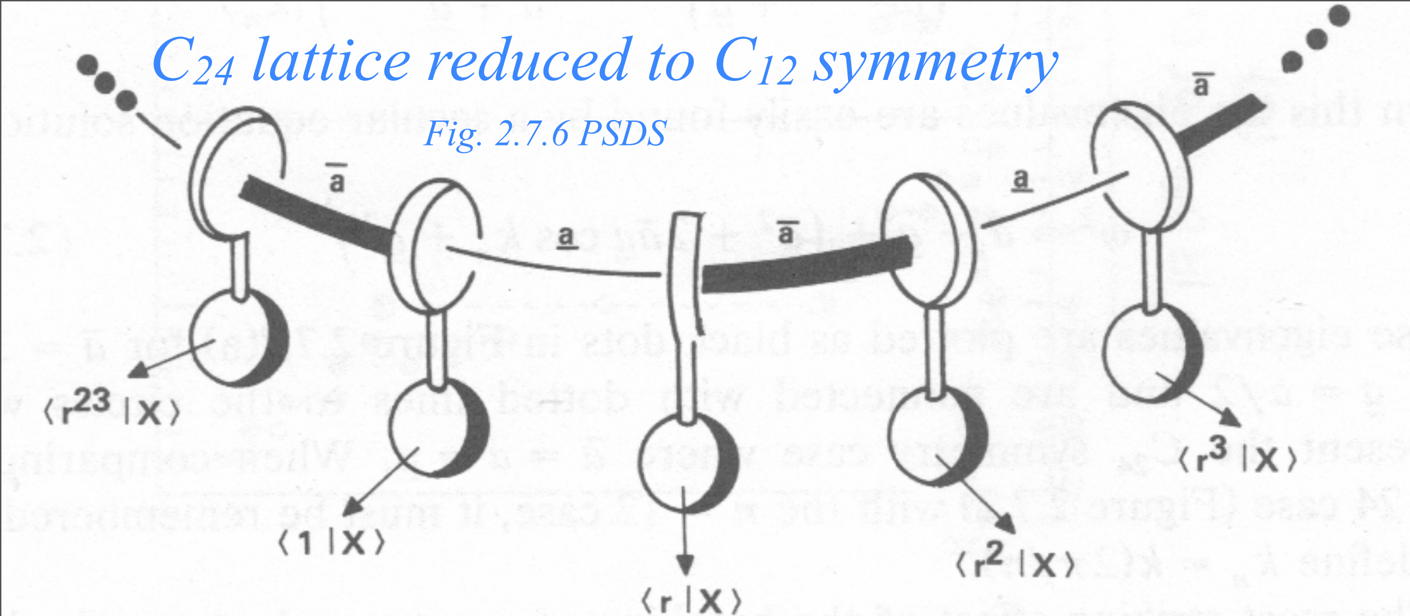

Fig. 2.7.6 PSDS

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

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

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

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

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

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

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

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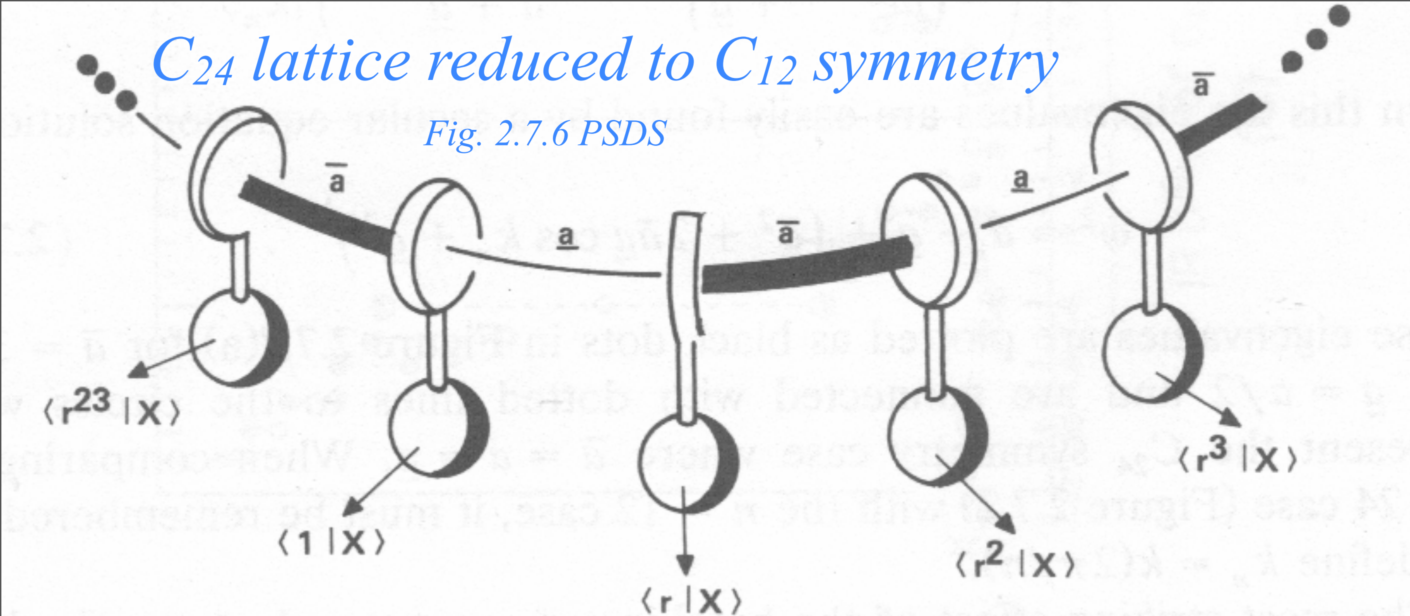

Fig. 2.7.6 PSDS

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

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Secular Eq.:

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

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

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

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

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

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

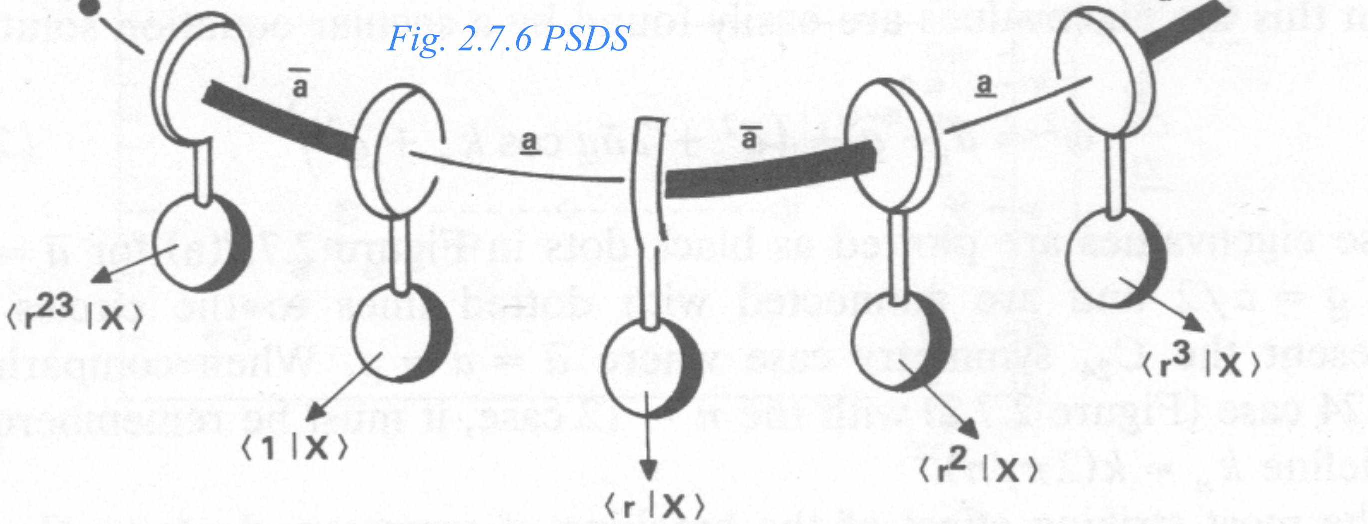

Fig. 2.7.6 PSDS

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

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

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

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

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

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

Secular Eq.:

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

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

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

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

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

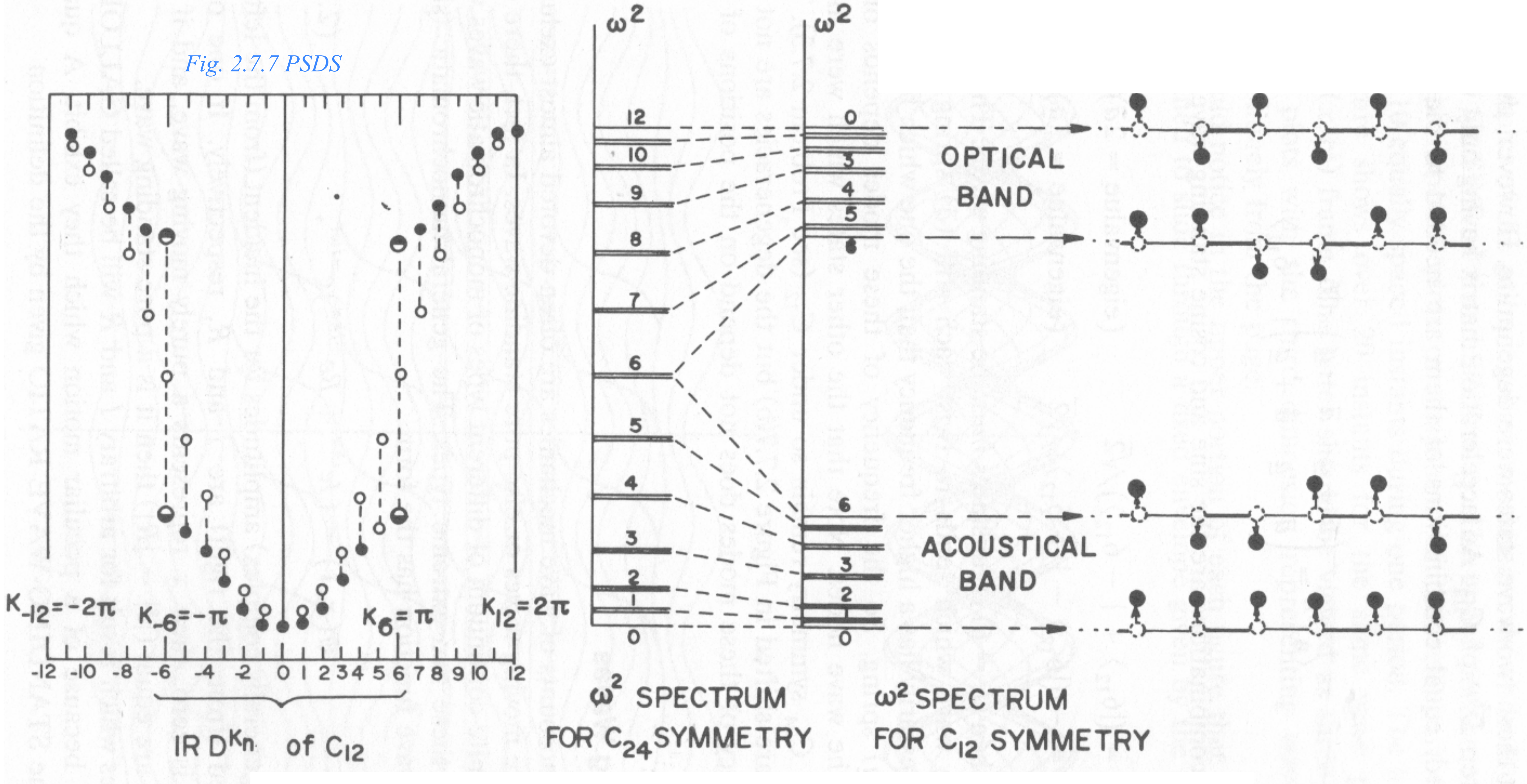

Figure 2.7.7 Band splitting due to C_{24}–C_{12} symmetry breaking.

Eigenvalues:

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

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

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

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

Fig. 2.7.7 PSDS

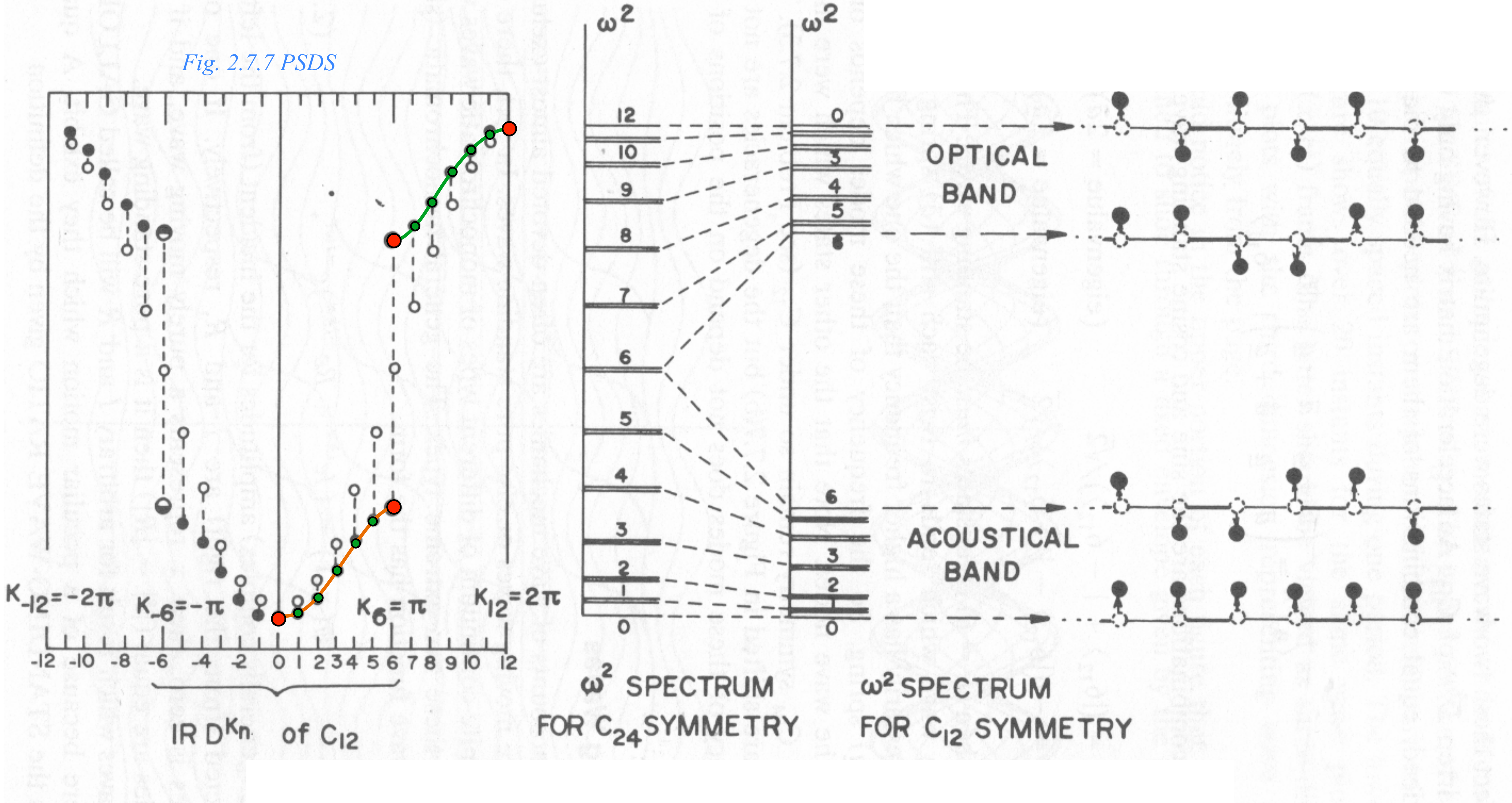

Figure 2.7.7 Band splitting due to C_{24}–C_{12} symmetry breaking.

Eigenvalues:

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

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

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

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

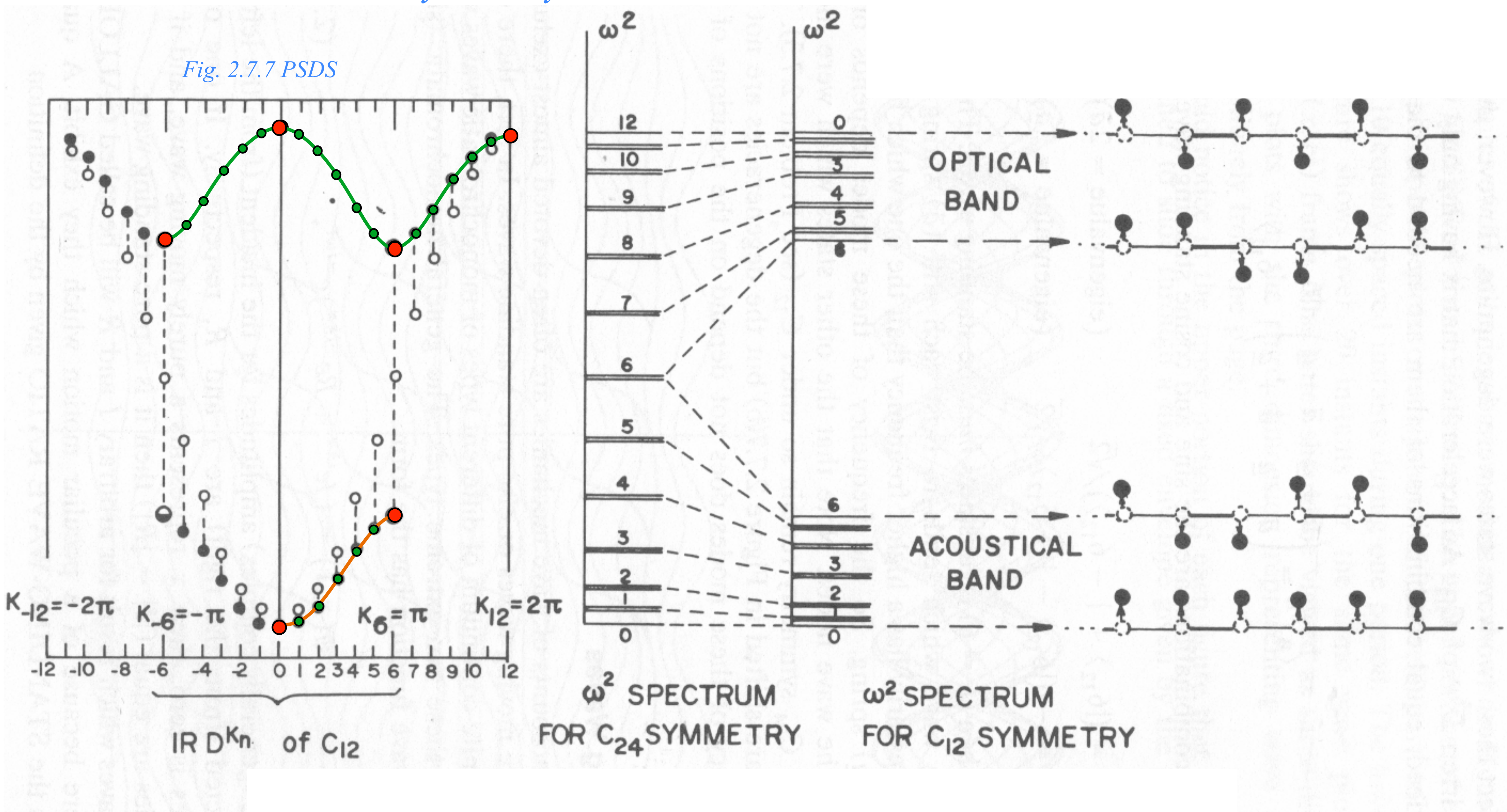

Figure 2.7.7 Band splitting due to C_{24}–C_{12} symmetry breaking.

Eigenvalues:

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

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

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

Breaking C_N cyclic coupling into linear chains

Review of 1D-Bohr-ring related to infinite square well (and review of revival)

Breaking C_{2N+2} to approximate linear N-chain

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Type-AB avoided crossing view of band-gaps

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

Spectral decomposition of D_2

Some D_2 modes

Outer product properties and the Group Zoo

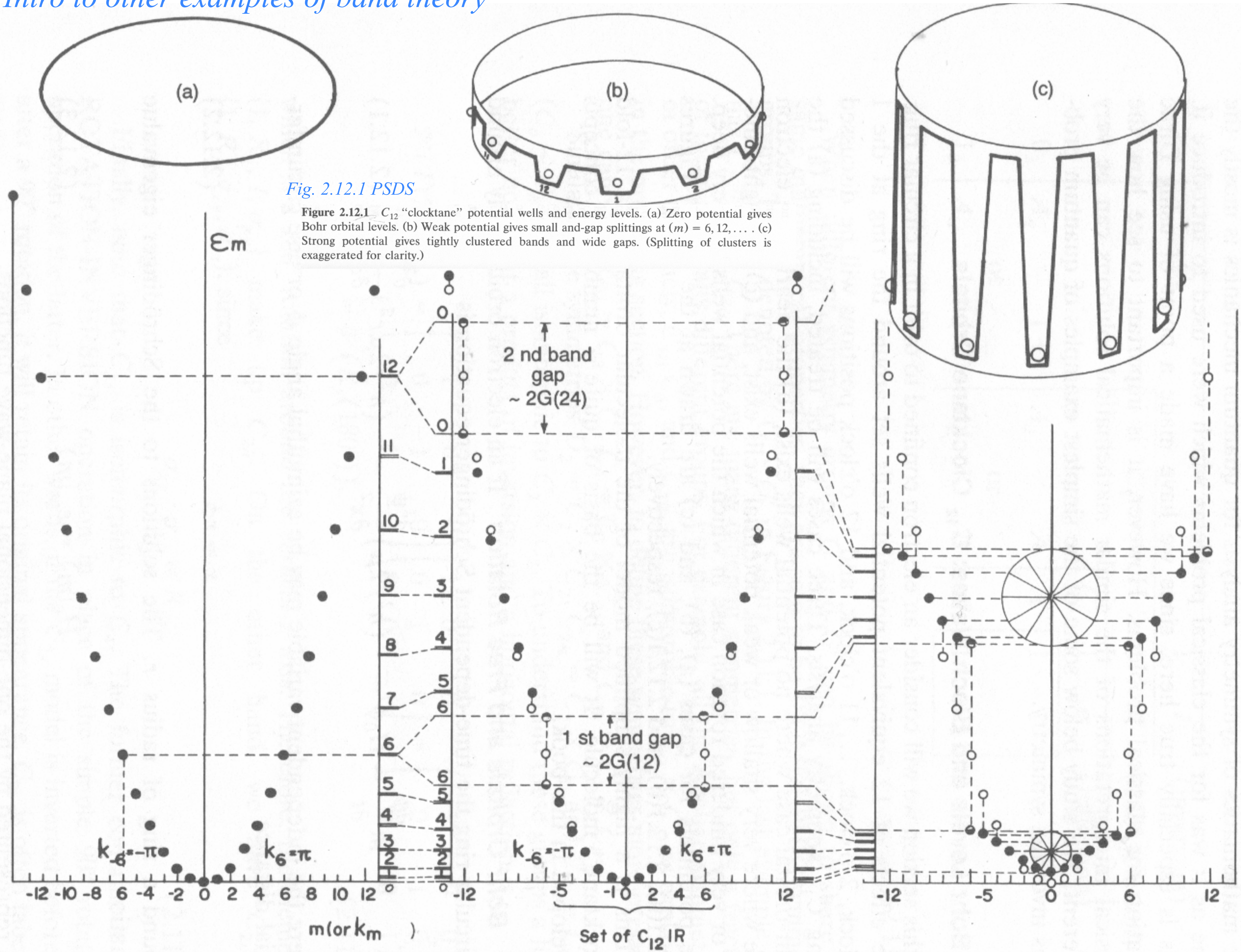


Figure 2.12.1 C_{12} "clocktane" potential wells and energy levels. (a) Zero potential gives Bohr orbital levels. (b) Weak potential gives small and-gap splittings at $(m) = 6, 12, \ldots$. (c) Strong potential gives tightly clustered bands and wide gaps. (Splitting of clusters is exaggerated for clarity.)

Crossing equations for a pair of humps

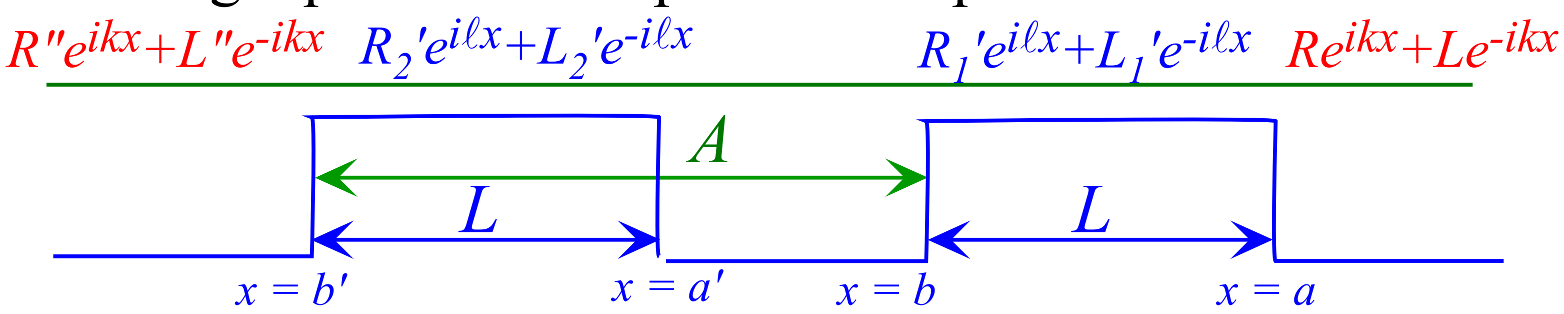


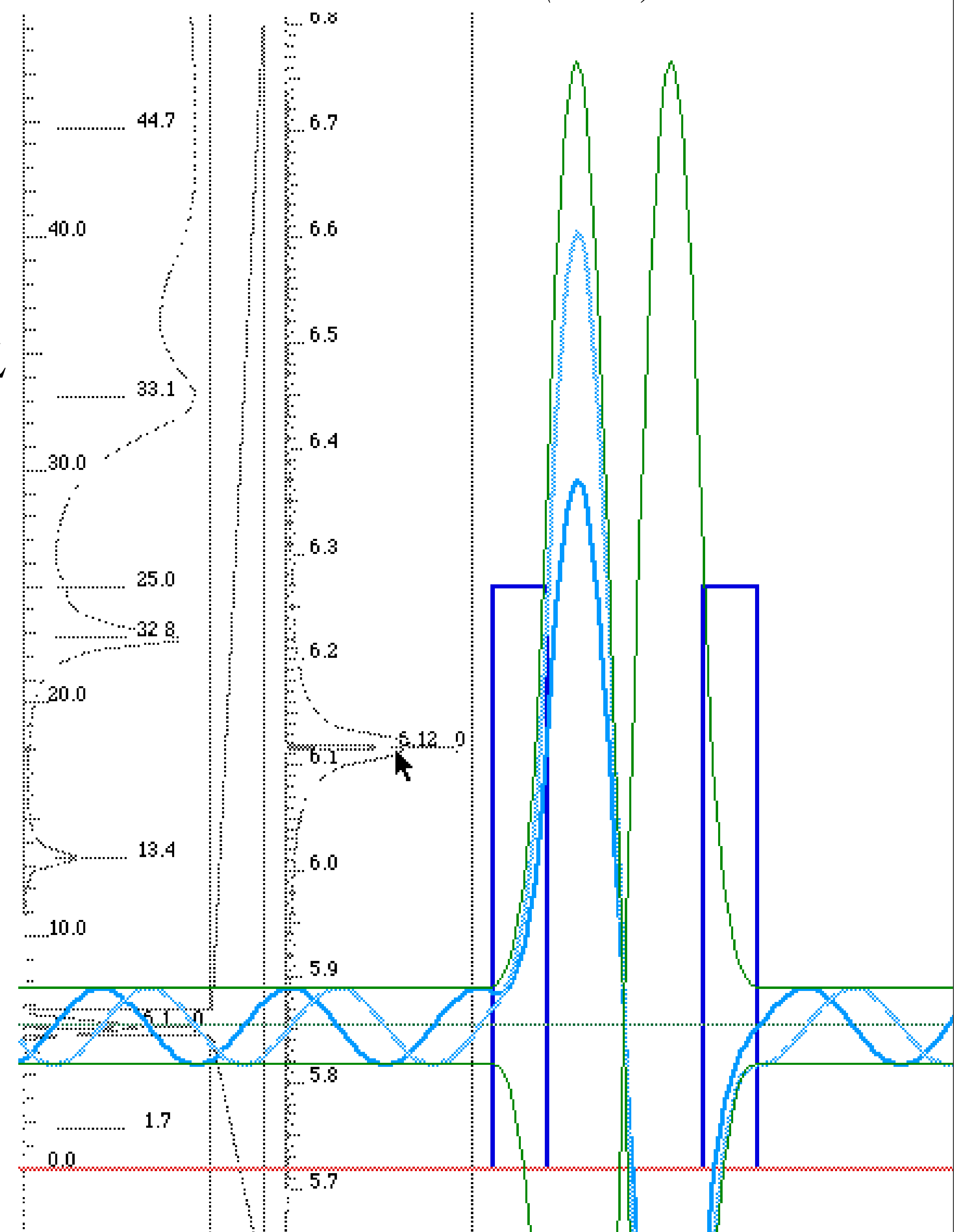
Fig. 14.1.5 C₂-symmetric double barrier .

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

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

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

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



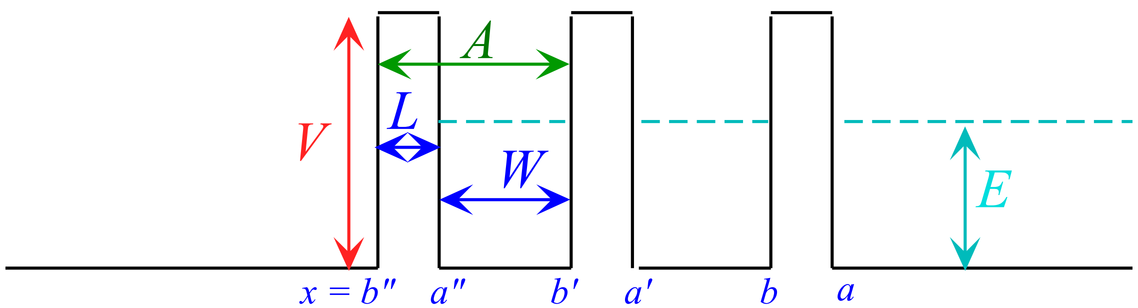
Intro to other examples of band theory

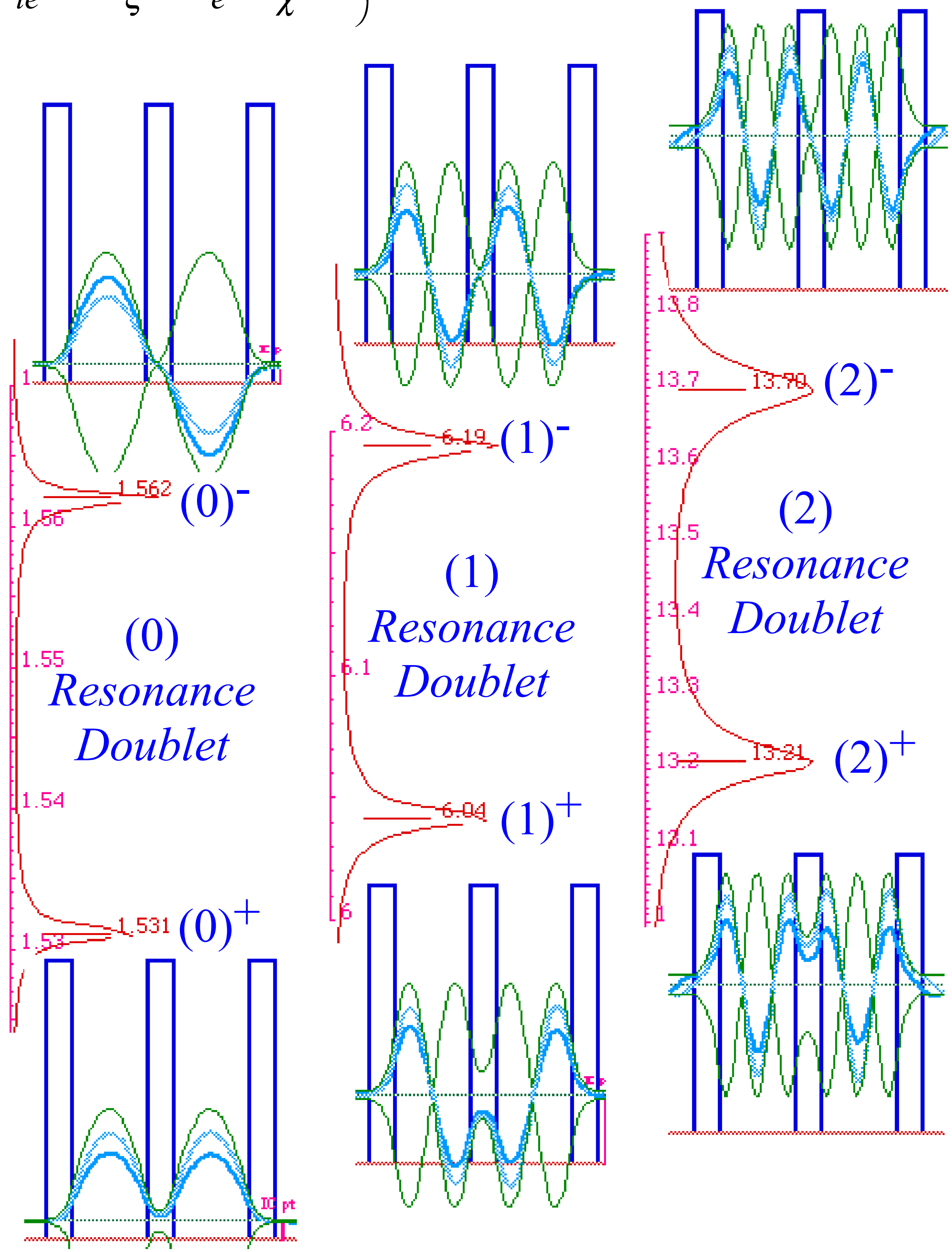
$$C^{3-barrier} = C'' \cdot C' \cdot C$$

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

Crossing equations for three humps

Fig. 14.1.10 Triple-barrier double-well potential





Intro to other examples of band theory

Bohr-It simulations assume ring-periodic-boundary conditions

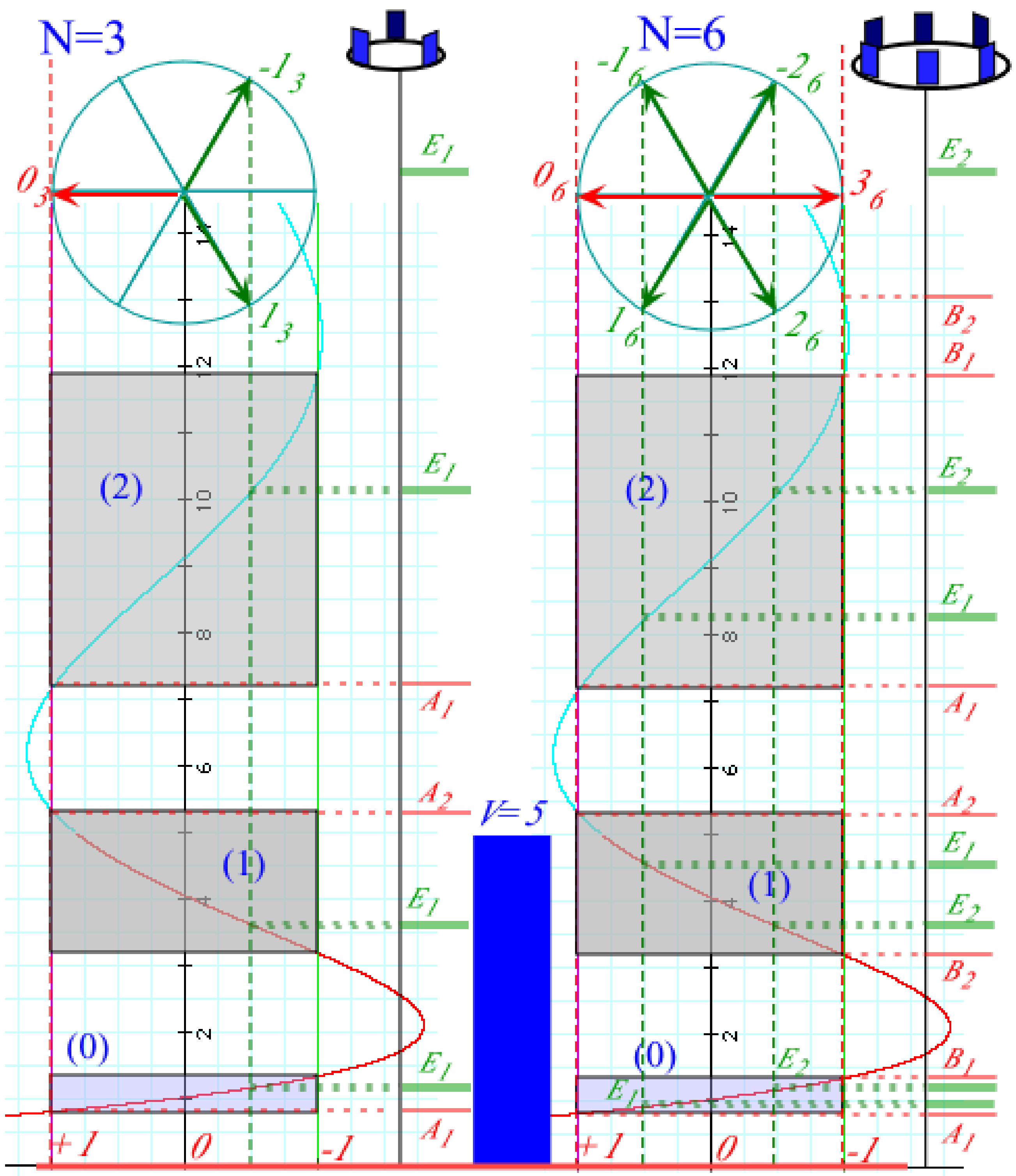


Fig. 14.2.8 Multiplets for V=5.
(W=15nm well ,L=5nm barrier) for (N=3)-ring and (N=6)-ring.

Intro to other examples of band theory

Bohr-It simulations assume ring-periodic-boundary conditions

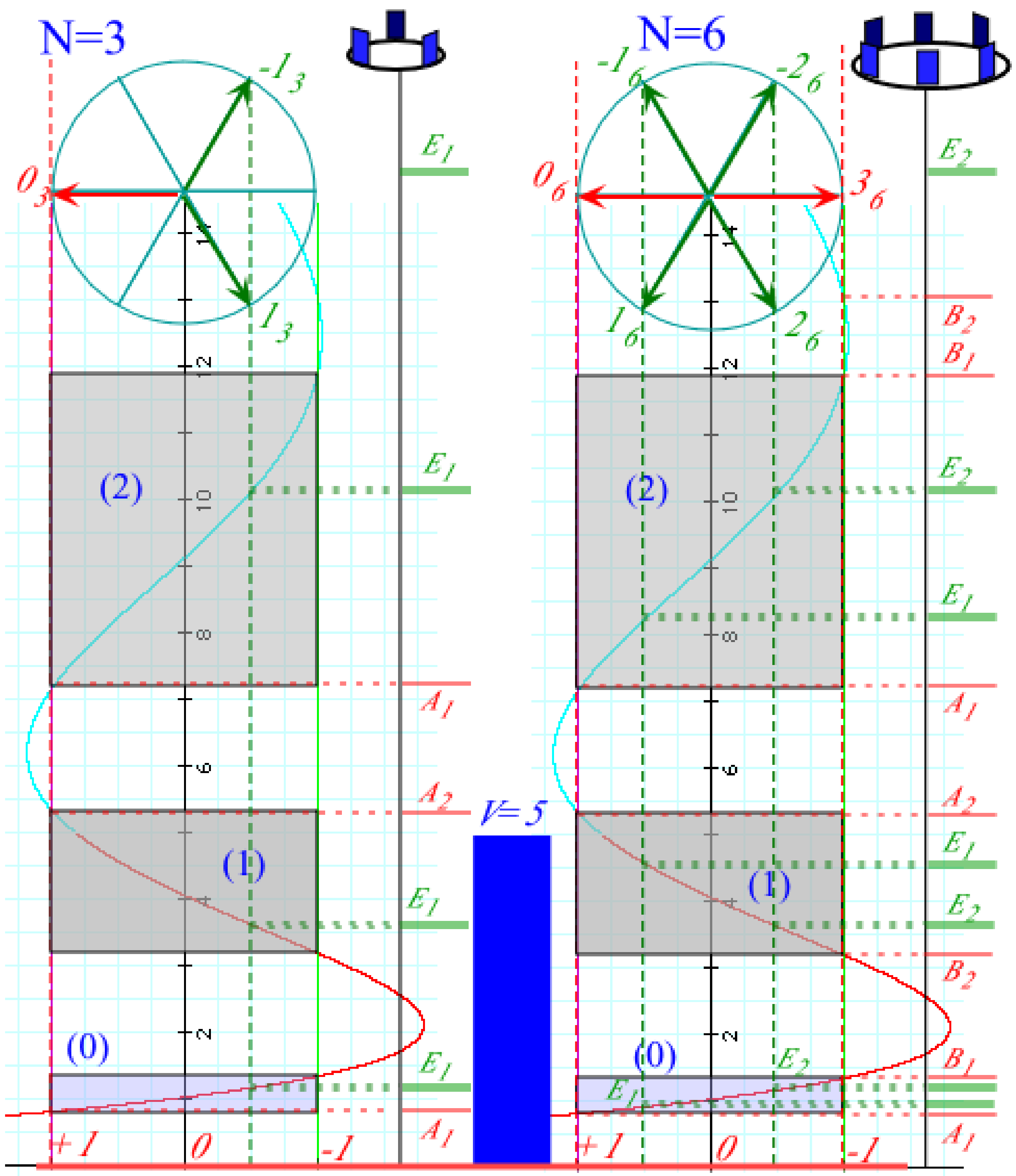


Fig. 14.2.8 Multiplets for V=5.
(W=15nm well ,L=5nm barrier) for (N=3)-ring and (N=6)-ring.

Band-It simulations line-non-periodic scattering conditions

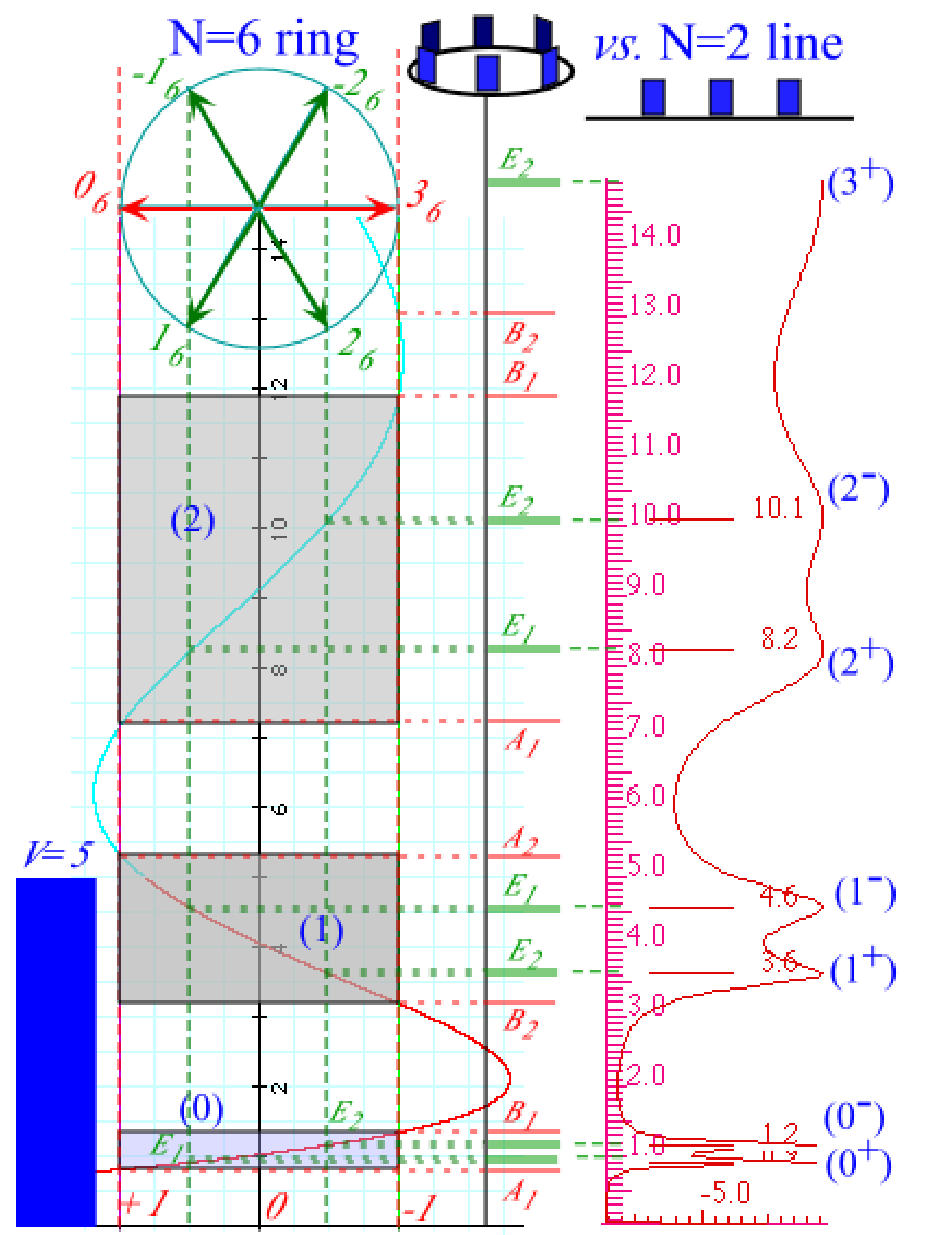


Fig. 14.2.9 (N=6)-ring and (N=2)-line potential.
(V=5, W=15nm well ,L=5nm barrier)

Breaking C_N cyclic coupling into linear chains

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*Type-*AB *avoided crossing view of band-gaps*

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Some D_2 modes

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Pure Type-B Hamiltonian

NH$_3$ (Ammonia)

Fig. 2.12.7 PSDS

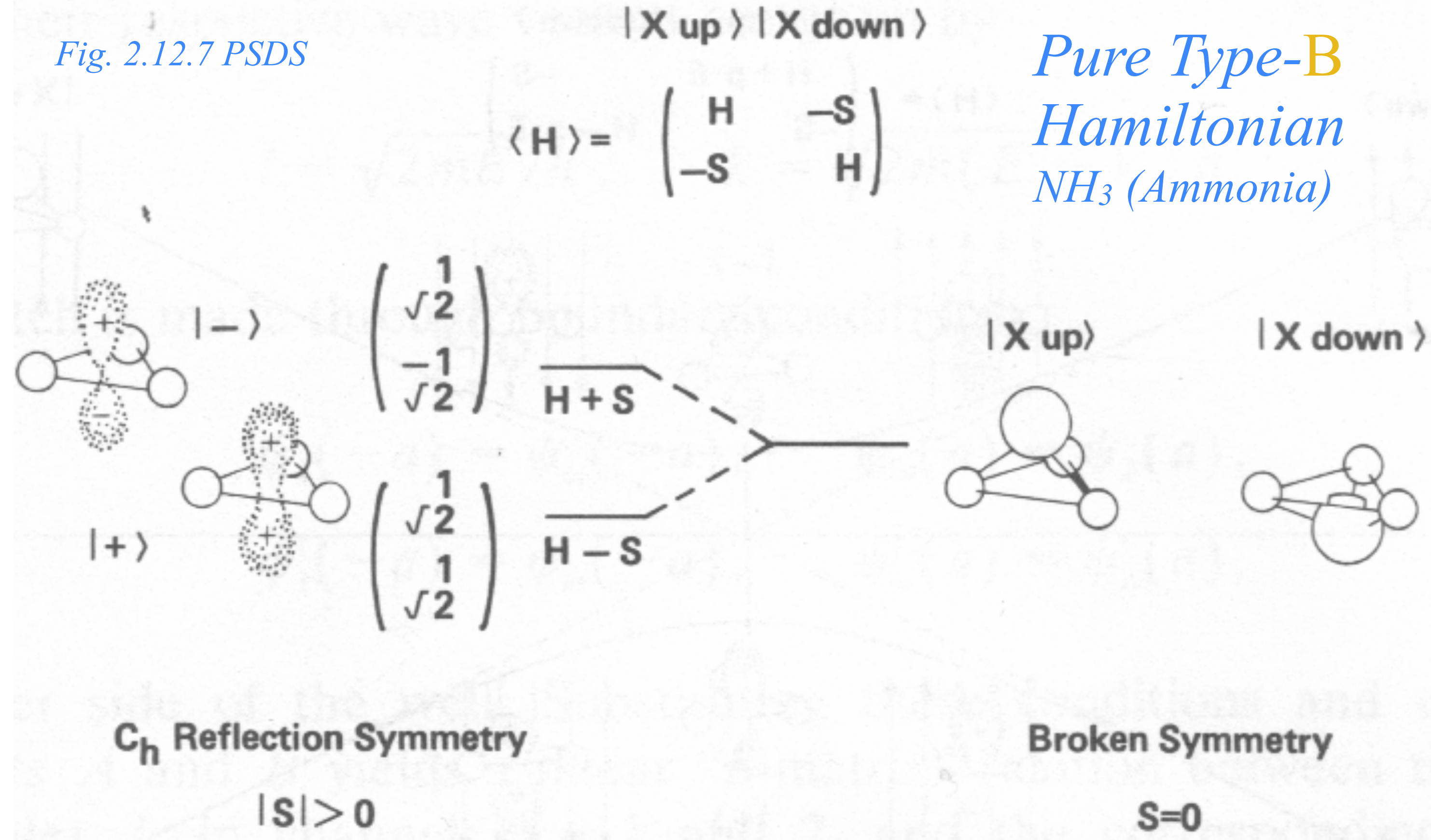
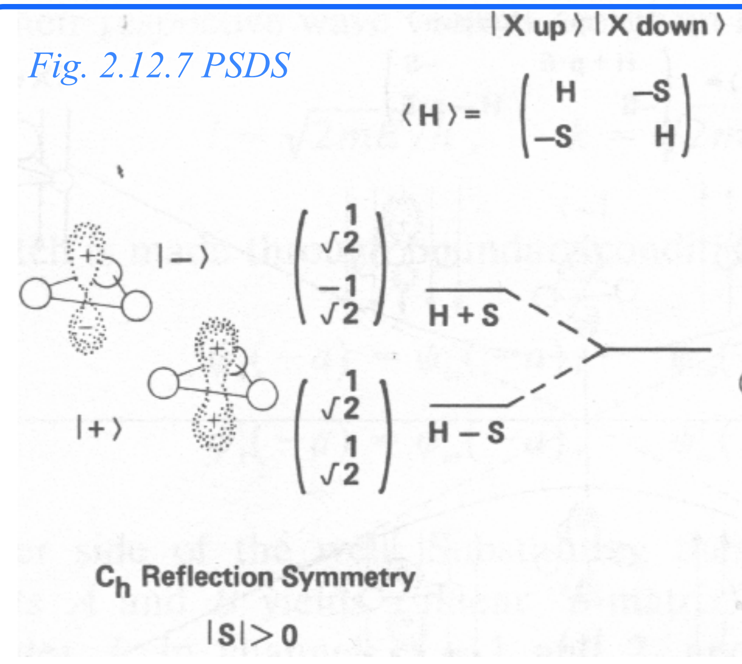


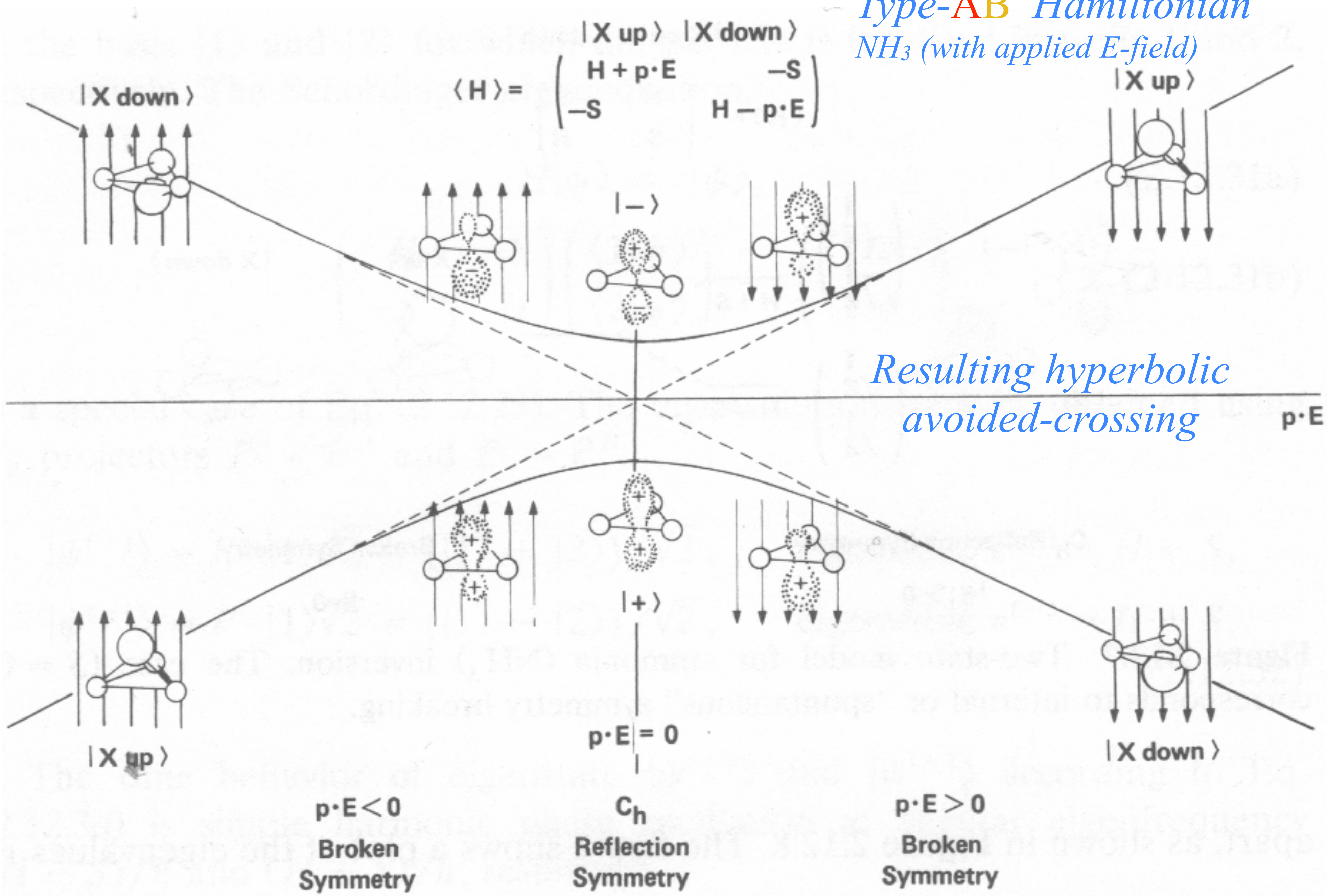
Fig. 2.12.7 PSDS

Pure Type-B Hamiltonian
NH_3 (Ammonia)



Type-AB Hamiltonian
NH_3 (with applied E-field)

Fig. 2.12.8 PSDS



Resulting hyperbolic avoided-crossing

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

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

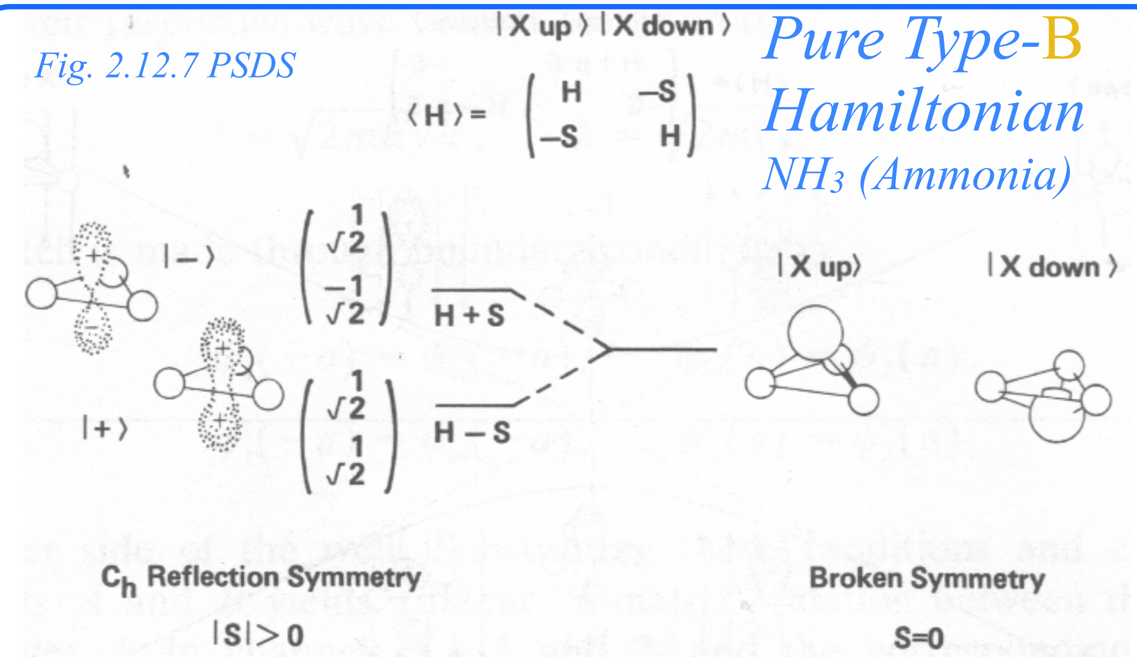
$$=\frac{1}{2}\begin{pmatrix}1&1\\1&-1\end{pmatrix}\begin{pmatrix}+A&B\\B&-A\end{pmatrix}\begin{pmatrix}1&1\\1&-1\end{pmatrix}$$

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

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

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

Fig. 2.12.7 PSDS

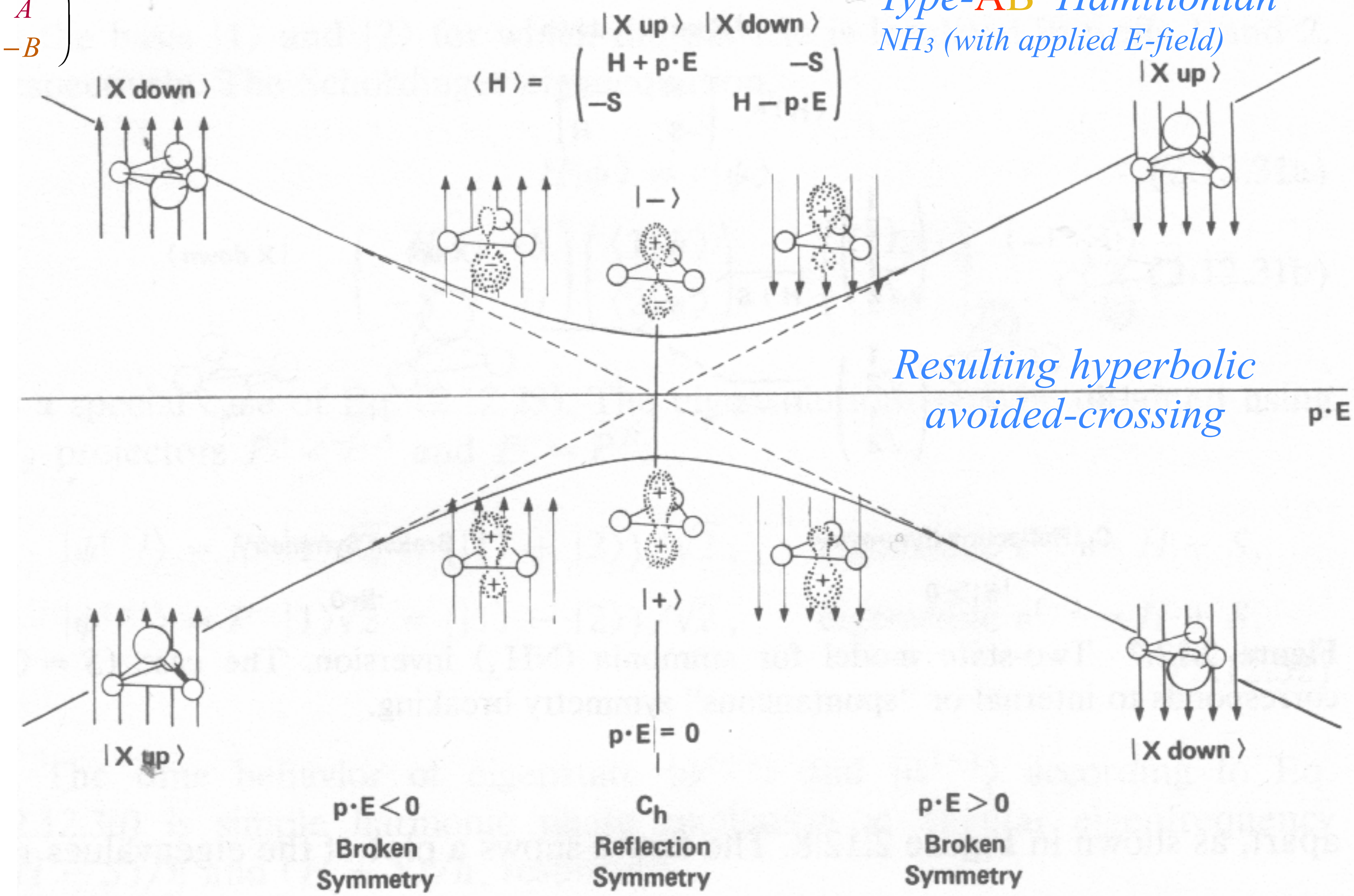


Pure Type-B Hamiltonian
NH_3 (Ammonia)

Type-AB Hamiltonian
NH_3 (with applied E-field)

Review of
Lecture 10
p. 65 to 73

Fig. 2.12.8 PSDS



Resulting hyperbolic avoided-crossing

A to B to A Symmetry breaking described by hyperbolic eigenvalues of $A\boldsymbol{\sigma}_A + B\boldsymbol{\sigma}_B = \mathbf{H} = \begin{pmatrix} +A & B \\ B & -A \end{pmatrix}$

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

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

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

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

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

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

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

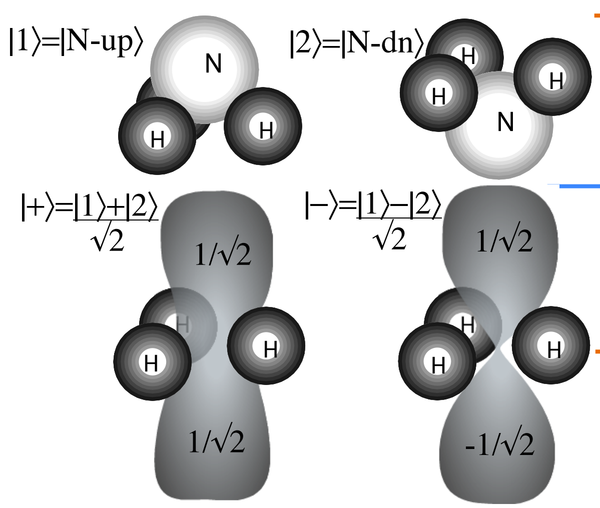


Fig. 10.3.2 Ammonia (NH_3) inversion states
(a) Base states (b) C_2-Eigenstates

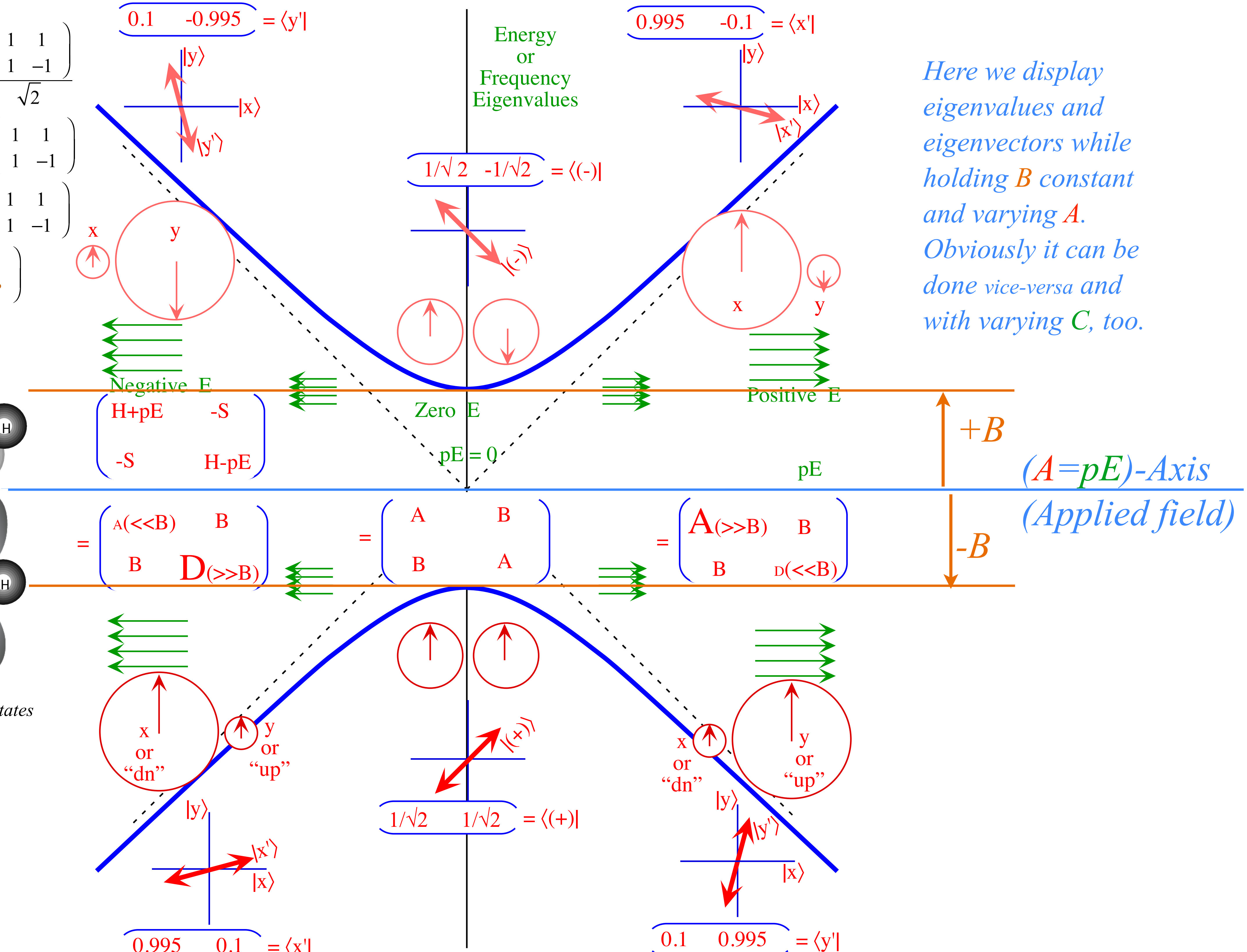


Fig. 10.3.1 (b) Wigner avoided level crossing. (Fixed tunneling B=-S and variable A-D=pE field.)

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.

Review of Lecture 10 p. 73

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Some D_2 modes

Outer product properties and the Crystal-Point Group Zoo

Finally! Symmetry groups that are not just C_N (And some that are)

Fig. 2.11.1 PSDS

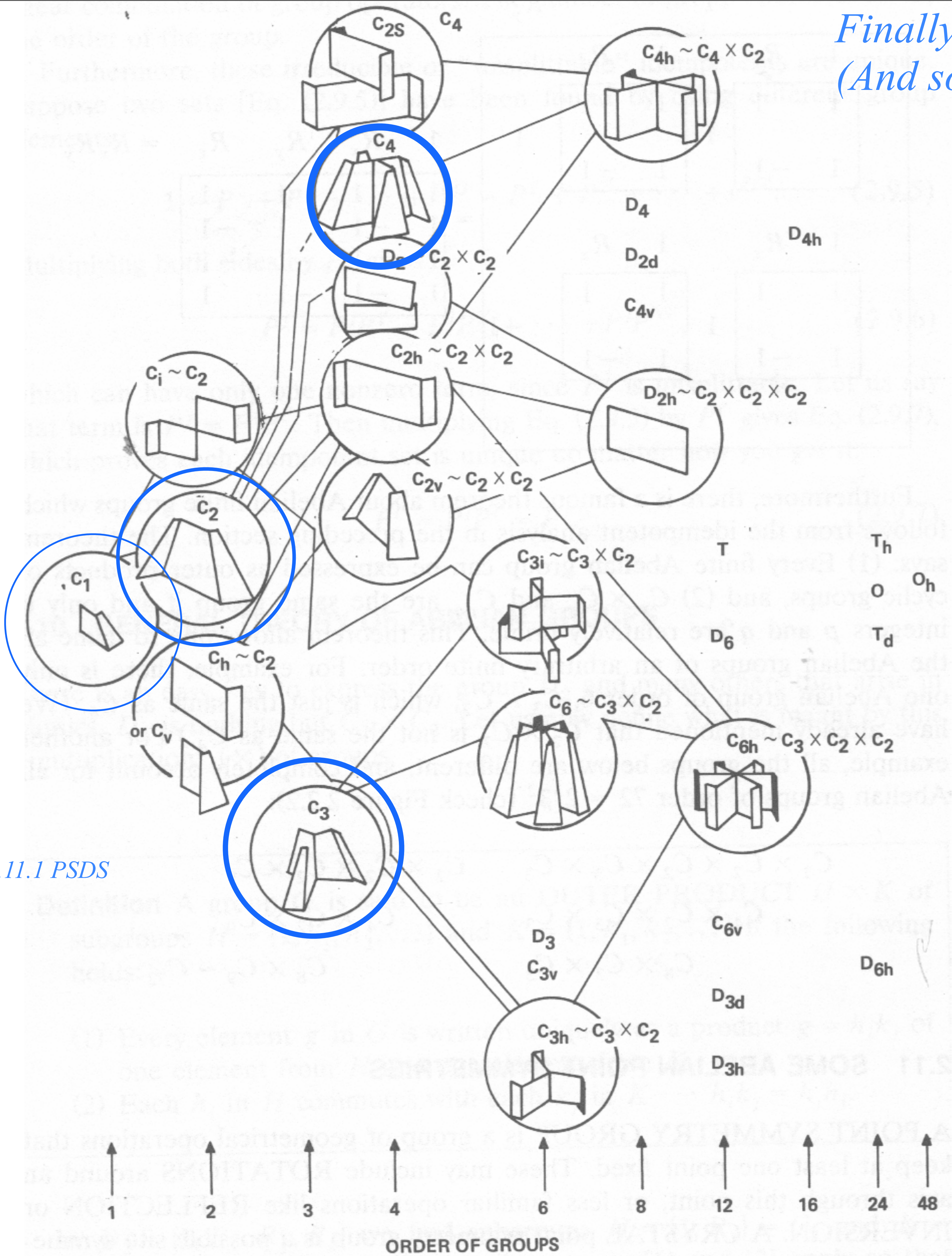


Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

Finally! Symmetry groups that are not just C_N
(And some that are)
Starting with D_2

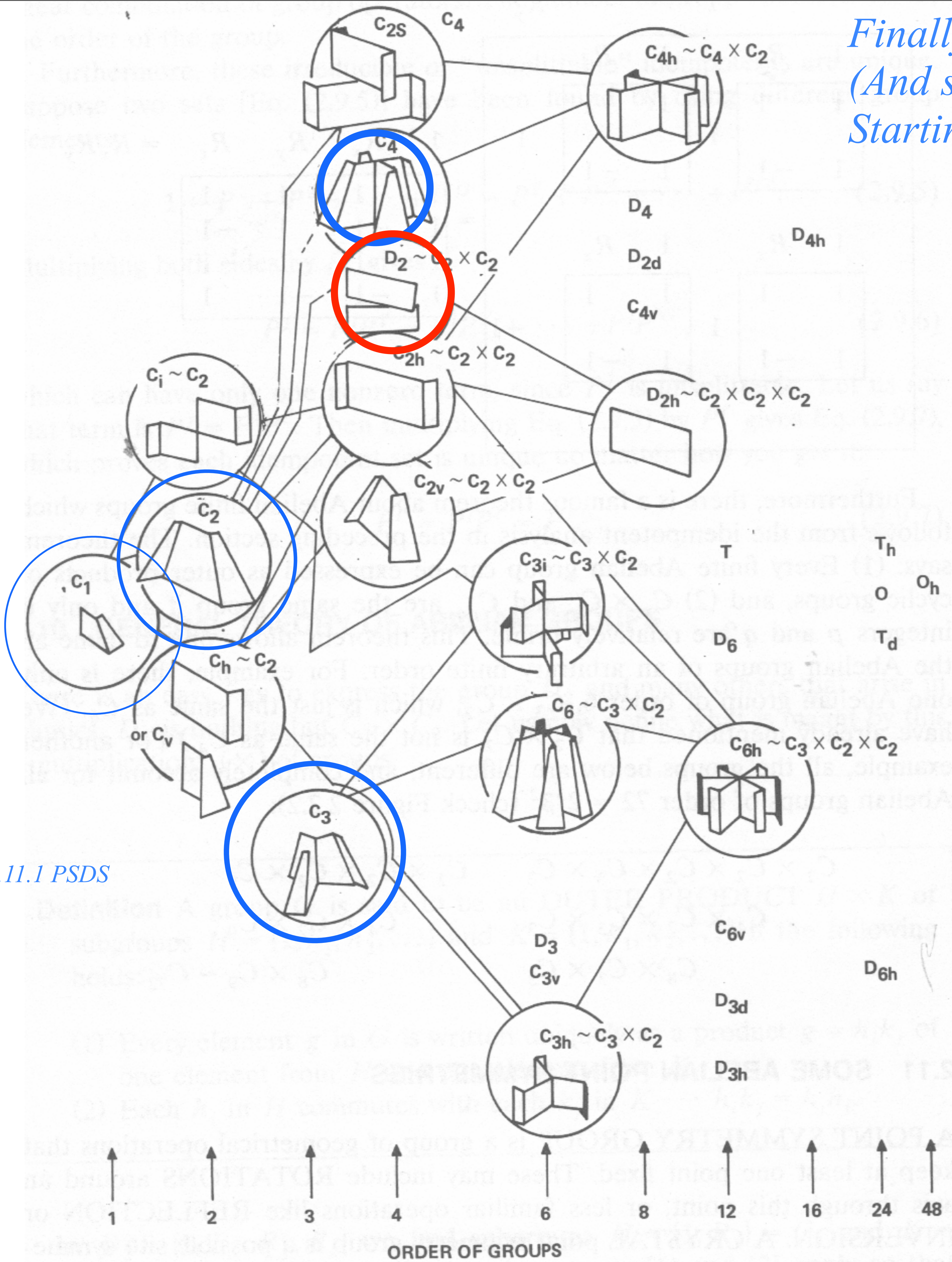


Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

Fig. 2.11.1 PSDS

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

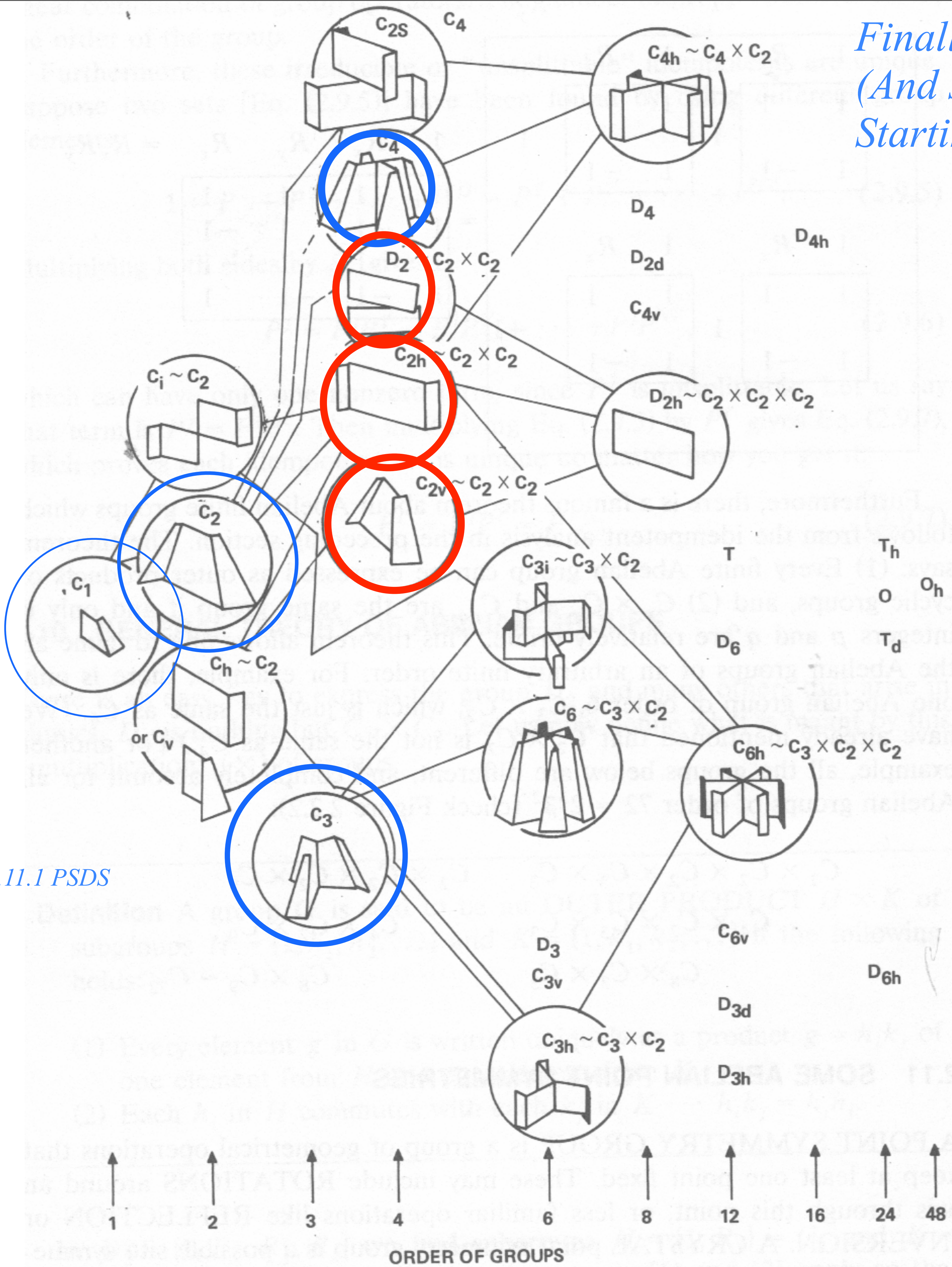
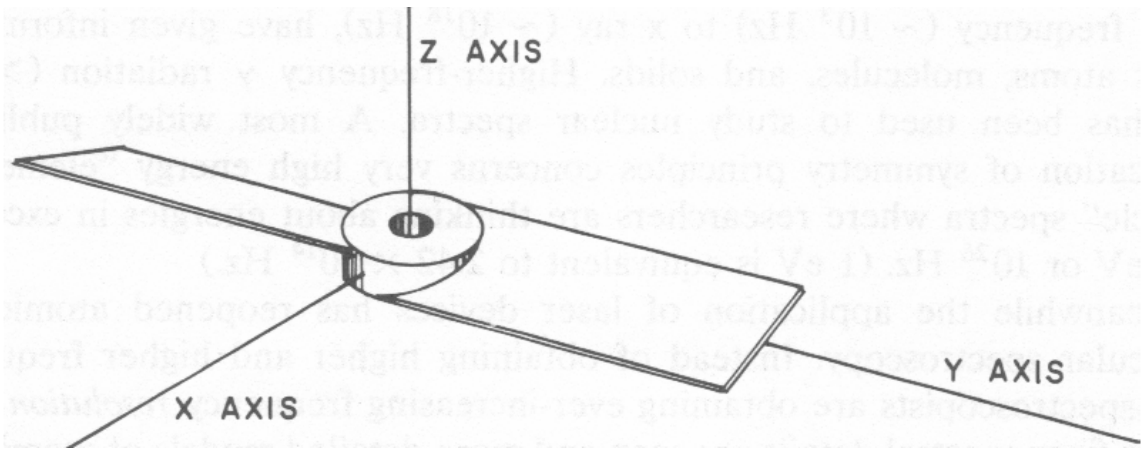


Fig. 2.11.1 PSDS

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.

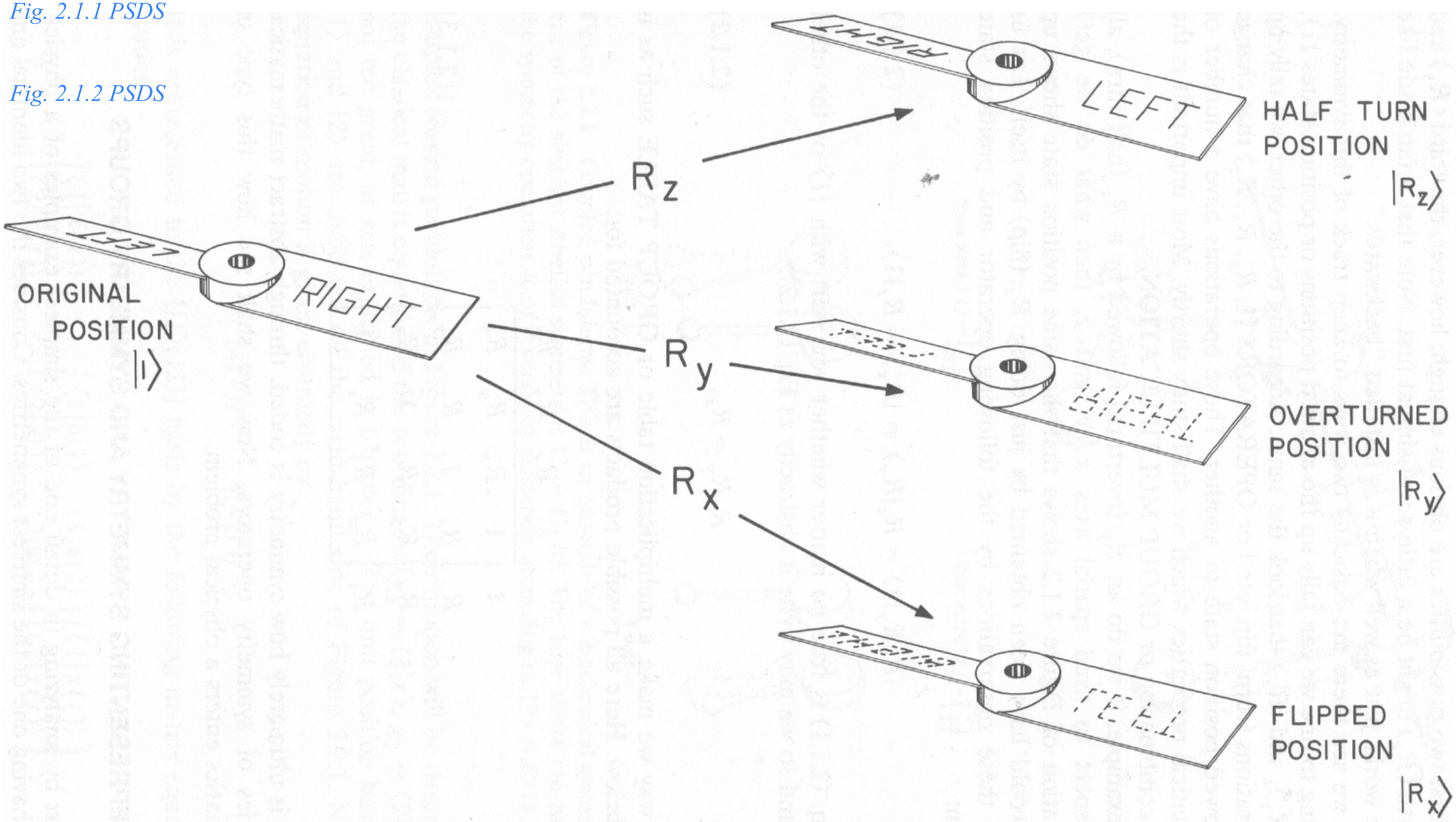
D_2 Symmetry (The 4-Group)



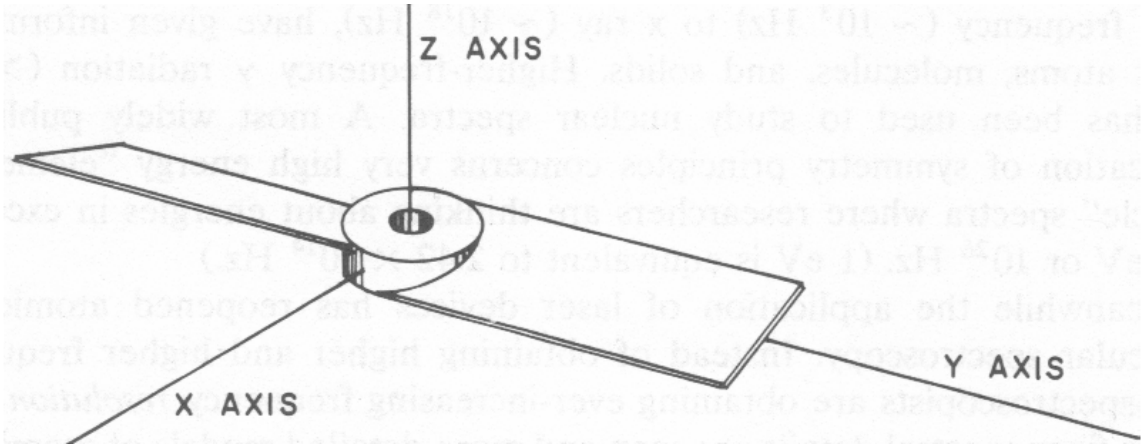
1 :	THE ORIGINAL POSITION	Don't touch the fan blade.
R_z:	THE HALF-TURN POSITION	Rotate it by 180° around its axle or the z axis.
R_y:	THE OVERTURNED POSITION	Overturn it 180° around the y axis.
R_x:	THE FLIPPED POSITION	Flip it 180° around the x axis.

Fig. 2.1.1 PSDS

Fig. 2.1.2 PSDS



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.
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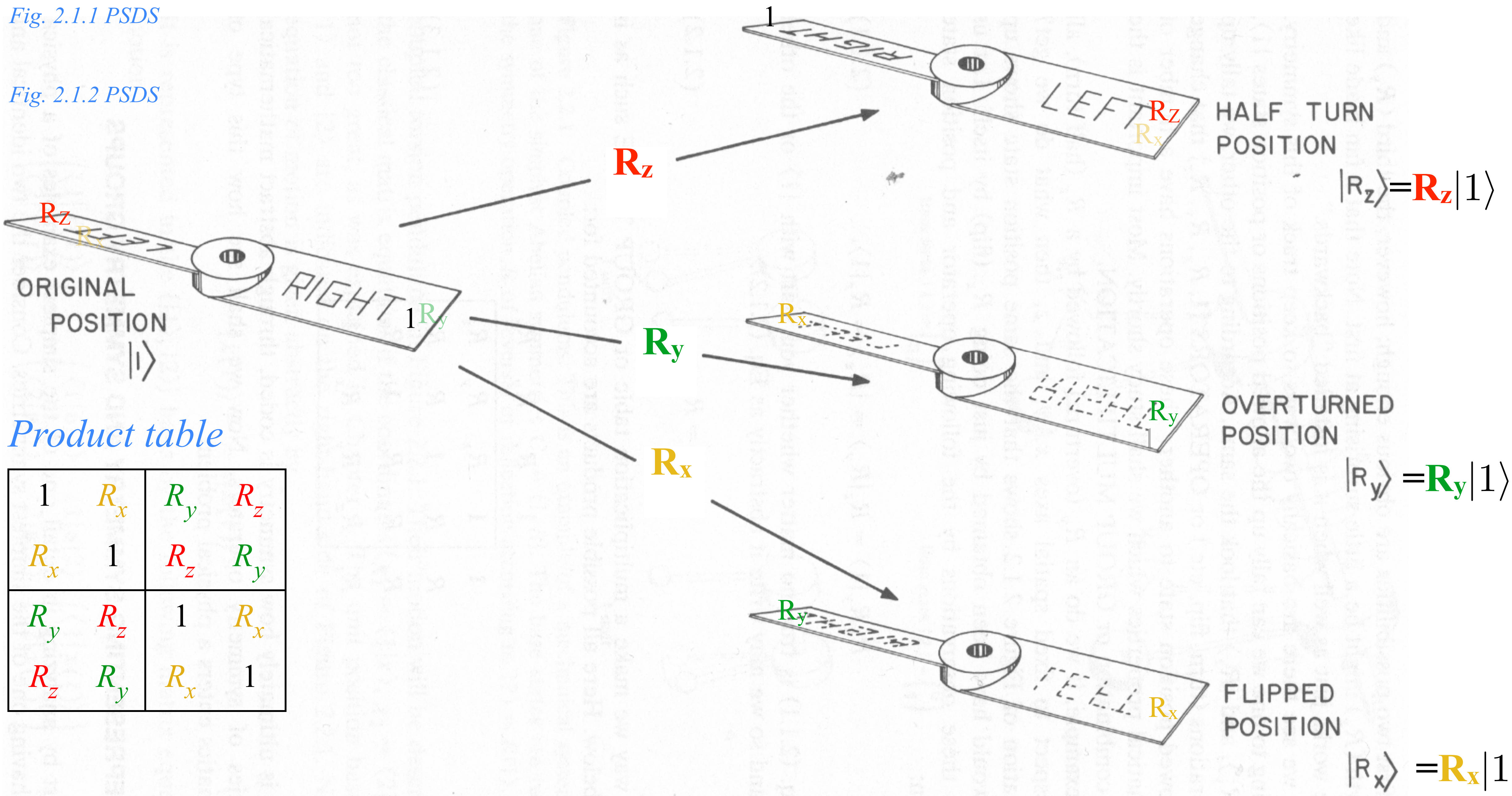
Fig. 2.1.1 PSDS

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

D_2 Symmetry (The 4-Group)

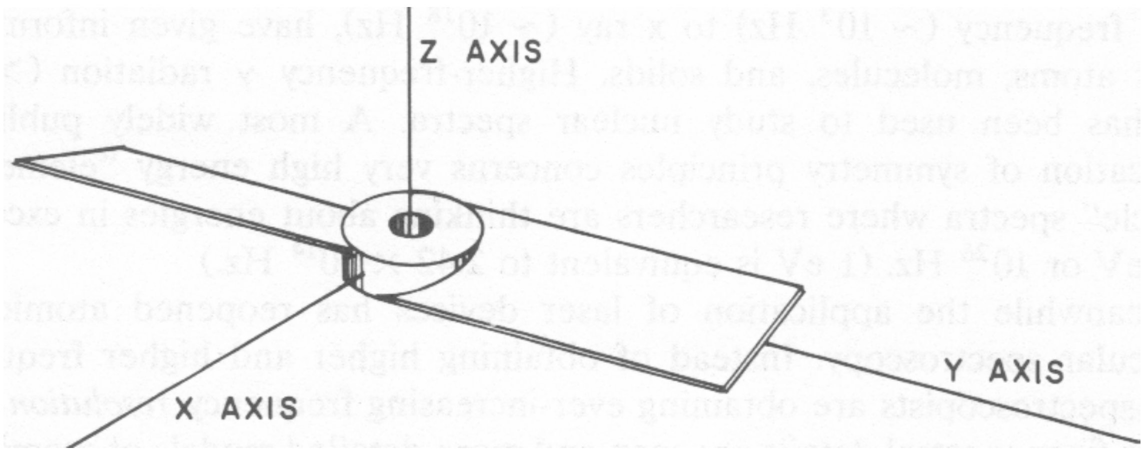


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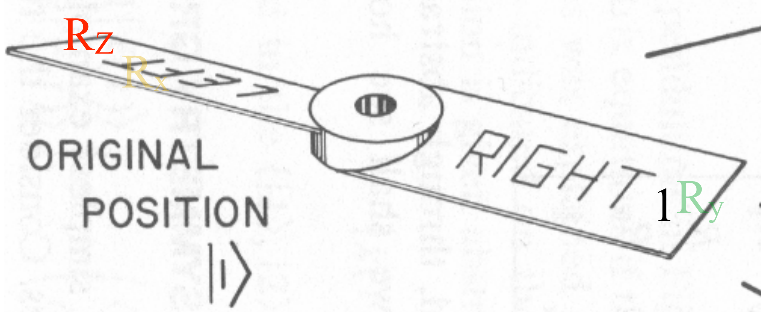
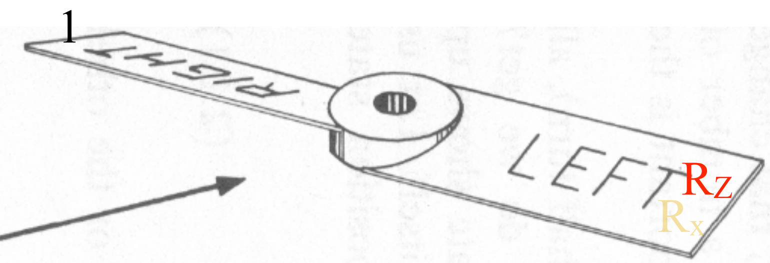
Fig. 2.1.1 PSDS

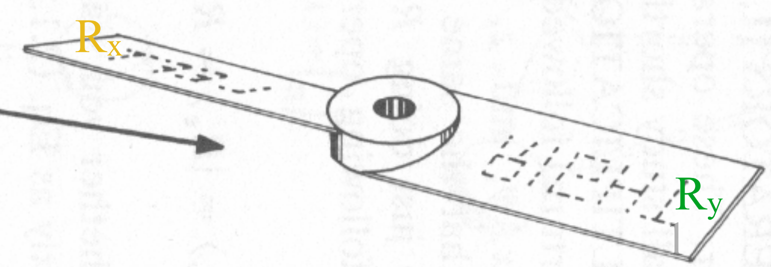
Fig. 2.1.2 PSDS





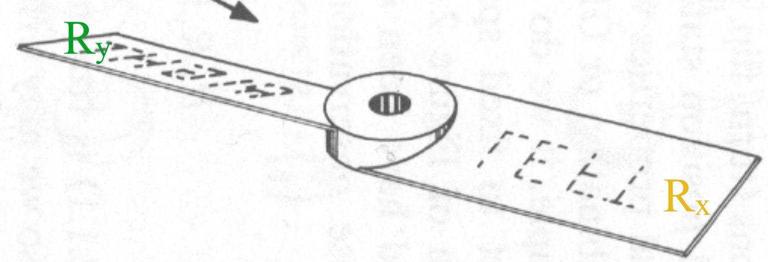
HALF TURN POSITION

$|R_z\rangle = \mathbf{R_z}|1\rangle$



OVERTURNED POSITION

$|R_y\rangle = \mathbf{R_y}|1\rangle$



FLIPPED POSITION

$|R_x\rangle = \mathbf{R_x}|1\rangle$

$\mathbf{R_z}$

$\mathbf{R_y}$

$\mathbf{R_x}$

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

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 (and review of revival)

Breaking C_{2N+2} to approximate linear N-chain

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

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 Group Zoo

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations:

$$\mathbf{R_x}^2 \mathbf{- 1 = 0}, \qquad \mathbf{R_y}^2 \mathbf{- 1 = 0}.$$

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

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

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

reducible projectors

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

D_2 spectral decomposition: The old "1=1•1 trick" again

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$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \quad\quad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

Completeness

D_2 spectral decomposition: The old "1=1•1 trick" again

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Completeness

$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \qquad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

Spec.decomps

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

D_2 spectral decomposition: The old "1=1•1 trick" again

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

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

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Completeness

Spec.decomps

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$(completeness\ is\ first)$

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

D_2 spectral decomposition: The old "1=1•1 trick" again

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reducible projectors

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Completeness

$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \qquad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

Spec.decomps

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(*then R_x eigenvalues*)

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

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

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reducible projectors

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Completeness

$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \qquad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

Spec.decomps

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(*...and so forth*)

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

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

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reducible projectors

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

Completeness

$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \qquad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

Spec.decomps

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

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

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

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
$+$	1	1
$-$	1	-1

$\times$

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
$+$	1	1
$-$	1	-1

$=$

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

Shortcut notation for getting D_2 character table

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
+	1	1
−	1	−1

$\times$

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
+	1	1
−	1	−1

$=$

$C_2^x \times C_2^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_x\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_y$	$\mathbf{R}_x\cdot\mathbf{R}_y$
$+\cdot+$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$-\cdot+$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$-1\cdot1$
$+\cdot-$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$-1\cdot(-1)$

$=$

D_2	$\mathbf{1}$	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$
$+\cdot+$	1	1	1	1
$-\cdot+$	1	-1	1	-1
$+\cdot-$	1	1	−1	−1
$-\cdot-$	1	-1	−1	1

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

reducible projectors

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$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \qquad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

Completeness

Spec.decomps

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

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

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

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
+	1	1
−	1	−1

$\times$

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
+	1	1
−	1	−1

$=$

$C_2^x \times C_2^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_x\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_y$	$\mathbf{R}_x\cdot\mathbf{R}_y$
$+\cdot+$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$-\cdot+$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$-1\cdot1$
$+\cdot-$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$-1\cdot(-1)$

Shortcut notation for getting D_2 character table

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
$+$	1	1
$-$	1	-1

$\times$

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
$+$	1	1
$-$	1	-1

$=$

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

$=$

D_2	$\mathbf{1}$	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$
$++=A_1$	1	1	1	1
$-+=A_2$	1	-1	1	-1
$+-=B_1$	1	1	-1	-1
$--=B_2$	1	-1	-1	1

Note common notation

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

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

reducible projectors

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

$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \qquad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

Completeness Spec.decomps

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

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

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

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

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

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

(*completeness is first*)

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

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

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

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

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
$+$	1	1
$-$	1	-1

$\times$

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
$+$	1	1
$-$	1	-1

$=$

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

Shortcut notation for getting D_2 character table

Breaking C_N cyclic coupling into linear chains

Review of 1D-Bohr-ring related to infinite square well (and review of revival)

Breaking C_{2N+2} to approximate linear N-chain

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

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 Group Zoo

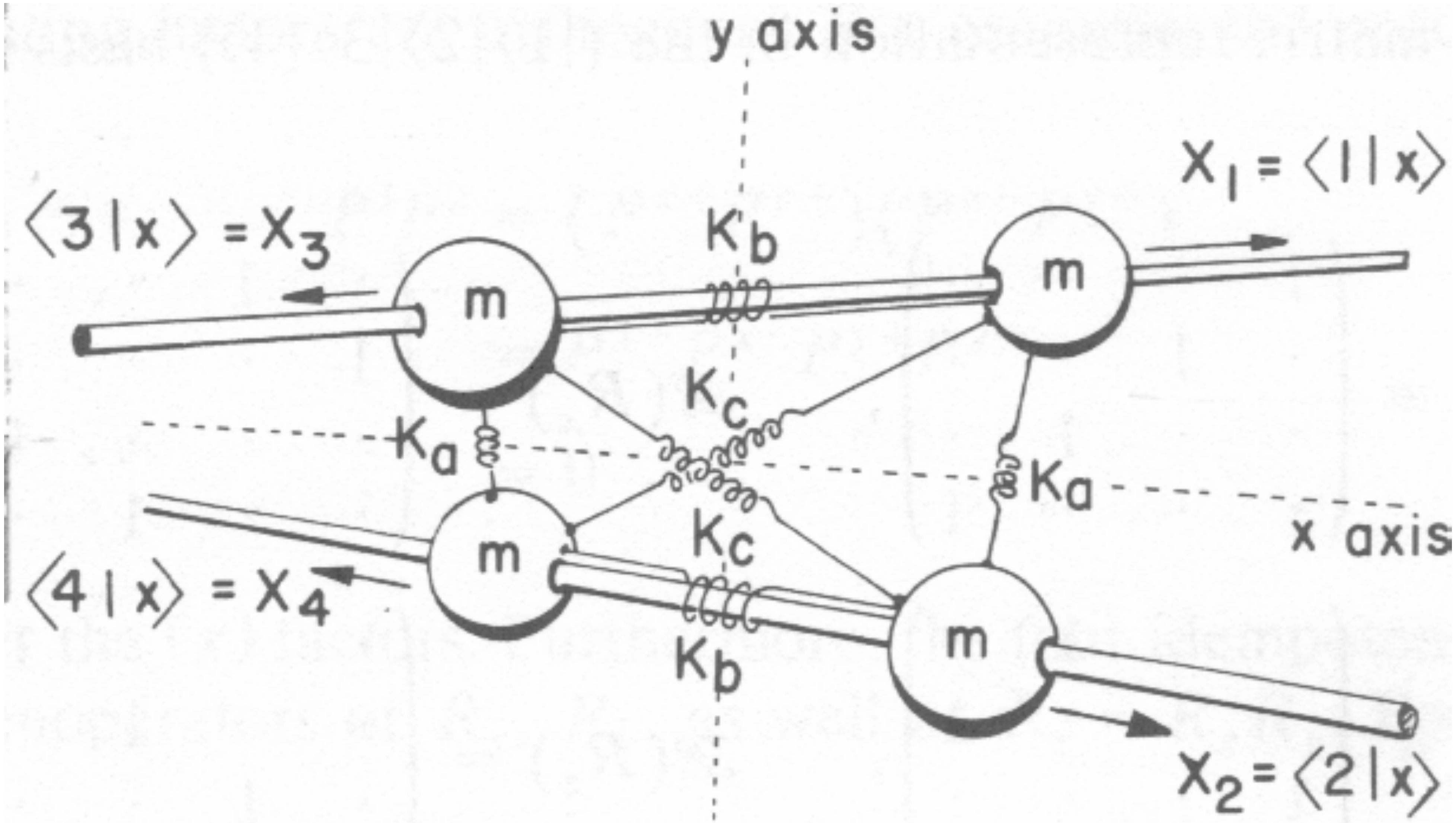


Fig. 2.8.1 PSDS

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

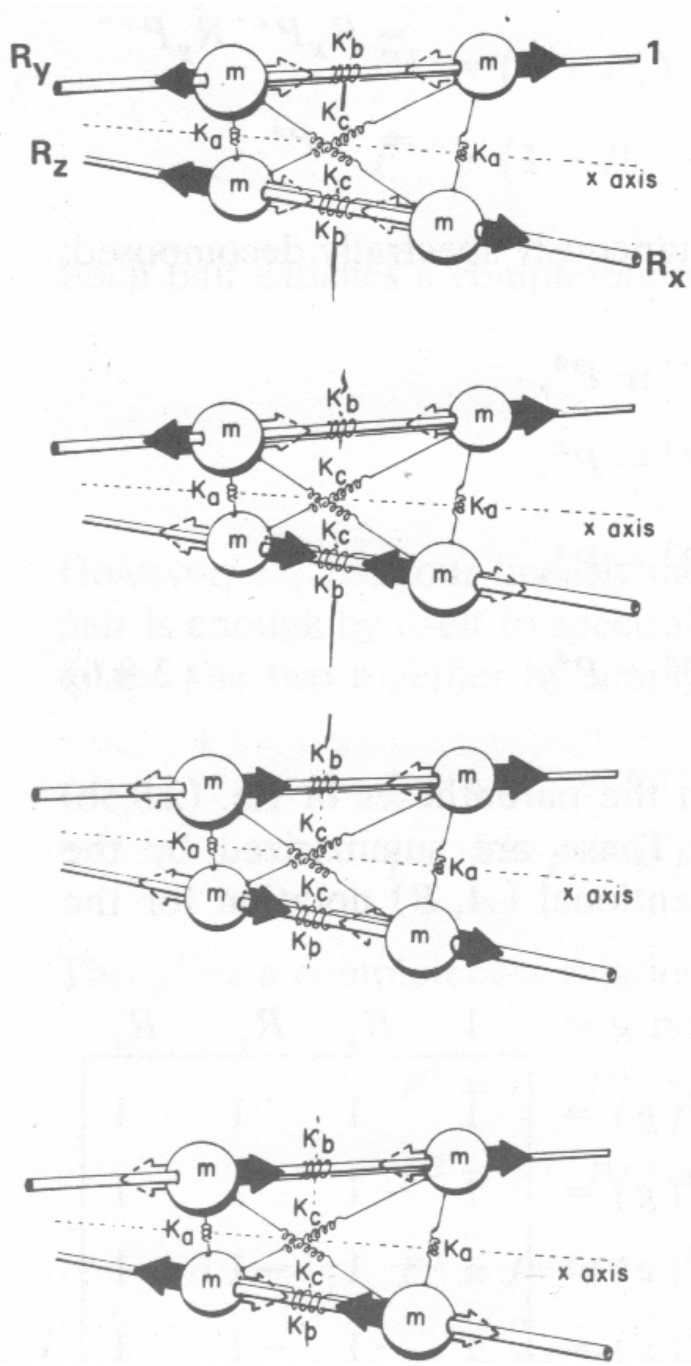
$$\begin{aligned} A &= -\left(k_a \cos^2(a,b) + k_b + k_c \cos^2(b,c)\right)/m, \\ a &= -k_a \cos^2(a,b)/m, \\ b &= -k_b/m, \\ c &= -k_c \cos^2(b,c)/m. \end{aligned}$$

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

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

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

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



$$\begin{pmatrix}1\\1\\1\\1\end{pmatrix}/2 \qquad (A+a+b+c)^{1/2}$$

$$\begin{pmatrix}1\\-1\\1\\-1\end{pmatrix}/2 \qquad (A-a+b-c)^{1/2}$$

$$\begin{pmatrix}1\\1\\-1\\-1\end{pmatrix}/2 \qquad (A+a-b-c)^{1/2}$$

$$\begin{pmatrix}1\\-1\\-1\\1\end{pmatrix}/2 \qquad (A-a-b+c)^{1/2}$$

Fig. 2.8.2 PSDS

Breaking C_N cyclic coupling into linear chains

Review of 1D-Bohr-ring related to infinite square well (and review of revival)

Breaking C_{2N+2} to approximate linear N-chain

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

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 Group Zoo* ⬅

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

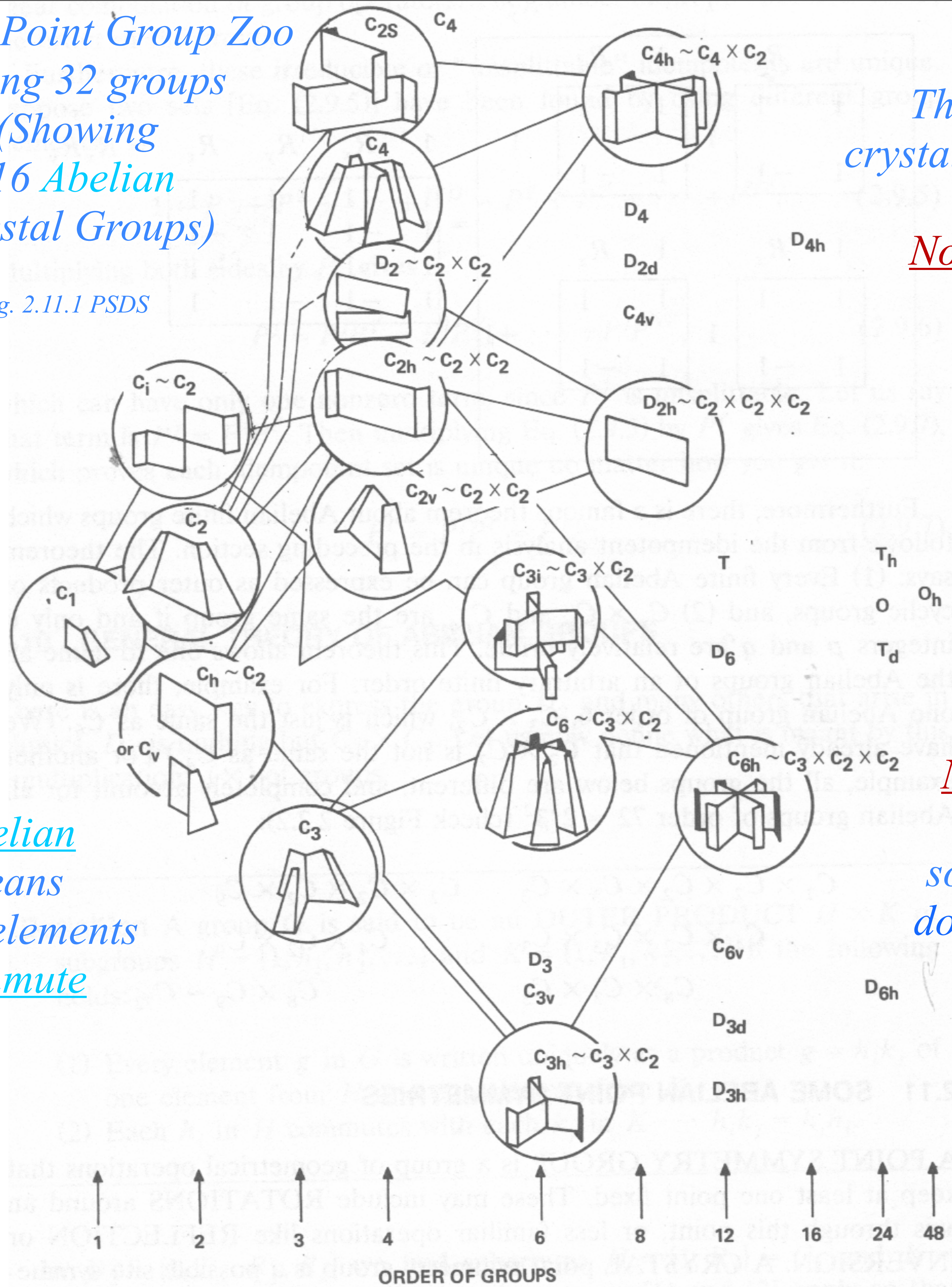


Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

Non-Abelian
means
some elements
do not commute

Abelian
means
all its elements
commute

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

From Lecture 12.6 p. 134
Character Trace of
n-fold rotation
where: $\ell^j = 2j+1$
is U(2) irrep dimension

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

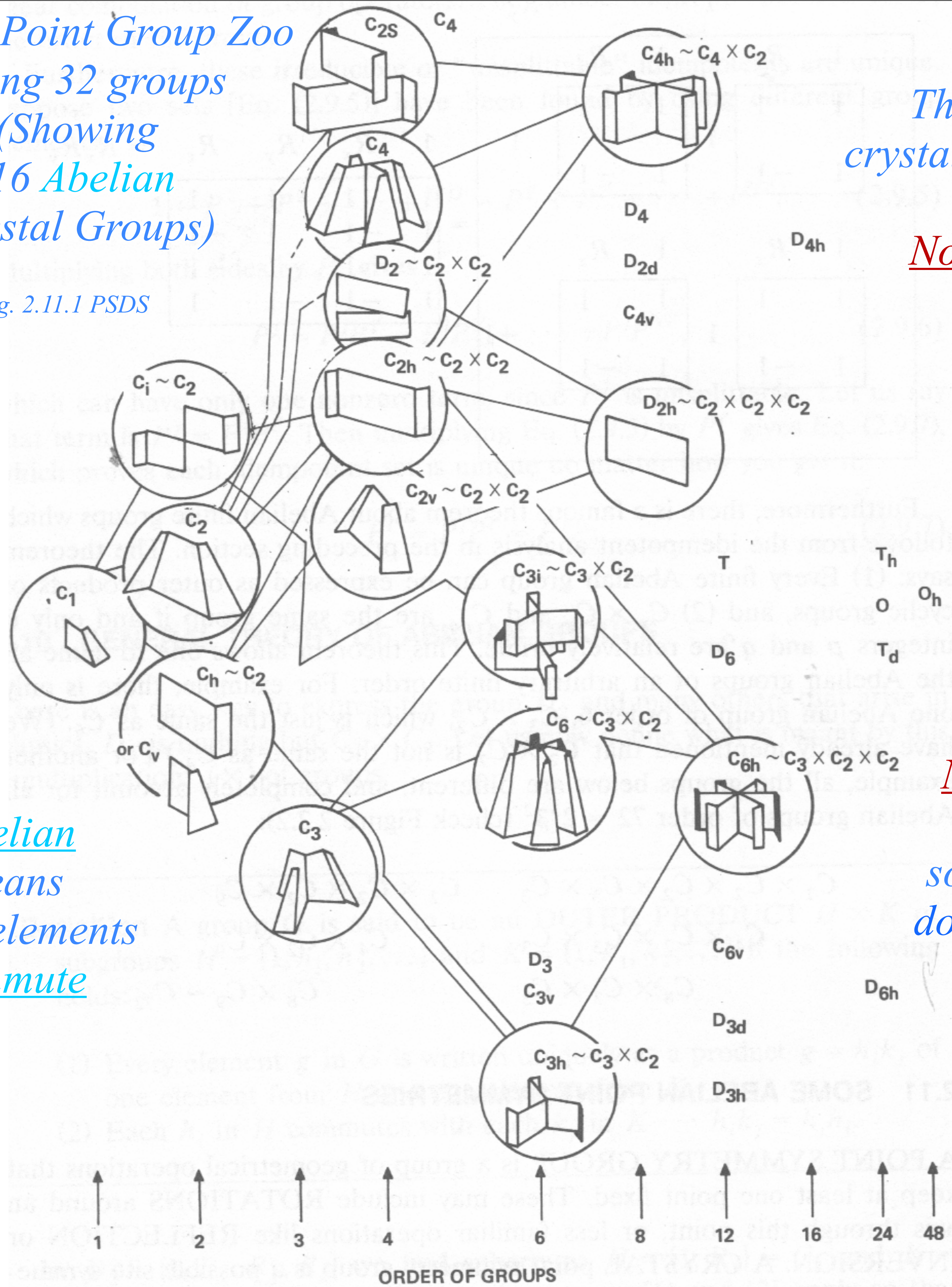


Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

Non-Abelian
means
some elements
do not commute

Abelian
means
all its elements
commute

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

Fig. 2.11.1 PSDS

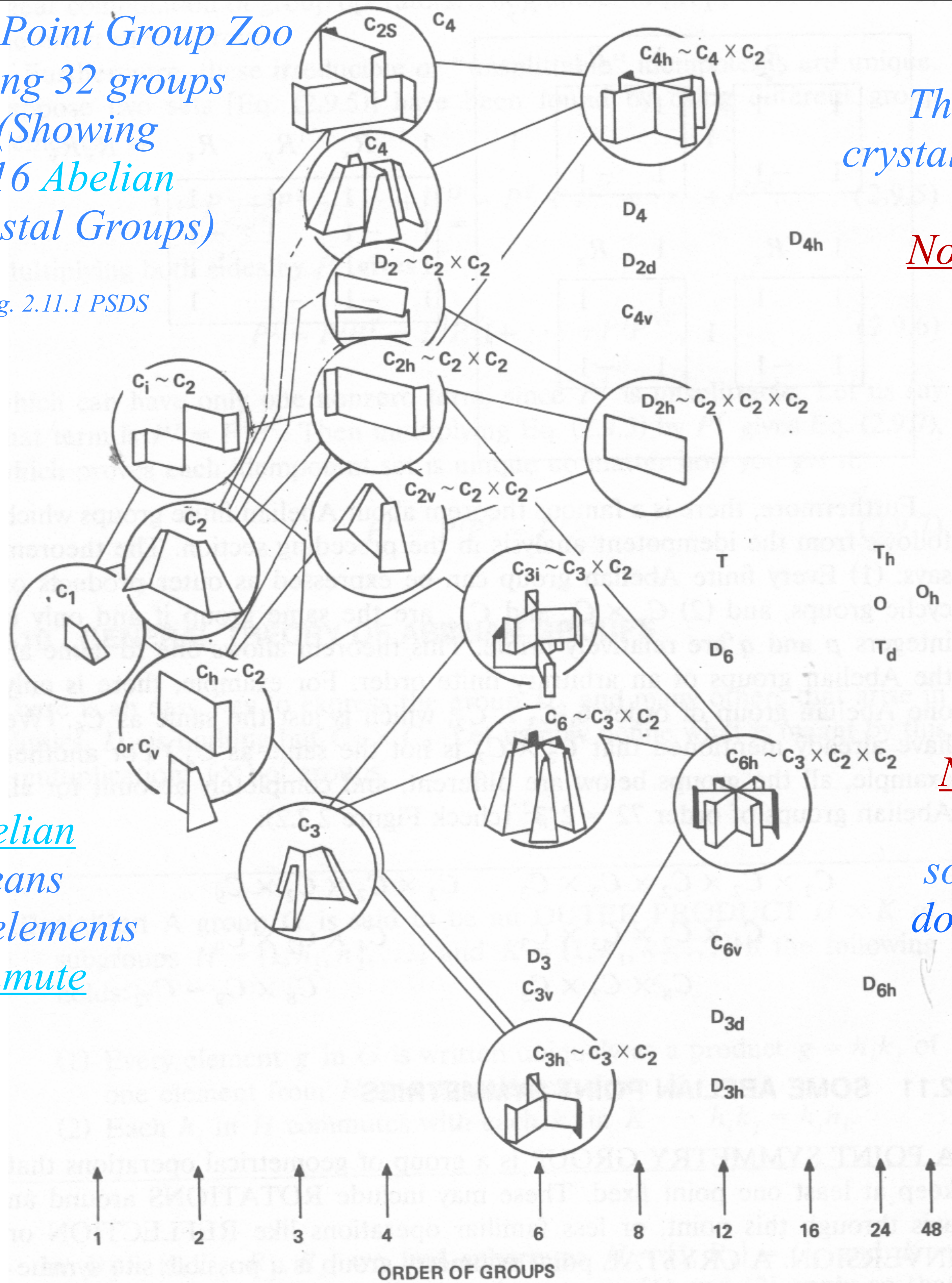


Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

Abelian means all its elements commute

The other 16 crystal-point groups are Non-Abelian

Non-Abelian means some elements do not commute

From Lecture 12.6 p. 134 Character Trace of n-fold rotation where: $\ell^j = 2j+1$ is U(2) irrep dimension

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

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

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

$$\frac{\sin\frac{3\pi}{2}}{\sin\frac{\pi}{2}} = -1 \ (n=2 \text{ ok})$$

$$\frac{\sin\frac{3\pi}{3}}{\sin\frac{\pi}{3}} = +1 \ (n=3 \text{ ok})$$

$$\frac{\sin\frac{3\pi}{4}}{\sin\frac{\pi}{4}} = +1 \ (n=4 \text{ ok})$$

$$\frac{\sin\frac{3\pi}{5}}{\sin\frac{\pi}{5}} = G^+ \ (n=5 \text{ NO!})$$

$$\frac{\sin\frac{3\pi}{6}}{\sin\frac{\pi}{6}} = +2 \ (n=6 \text{ ok})$$

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

Fig. 2.11.1 PSDS

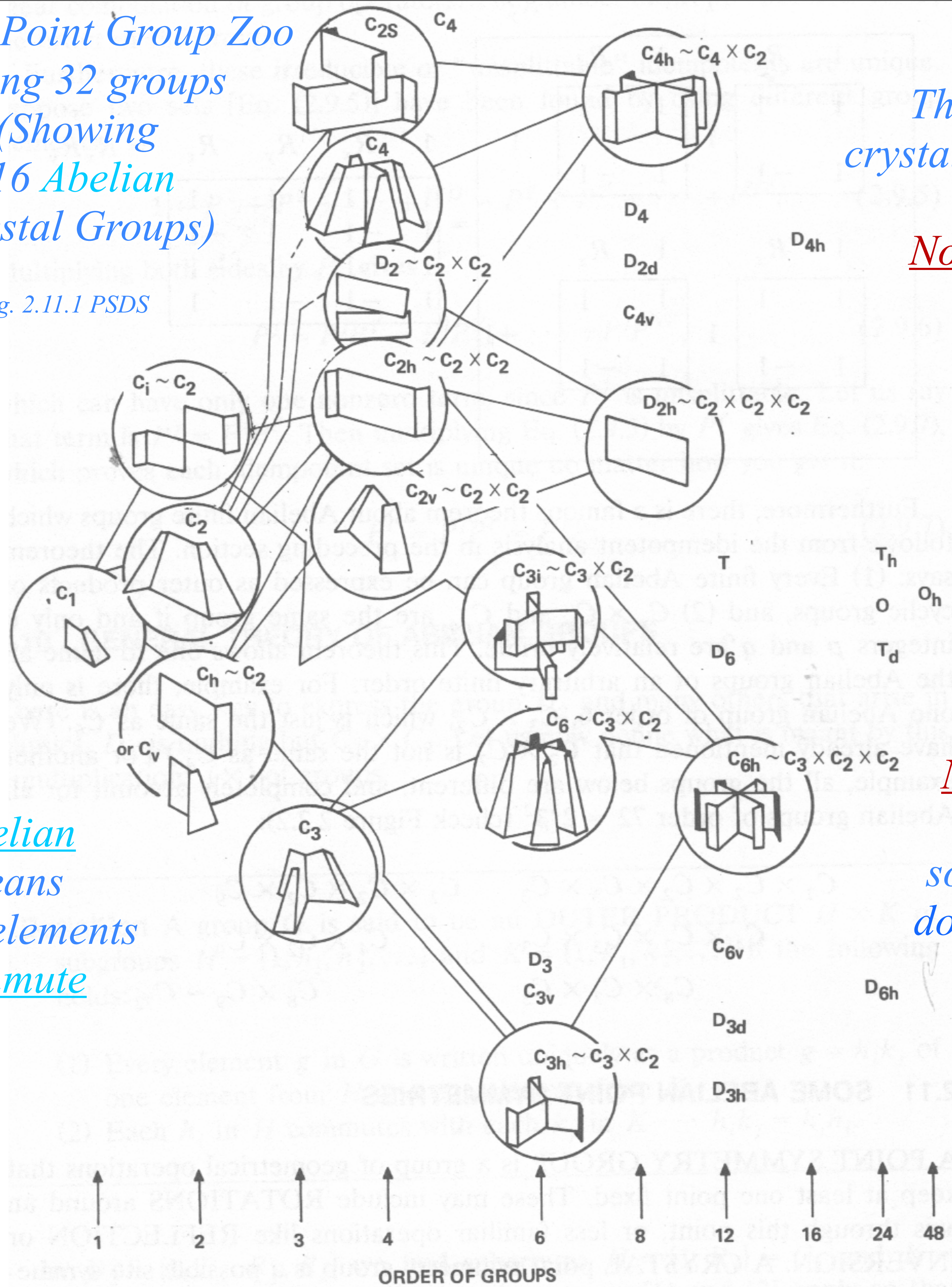


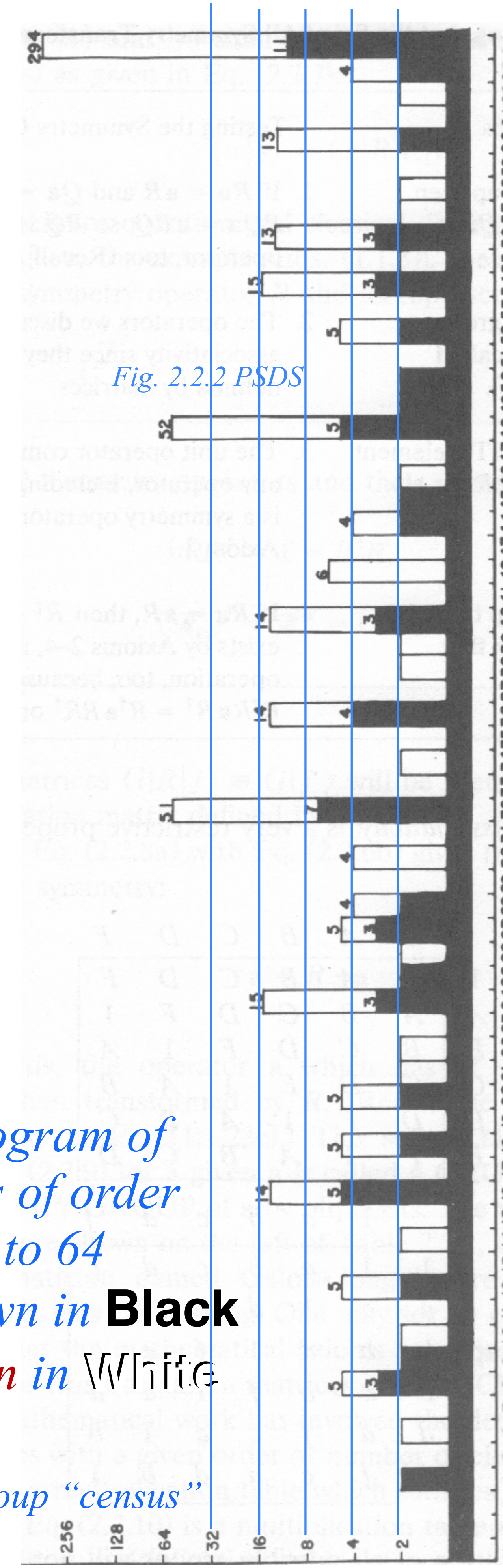
Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

The other 16
crystal-point groups
are
Non-Abelian

Abelian
means
all its elements
commute

Non-Abelian
means
some elements
do not commute

Fig. 2.2.2 PSDS



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

Group "census"

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

Fig. 2.11.1 PSDS

The other 16
crystal-point groups
are
Abelian

Abelian
means
all its elements
commute

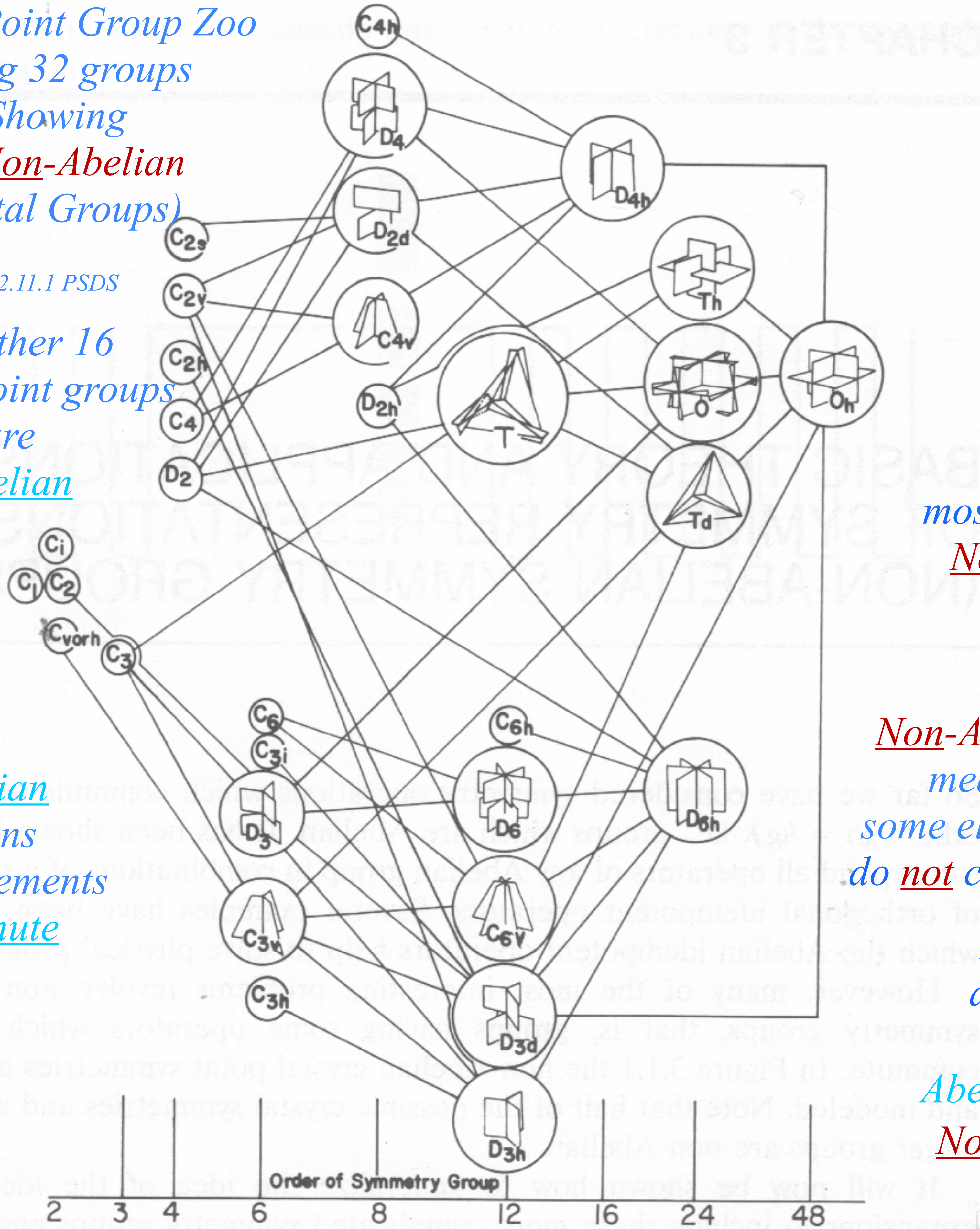
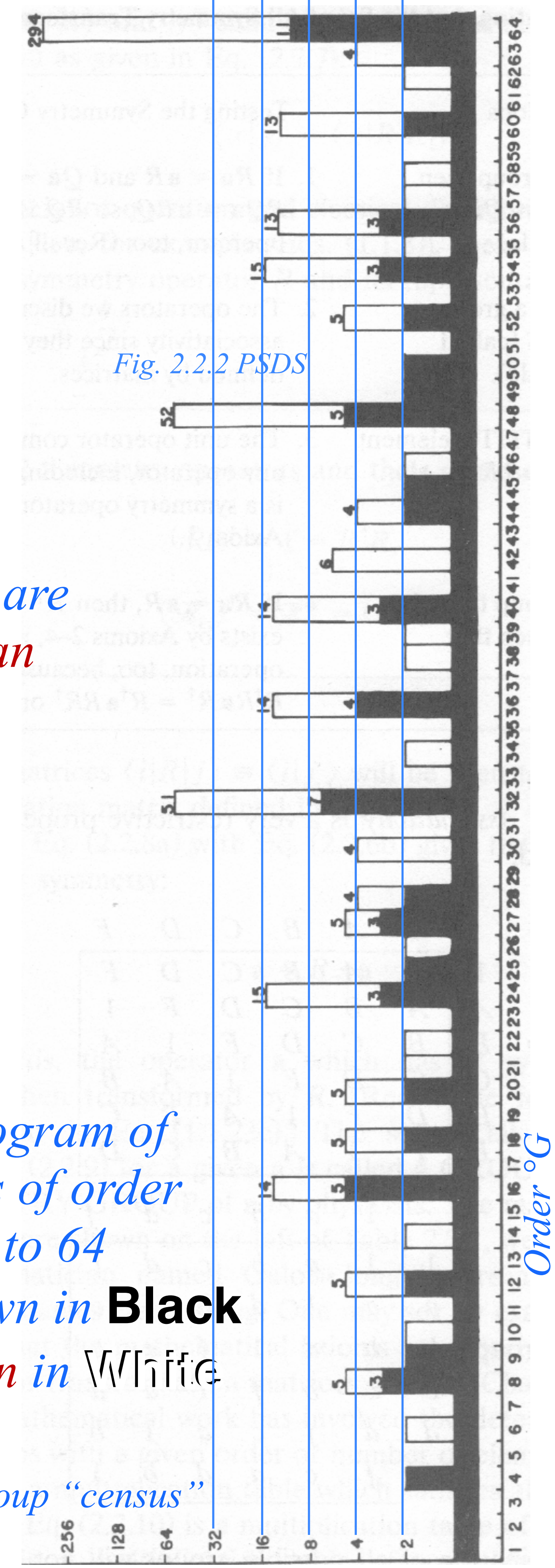


Figure 3.1.1 Crystal point symmetry groups. Models are sketched in circles for the 16 non-Abelian groups. (See also Figure 2.11.1.)

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	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{r}^2$
$(0)_3$	1	1	1
$(1)_3$	1	$e^{2\pi i/3}$	$e^{-2\pi i/3}$
$(2)_3$	1	$e^{-2\pi i/3}$	$e^{2\pi i/3}$

$\times$

C_2	$\mathbf{1}$	$\mathbf{R}$
$(0)_2$	1	1
$(1)_2$	1	-1

$=$

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

C_6 is product $\mathrm{C}_3\times \mathrm{C}_2$ *(but C_4 is NOT* $\mathrm{C}_2\times \mathrm{C}_2$*)*

C_3	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{r}^2$
$(0)_3$	1	1	1
$(1)_3$	1	$e^{2\pi i/3}$	$e^{-2\pi i/3}$
$(2)_3$	1	$e^{-2\pi i/3}$	$e^{2\pi i/3}$

$\times$

C_2	$\mathbf{1}$	$\mathbf{R}$
$(0)_2$	1	1
$(1)_2$	1	-1

$=$

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

$=$

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