Group Theory in Quantum Mechanics

Lecture 12 *(3.7.13)*

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)*
- *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 Group Zoo*

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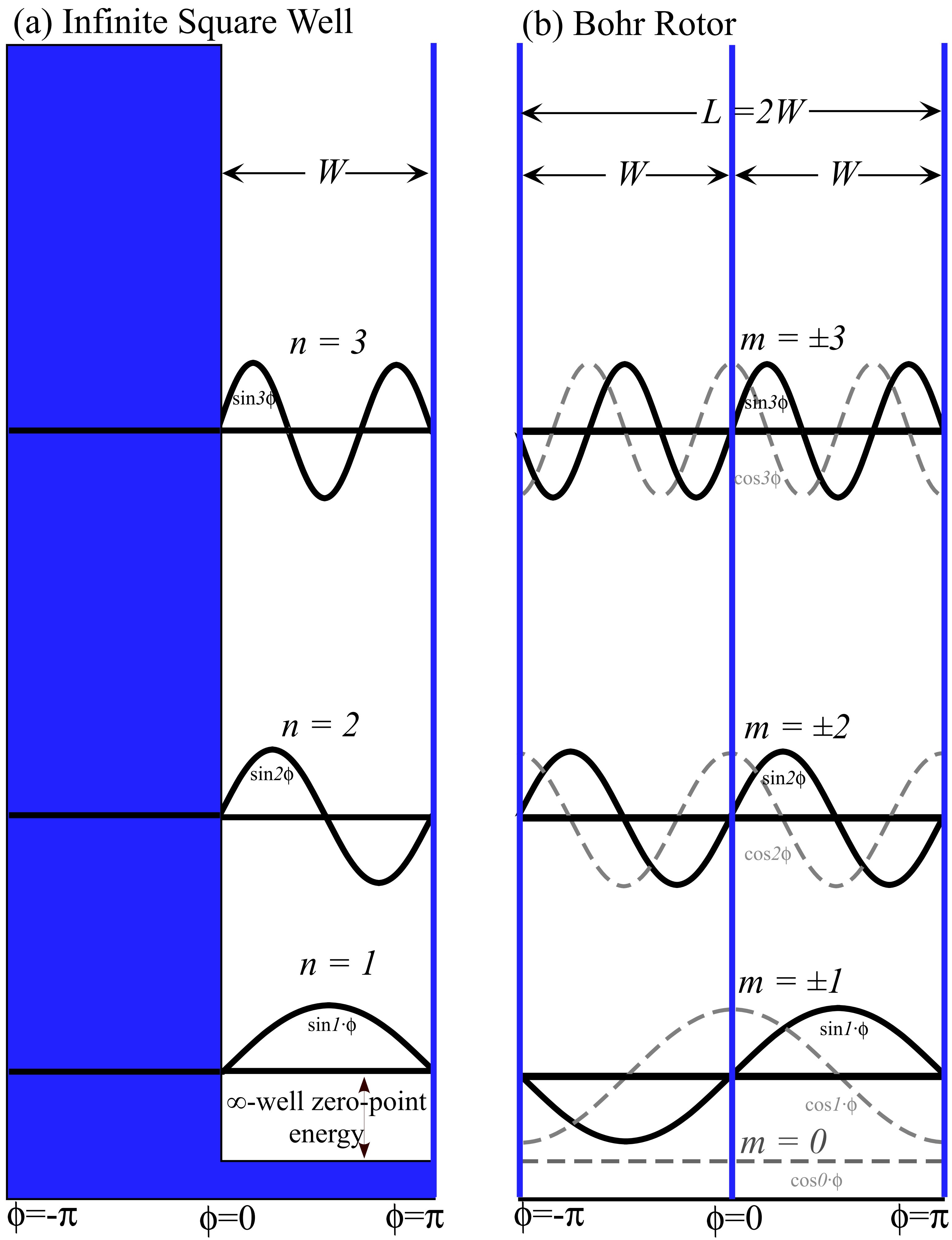
The "4-Group(s)" D_2 and C_{2v}

Spectral decomposition of D_2

Some D_2 modes

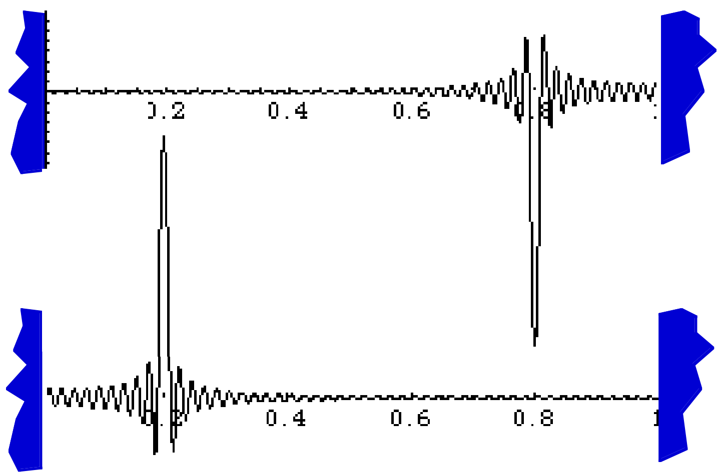
Outer product properties and the Group Zoo


(a) Infinite Square Well
(b) Bohr Rotor
L = 2W
W
W
W
n = 3
sin3ϕ
n = 2
sin2ϕ
n = 1
sin1·ϕ
∞-well zero-point energy
m = ±3
sin3ϕ
cos3ϕ
m = ±2
sin2ϕ
cos2ϕ
m = ±1
sin1·ϕ
cos1·ϕ
m = 0
cos0·ϕ
ϕ=-π
ϕ=0
ϕ=π
ϕ=-π
ϕ=0
ϕ=π

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

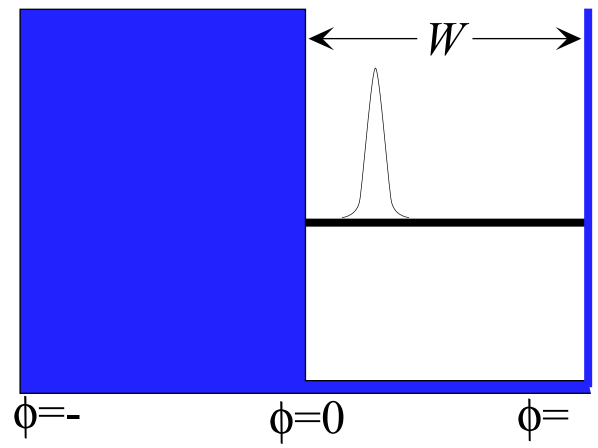
$t = 0.5000\tau_1$
$= 1.5\tau_{beat}$

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

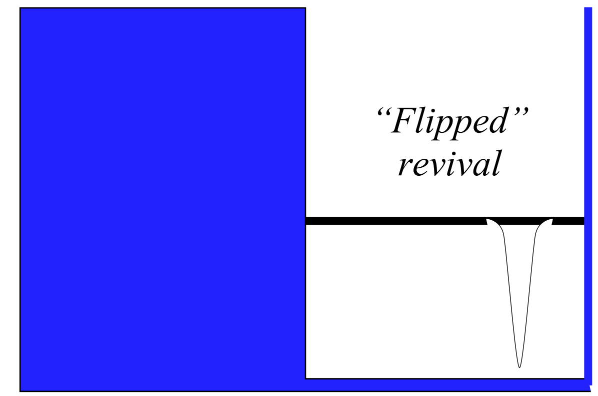


After only 50 round-trips
M's wave does a *partial revival*
as it makes an upside down-delta
function around *x=0.8W*.

(a) Infinite Square Well at t=0



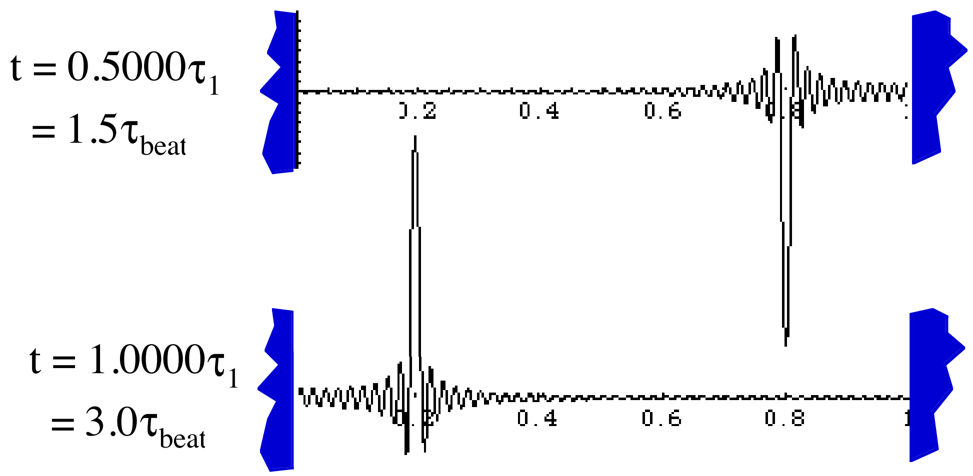
(c) Half-time revival at t=τ/2



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

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.



After only 50 round-trips
M's wave does a *partial revival*
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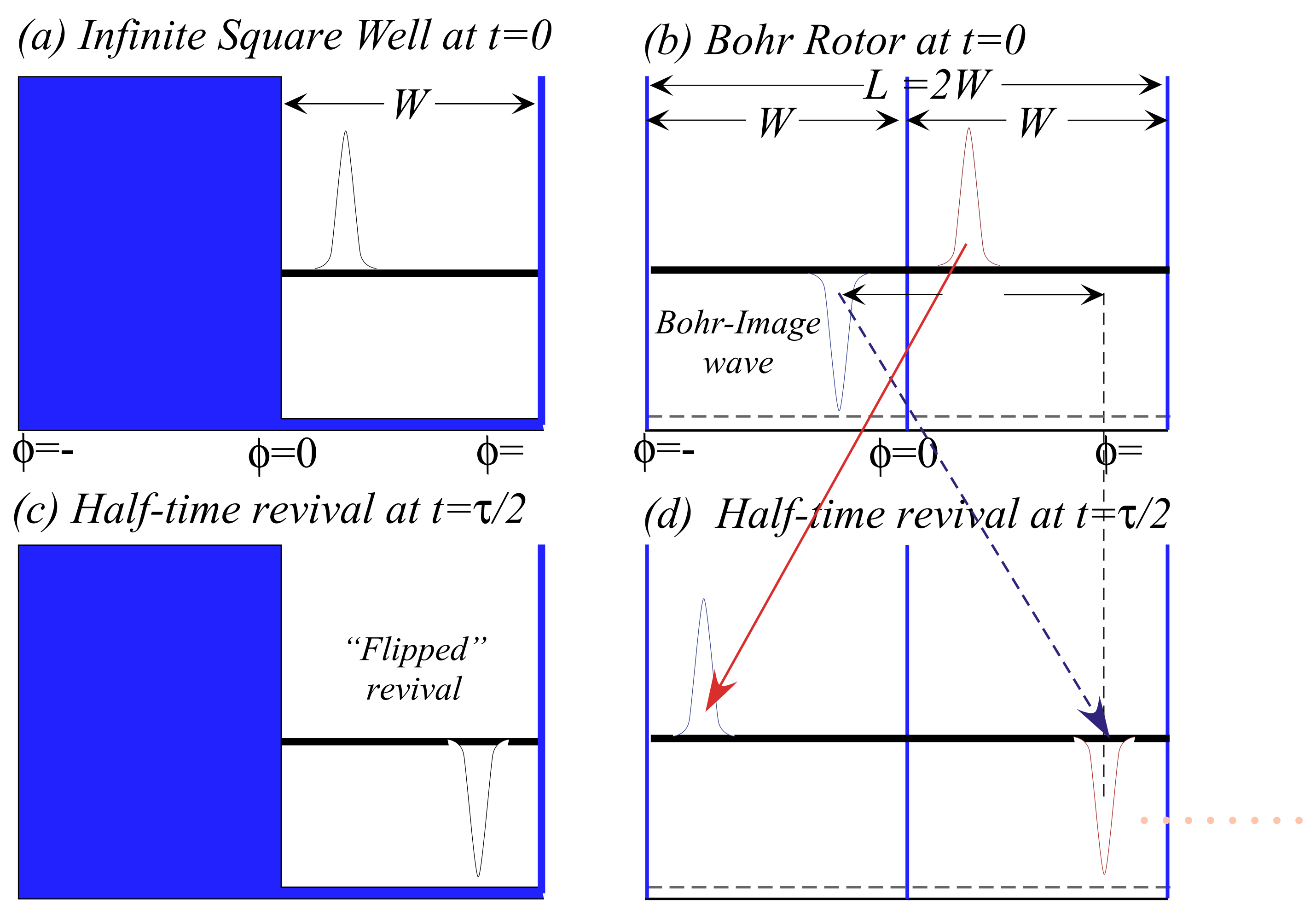

3. So how is the ∞-well "flipped revival explained?

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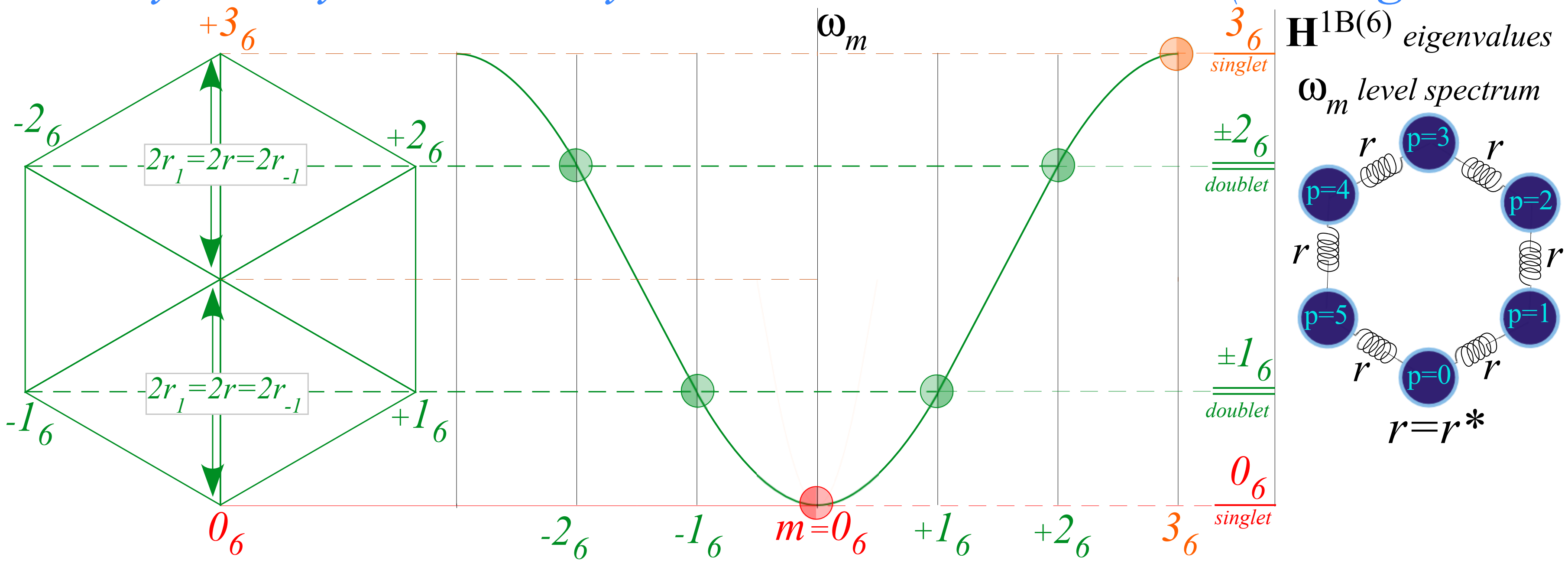
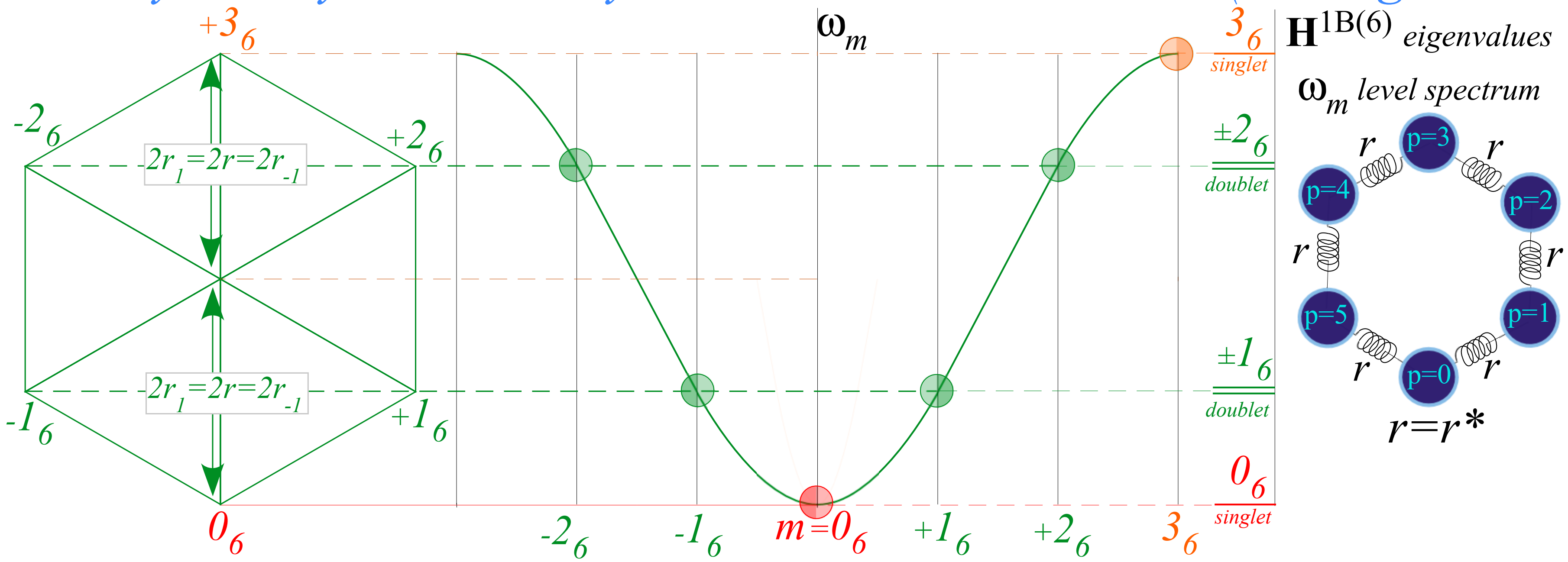
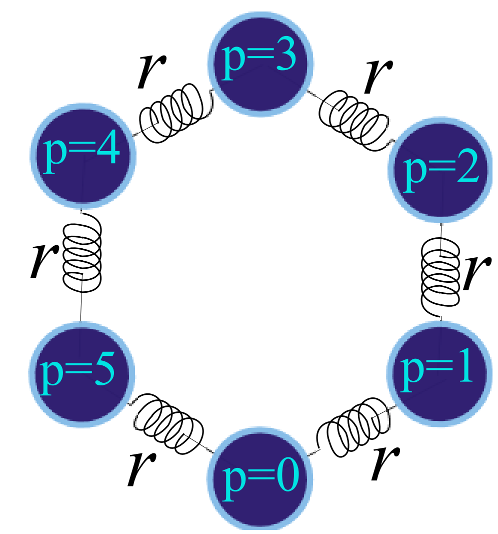
C_6 symmetry: Elementary Bloch Hamiltonian $\mathbf{H}^{1B(6)}$ (1st neighbor coupling)



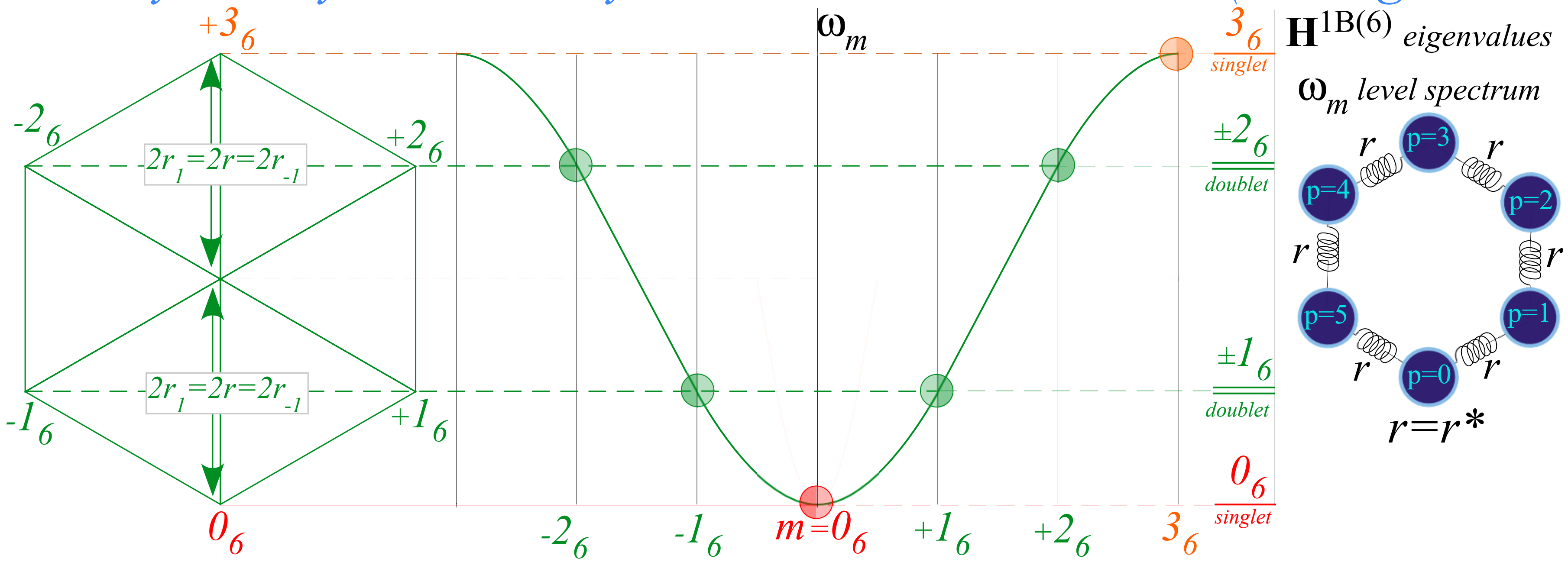
C_6 symmetry: Elementary Bloch Hamiltonian $\mathbf{H}^{1B(6)}$ (1^{st} neighbor coupling)



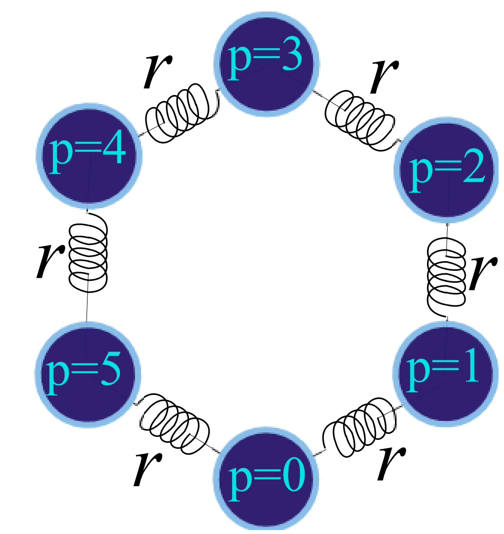
$$
\mathbf{H}^{1B(6)}\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}
=
\begin{array}{c}
\begin{array}{cccccc} p=0 & 1 & 2 & 3 & 4 & 5 \end{array}\\
\begin{pmatrix}
2r & -r & \cdot & \cdot & \cdot & -r\\
-r & 2r & -r & \cdot & \cdot & \cdot\\
\cdot & -r & 2r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



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



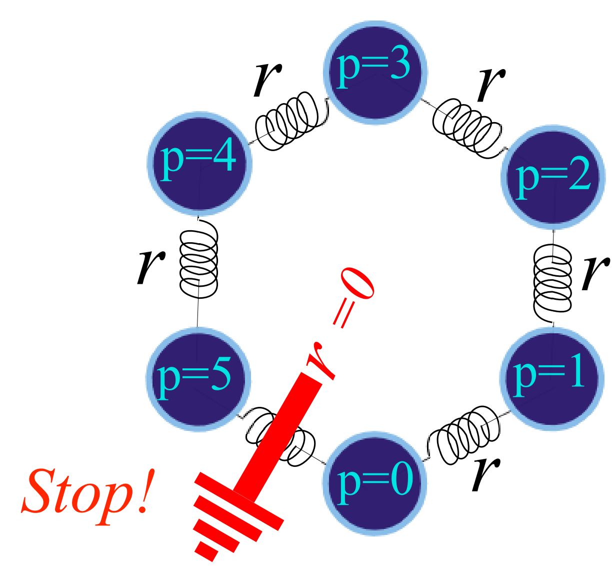
$$
\mathbf{H}^{1B(6)}\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}=
\begin{array}{c}
\begin{array}{cccccc} p=0 & 1 & 2 & 3 & 4 & 5 \end{array}\\
\begin{pmatrix}
2r & -r & \cdot & \cdot & \cdot & -r\\
-r & 2r & -r & \cdot & \cdot & \cdot\\
\cdot & -r & 2r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



$\mathbf{H}^{1B(6)}$ eigensolutions are very sensitive to zeroing or constraing 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 $\mathbf{H}^{\mathrm{EB}(14)}$

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

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

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

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

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 $\mathbf{H}^{\mathrm{EB}(14)}$

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

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

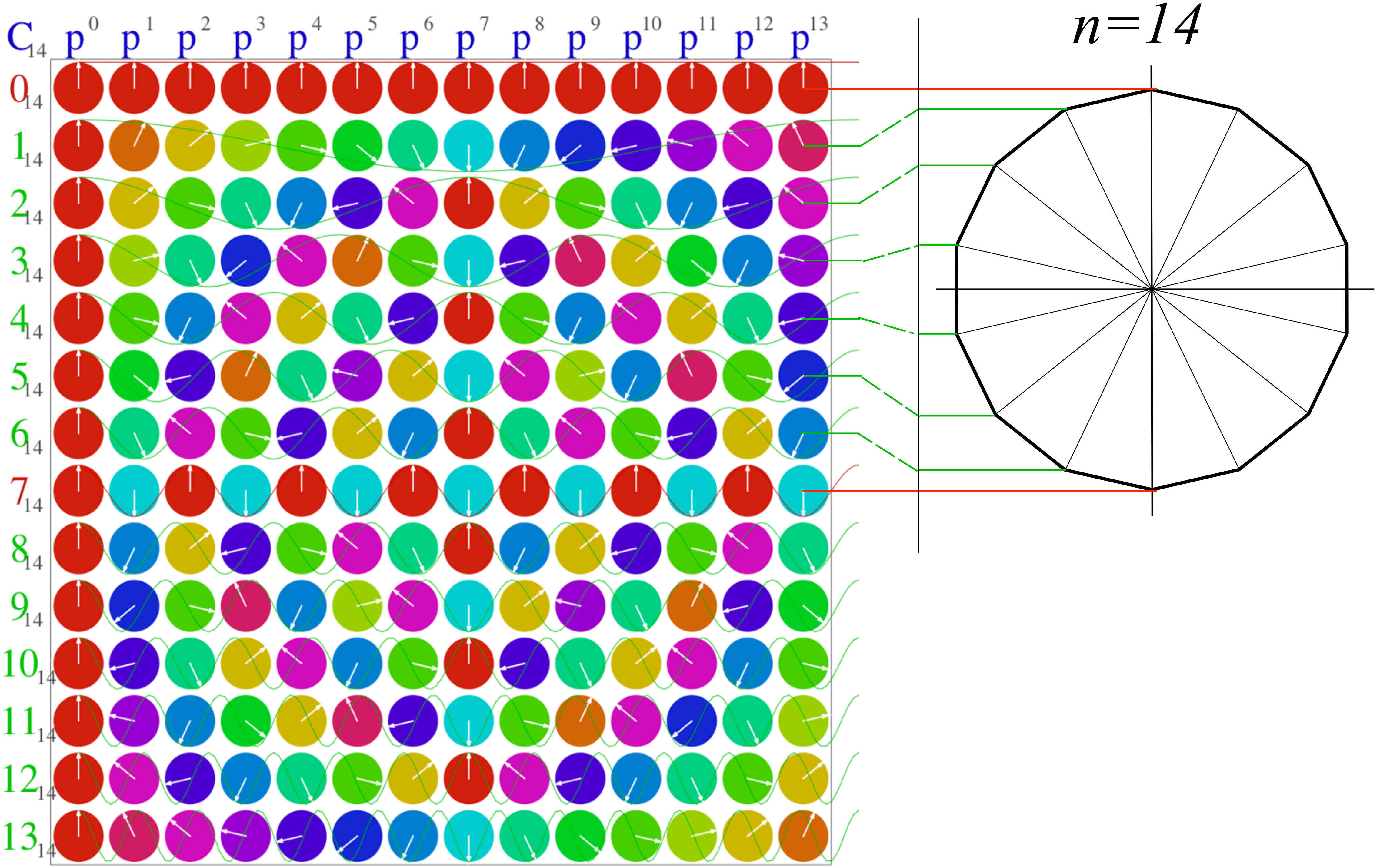
$\mathbf{H}^{\mathrm{EB}(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{\mathrm{CM}(6)}$

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

where:

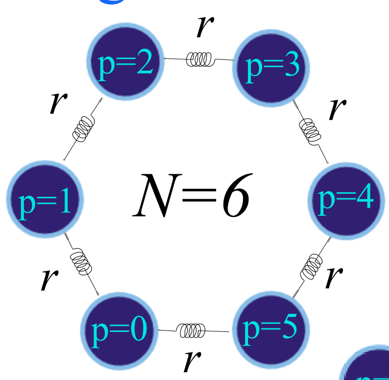
$$\omega^{m(14)} = 2r\left(1 - \cos\frac{2\pi m}{14}\right)$$

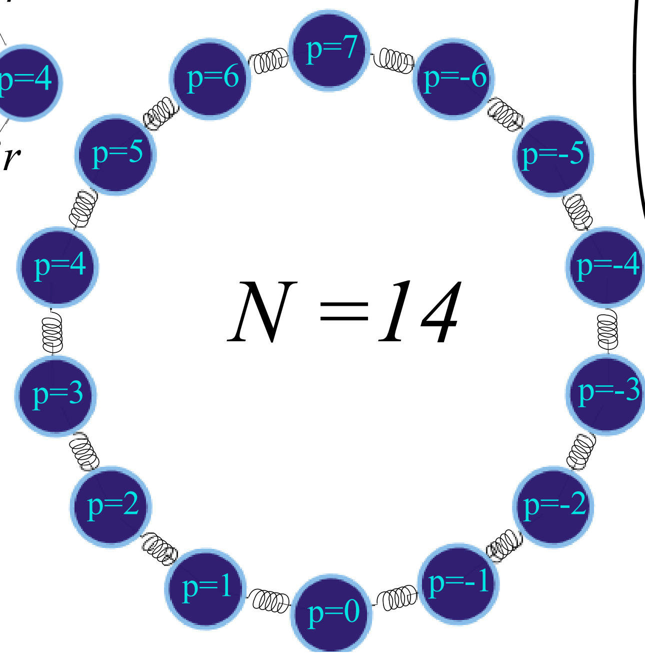
$\mathbf{H}^{EB(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{CM(6)}$ using its sine-waves only



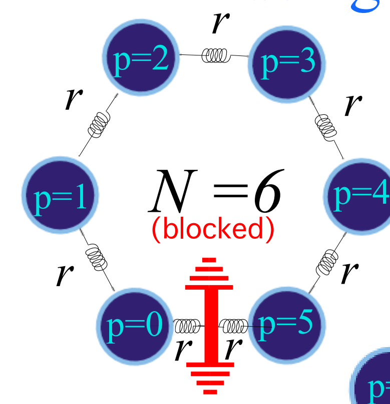
$\mathbf{H}^{EB(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{CM(6)}$ using its sine-waves only

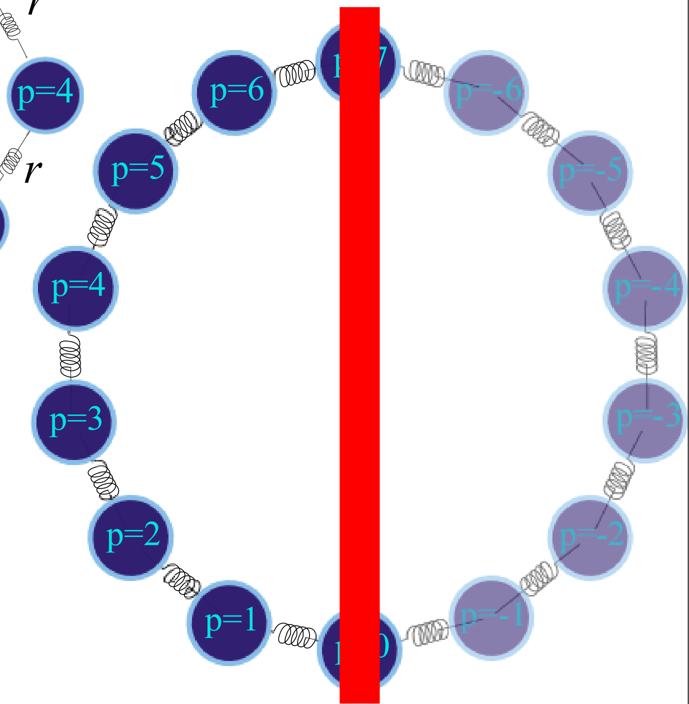
$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & -r \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ -r & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$





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





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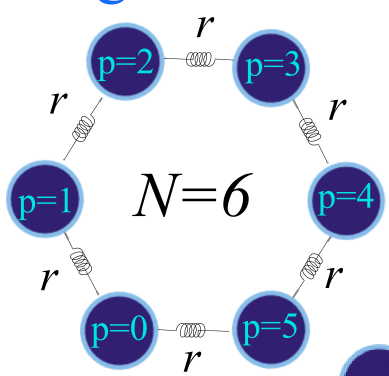
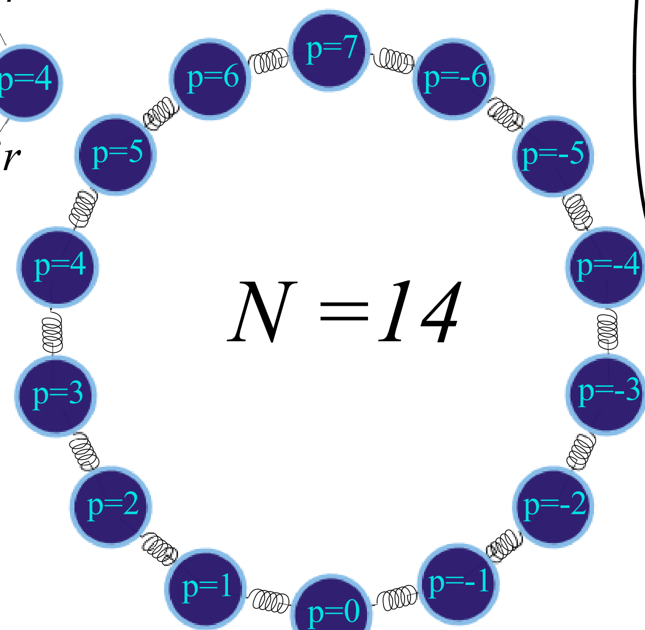
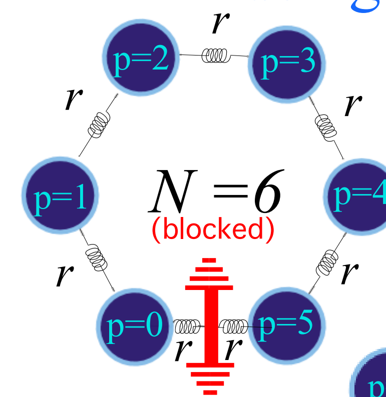
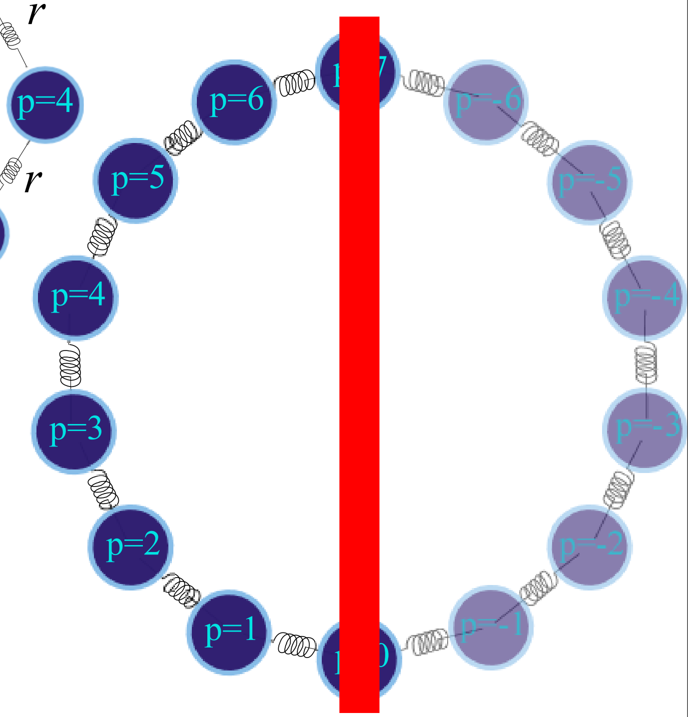
$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & -r \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ -r & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$



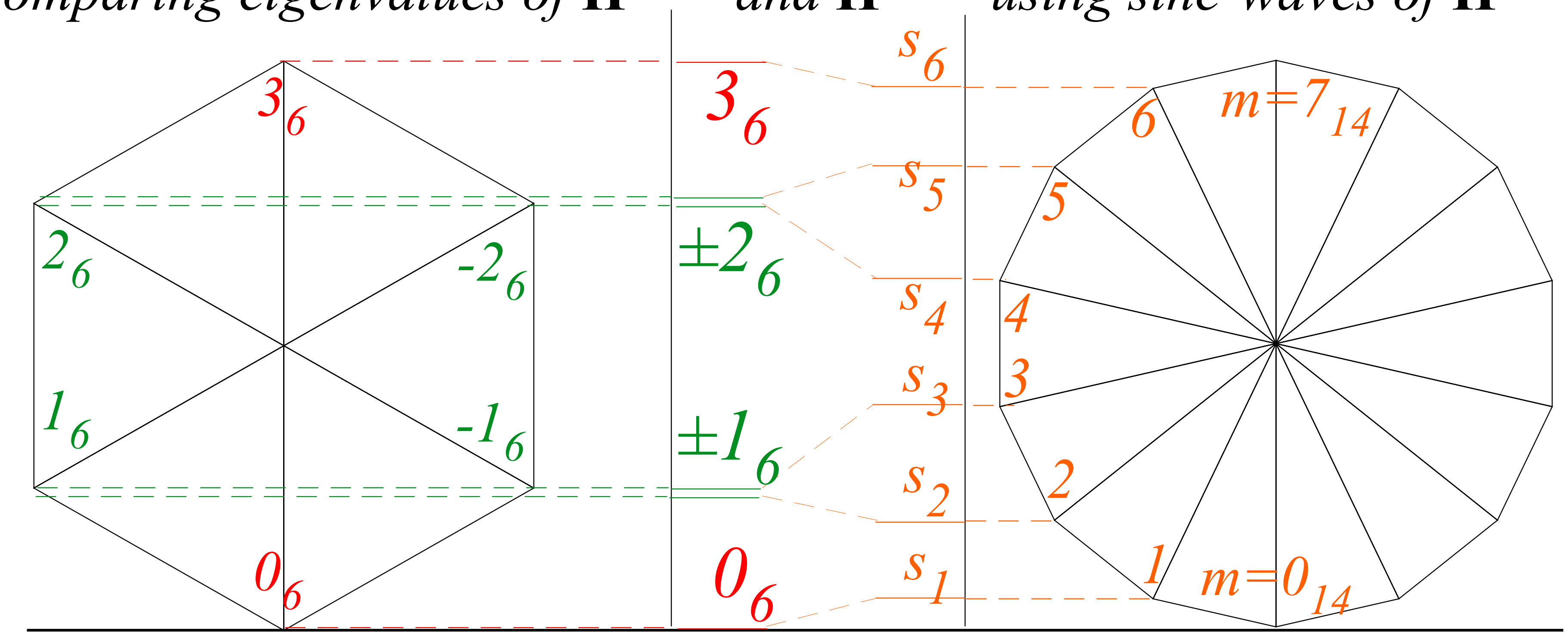


$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & 0 \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ 0 & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$



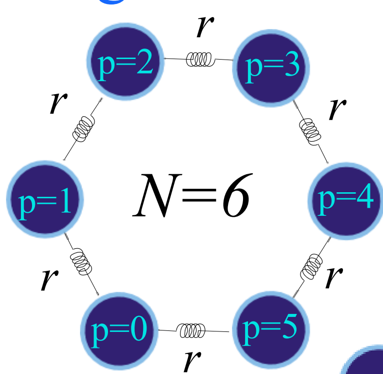


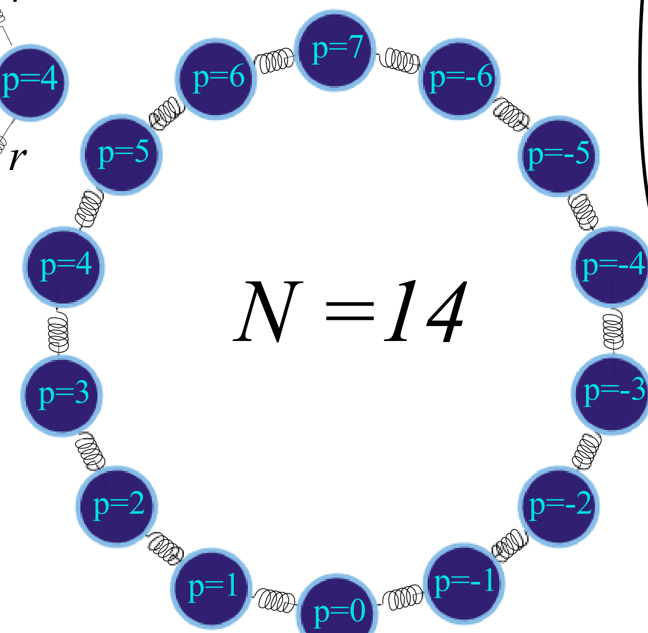
Comparing eigenvalues of $\mathbf{H}^{EB(6)}$ *and* $\mathbf{H}^{CM(6)}$*using sine-waves of* $\mathbf{H}^{EB(14)}$



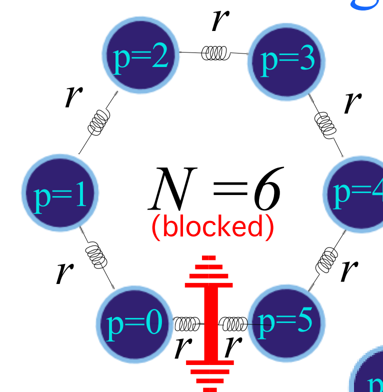
$\mathbf{H}^{EB(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{CM(6)}$ using its sine-waves only

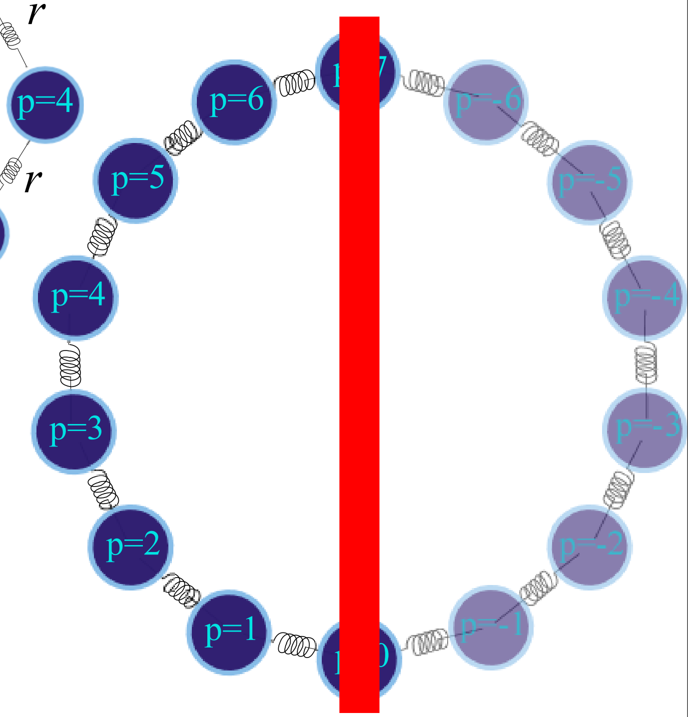
$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & -r \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ -r & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$



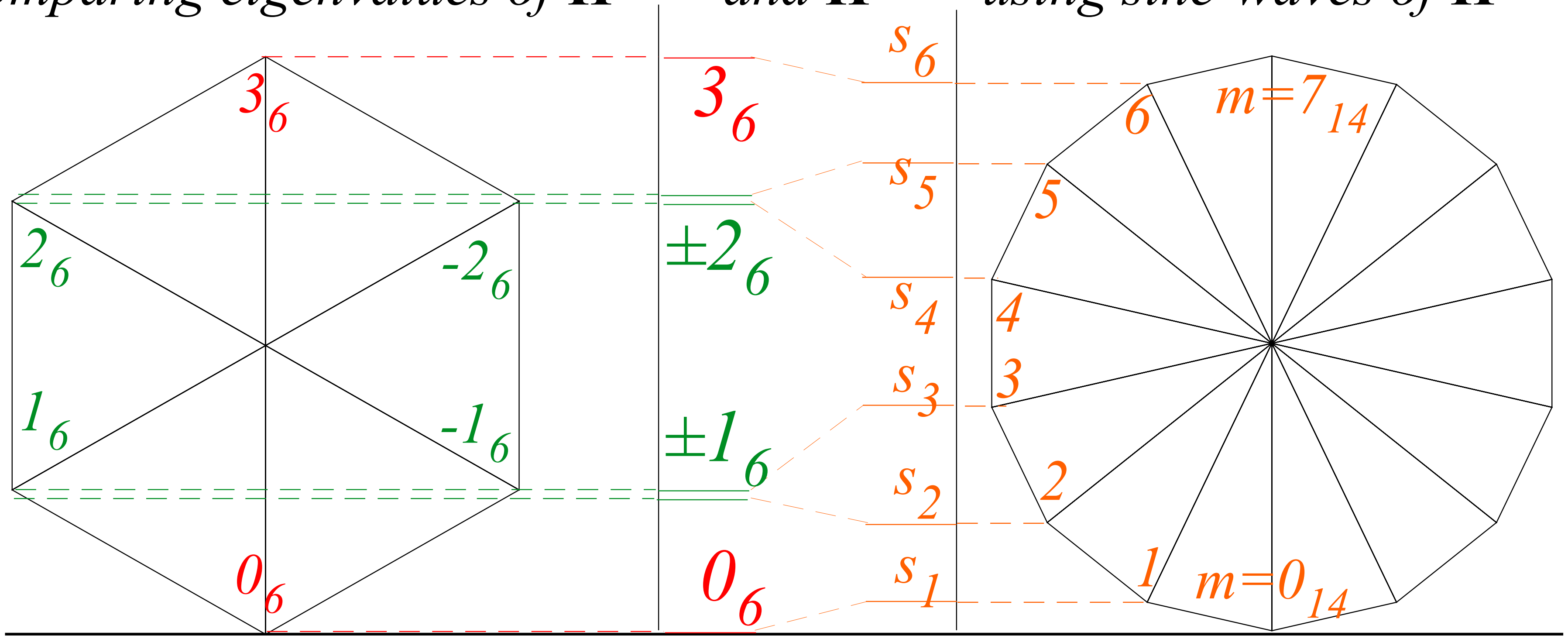


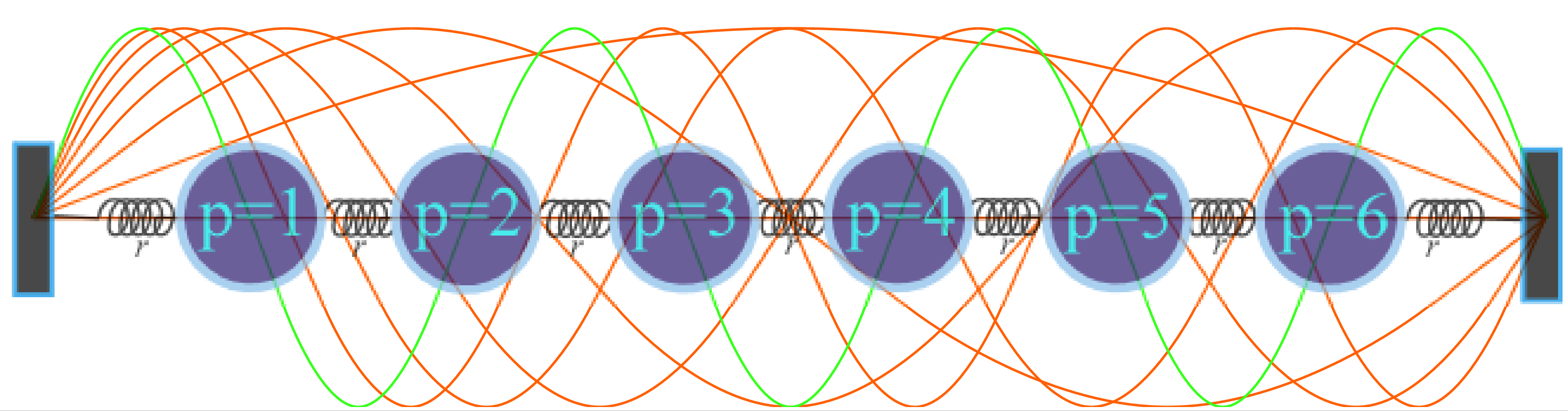
$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & 0 \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ 0 & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$





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





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

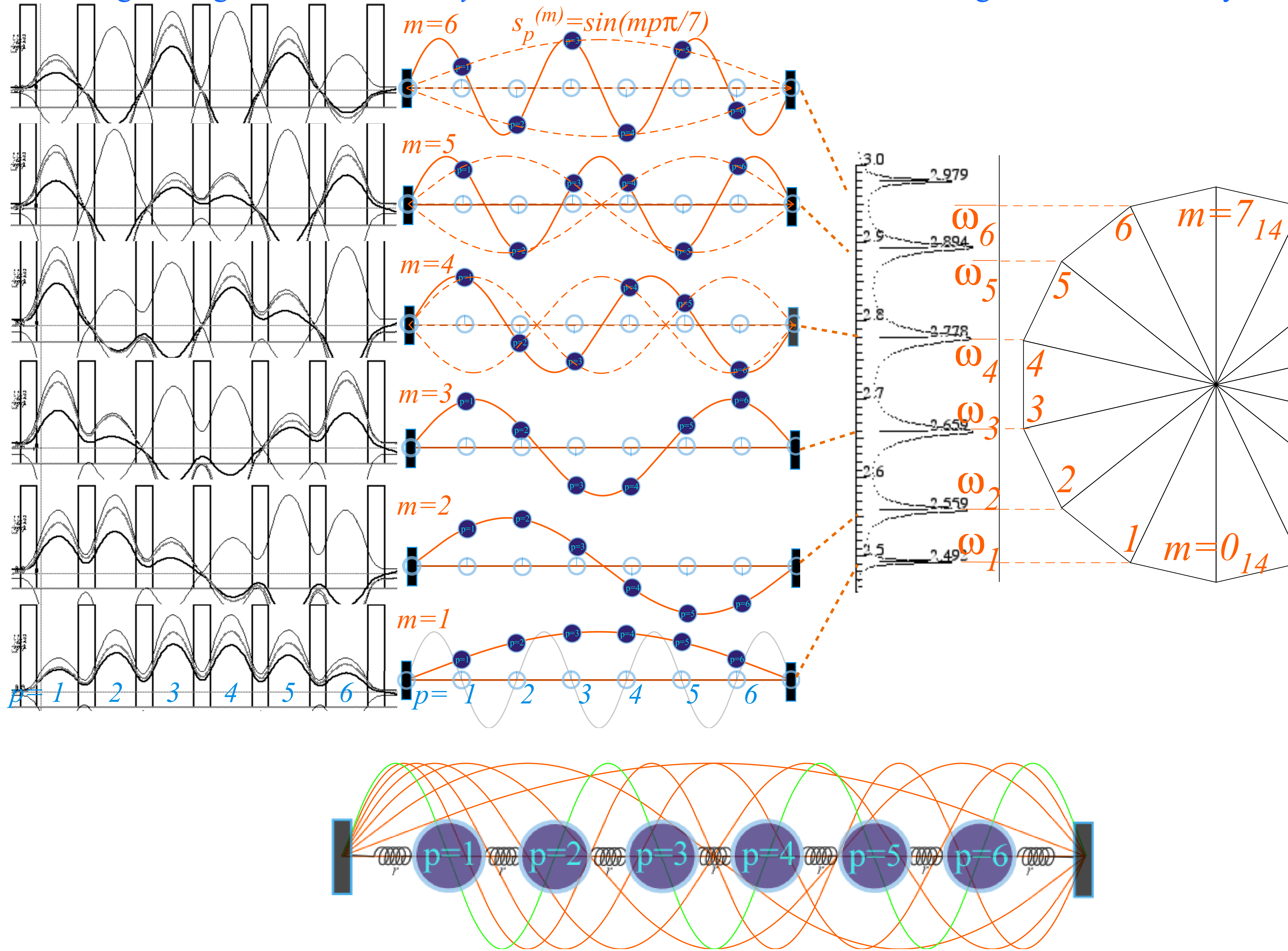
The "4-Group(s)" D_2 and C_{2v}

Spectral decomposition of D_2

Some D_2 modes

Outer product properties and the Group Zoo

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



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

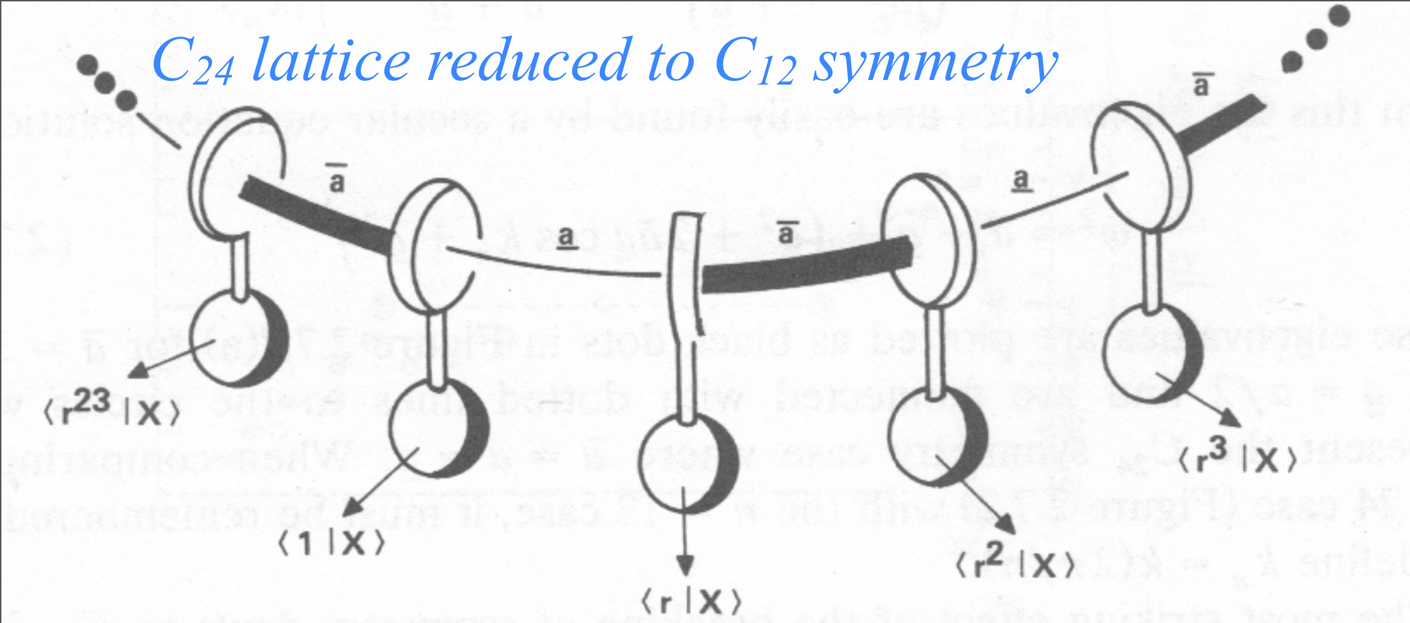

Fig. 2.7.6 PrinciplesSymmetryDynamics&Spectroscopy

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

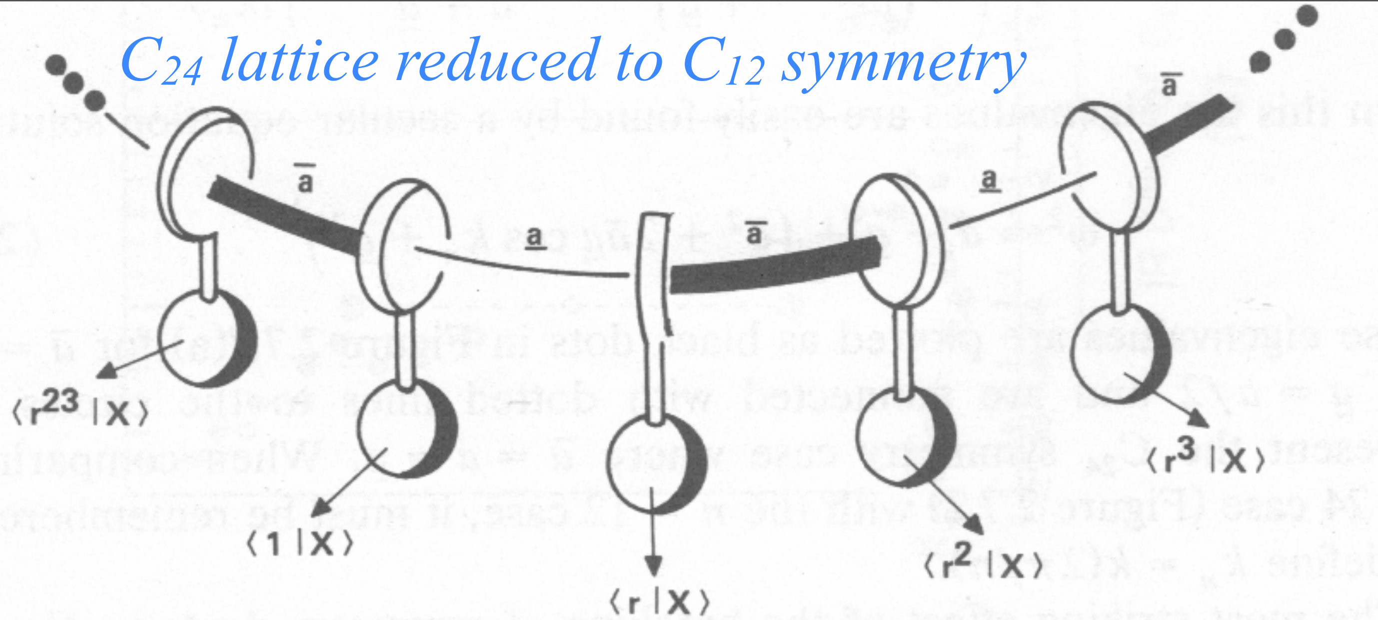

Fig. 2.7.6 PrinciplesSymmetryDynamics&Spectroscopy

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

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

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

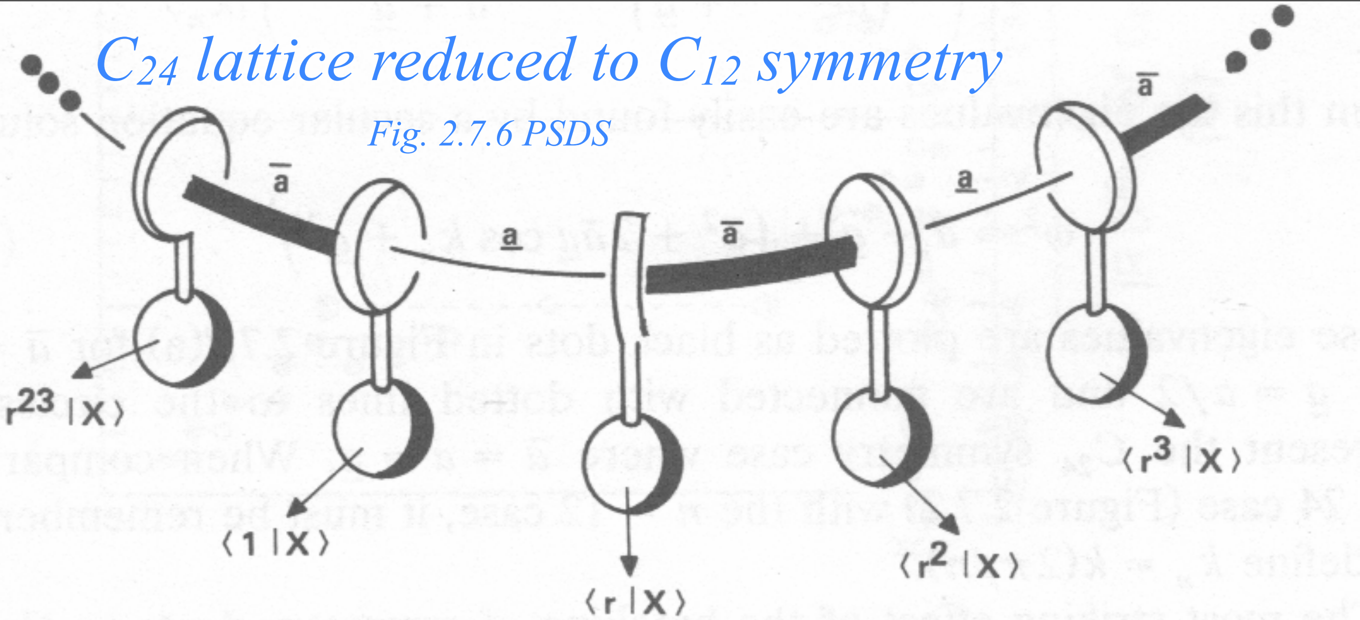

Fig. 2.7.6 PSDS

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

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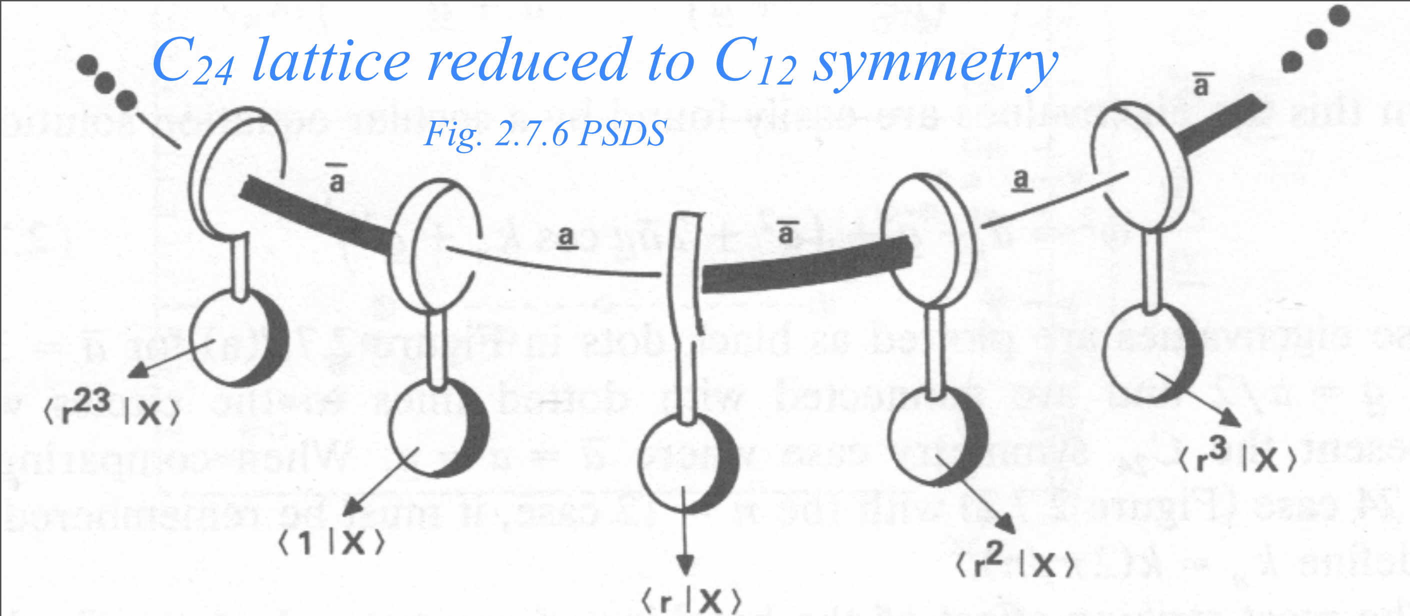
Only C_{12} symmetry projectors commute with **K***-matrix if* $\underline{a} \neq \bar{a}$

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



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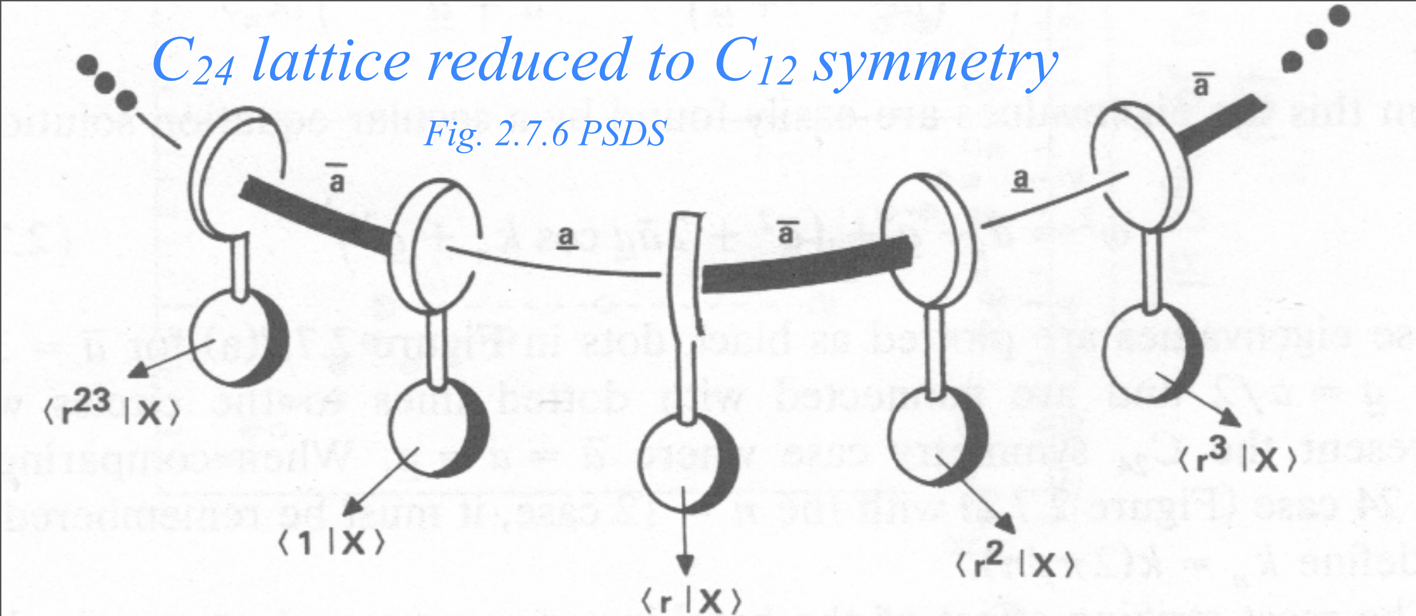
Only C_{12} *symmetry projectors commute with* **K**-*matrix if* $\underline{a} \neq \bar{a}$

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

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



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

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

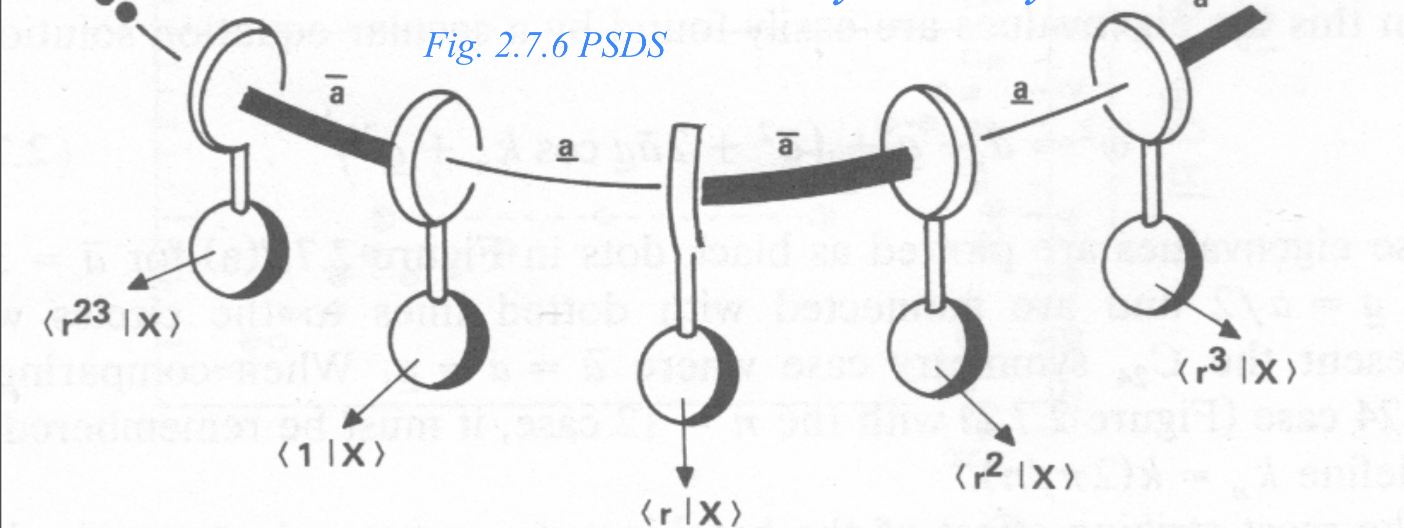

Fig. 2.7.6 PSDS

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

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

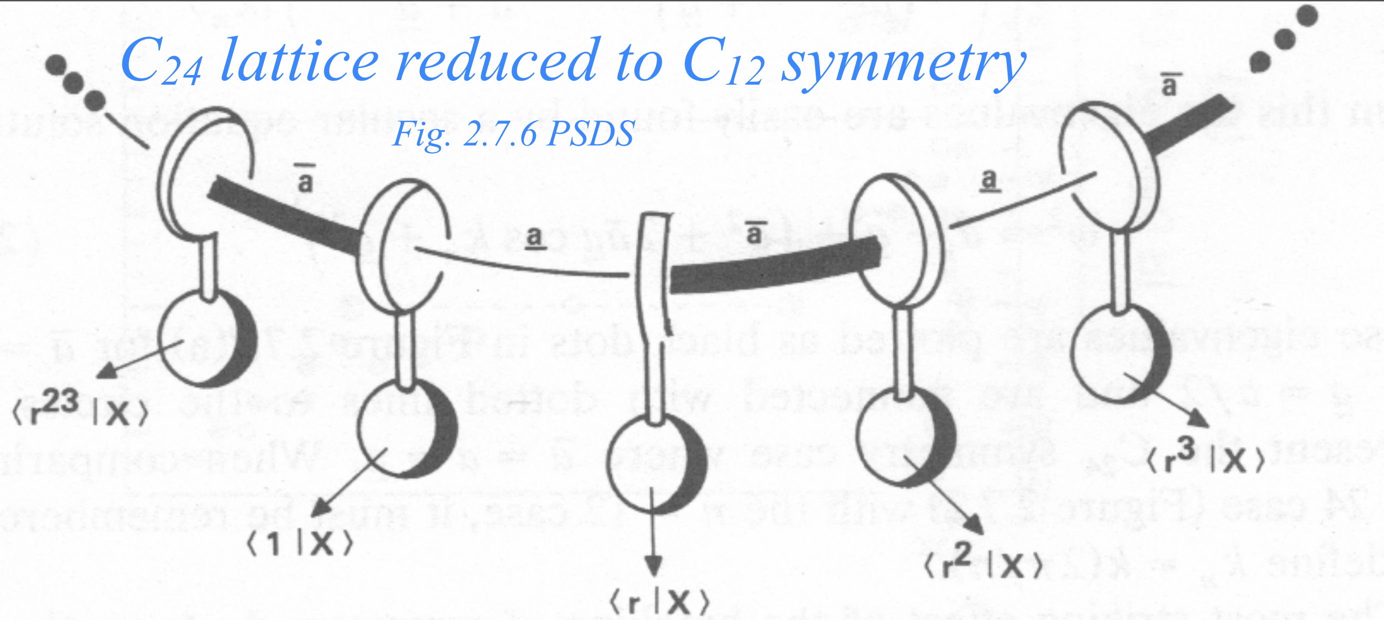

Fig. 2.7.6 PSDS

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

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

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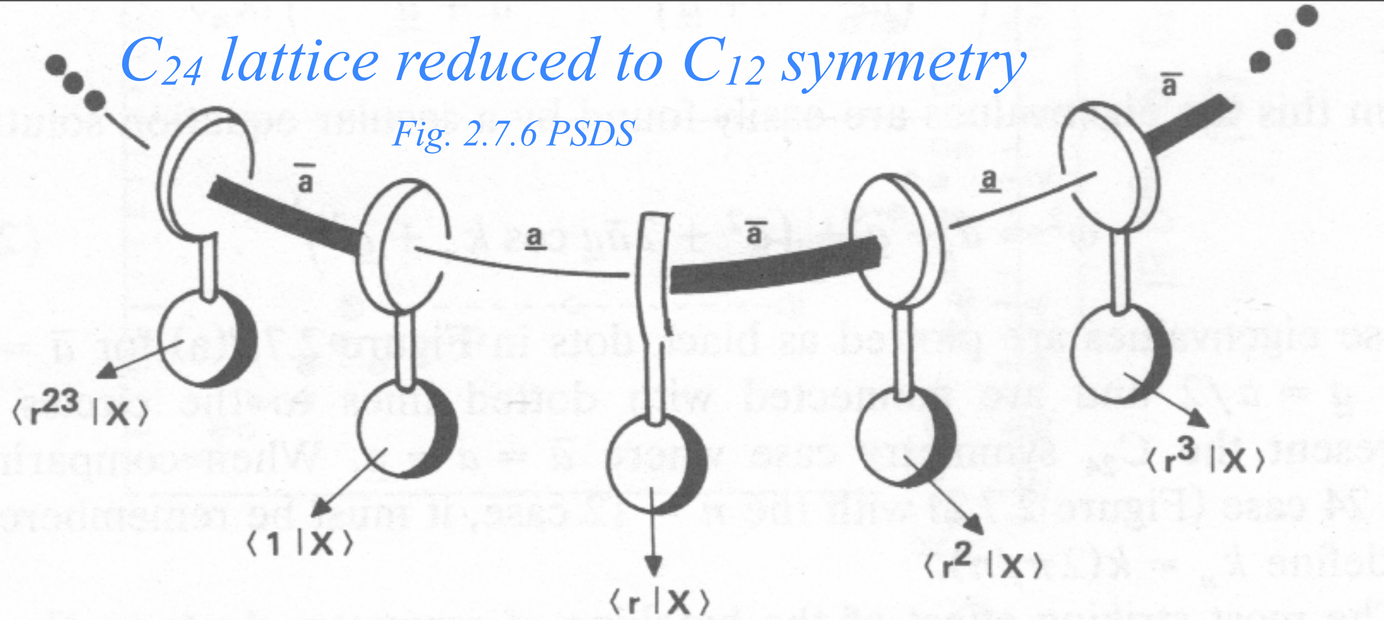

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$$\begin{pmatrix} \langle r^0|\mathbf{K}|r^0\rangle & \langle r^0|\mathbf{K}|r^1\rangle & \langle r^0|\mathbf{K}|r^2\rangle & \dots & \langle r^0|\mathbf{K}|r^{-1}\rangle \\ \langle r^1|\mathbf{K}|r^0\rangle & \langle r^1|\mathbf{K}|r^1\rangle & \langle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

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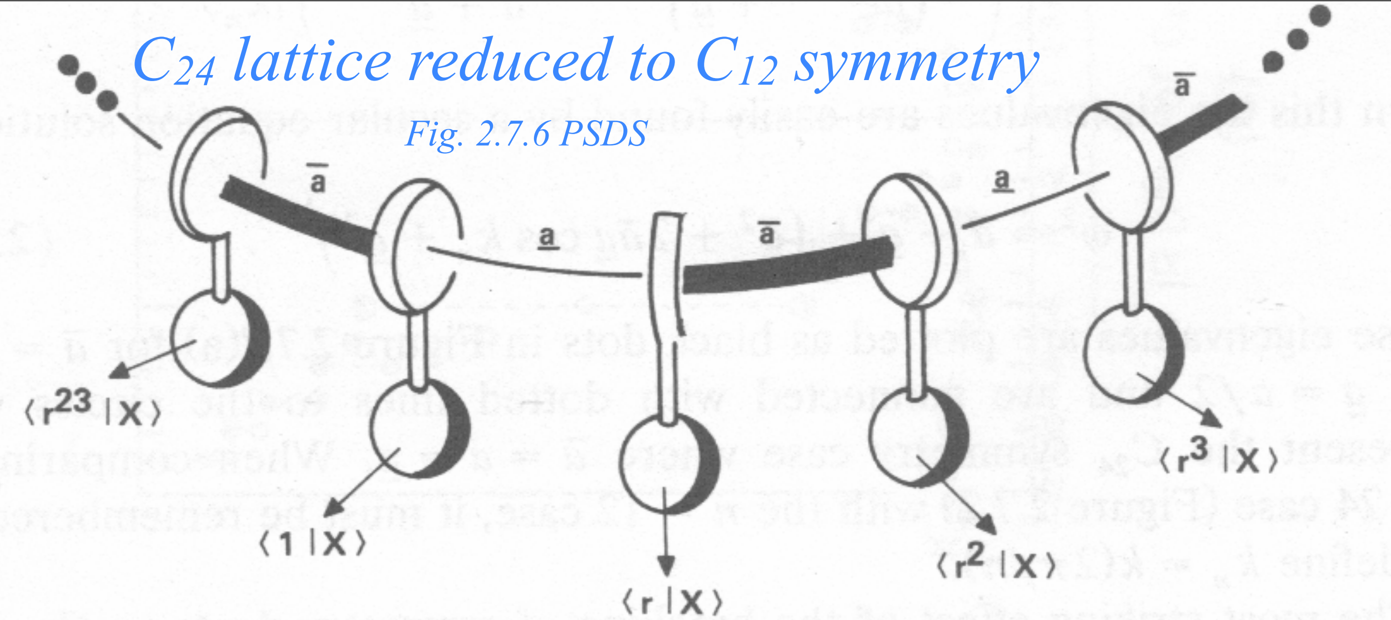
$$\begin{aligned}\langle k'_m|\mathbf{K}|k_m\rangle &= \langle r^1|\mathbf{P}^{(m)}\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle \cdot 12 = \langle r^1|\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle \cdot 12 \\ &= \langle r^1|\mathbf{K}|r^0\rangle + e^{-ik_m}\langle r^1|\mathbf{K}|r^2\rangle + e^{-2ik_m}\langle r^1|\mathbf{K}|r^4\rangle|r^5\rangle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

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



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

Only C_{12} symmetry projectors commute with $\mathbf{K}$*-matrix if* $\underline{a} \neq \bar{a}$

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

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

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

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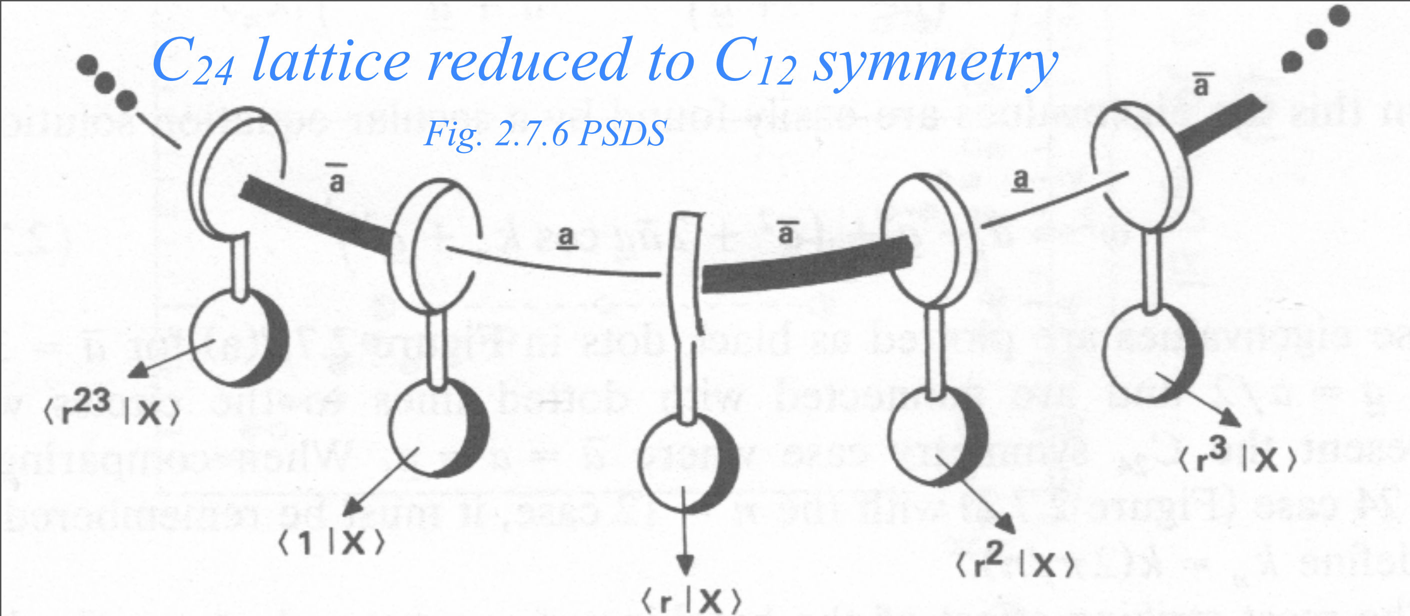

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Only C_{12} symmetry projectors commute with **K***-matrix if* $\underline{a} \neq \overline{a}$

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

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

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

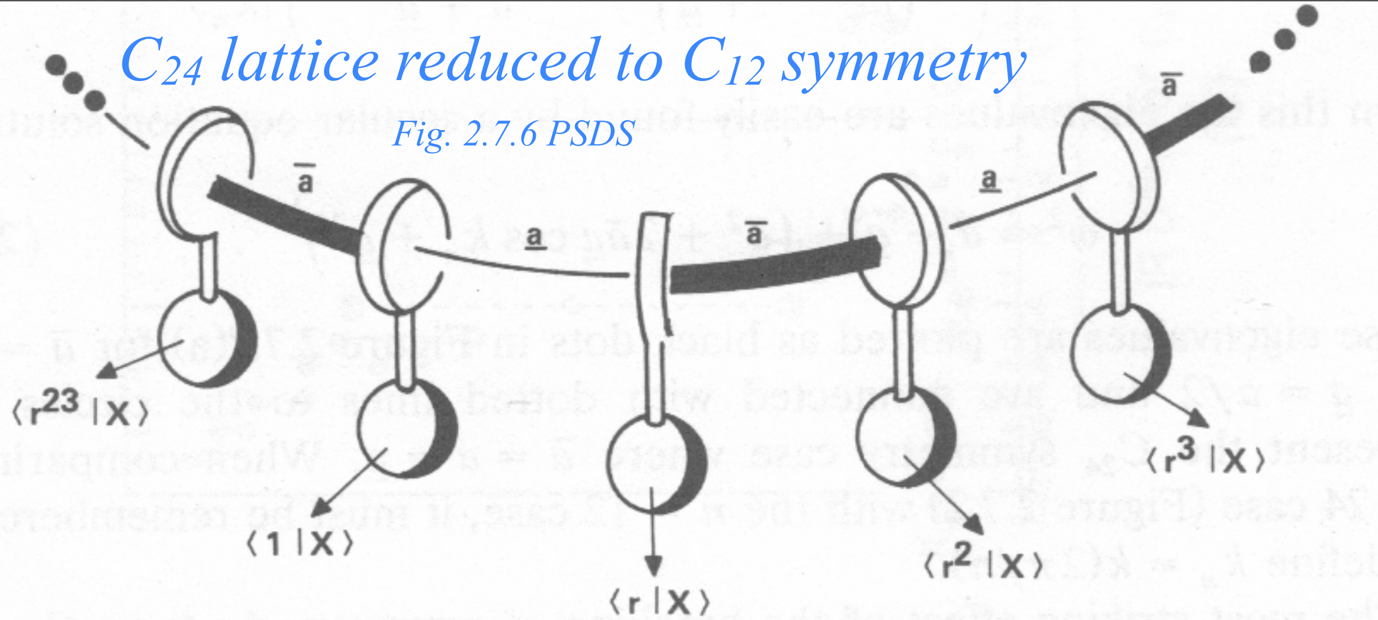

Fig. 2.7.6 PSDS

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

Only C_{12} symmetry projectors commute with **K**-*matrix if* $\underline{a} \neq \bar{a}$

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

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

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

Secular Eq.:

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

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

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

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

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

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

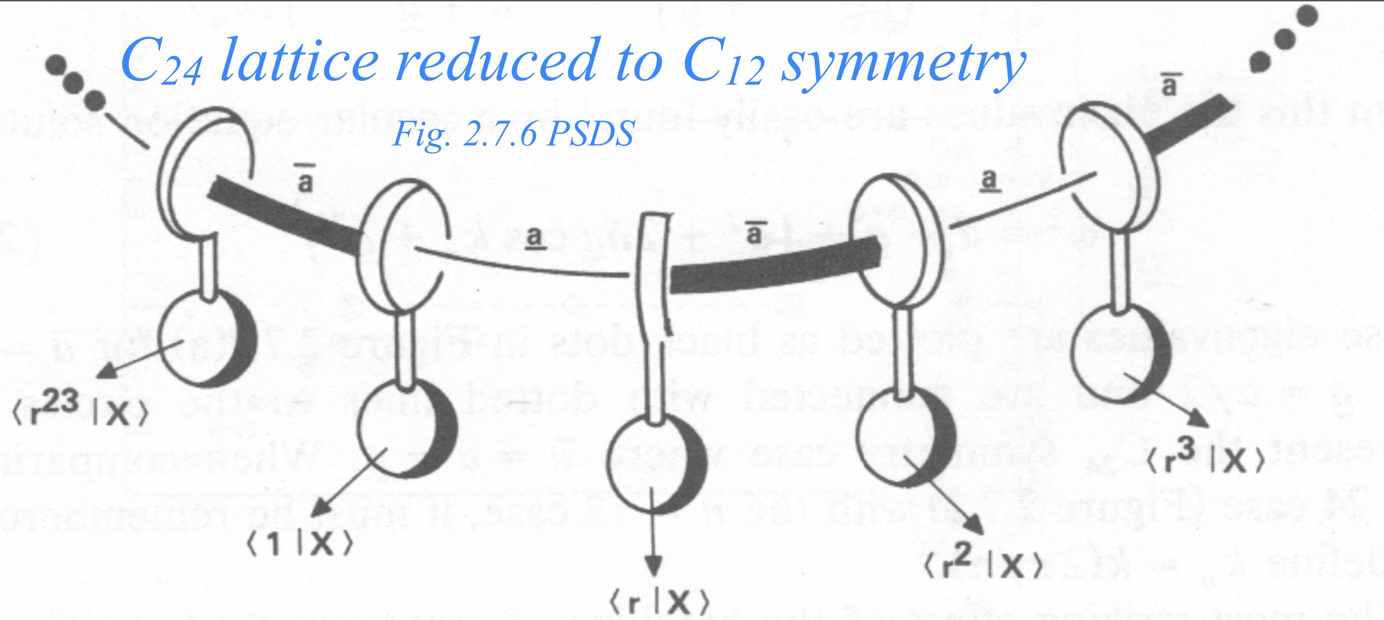

Fig. 2.7.6 PSDS

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

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

Only C_{12} symmetry projectors commute with **K**-*matrix if* $\underline{a} \neq \bar{a}$

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

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

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

Eigenvalues:

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

Fig. 2.7.7 PSDS

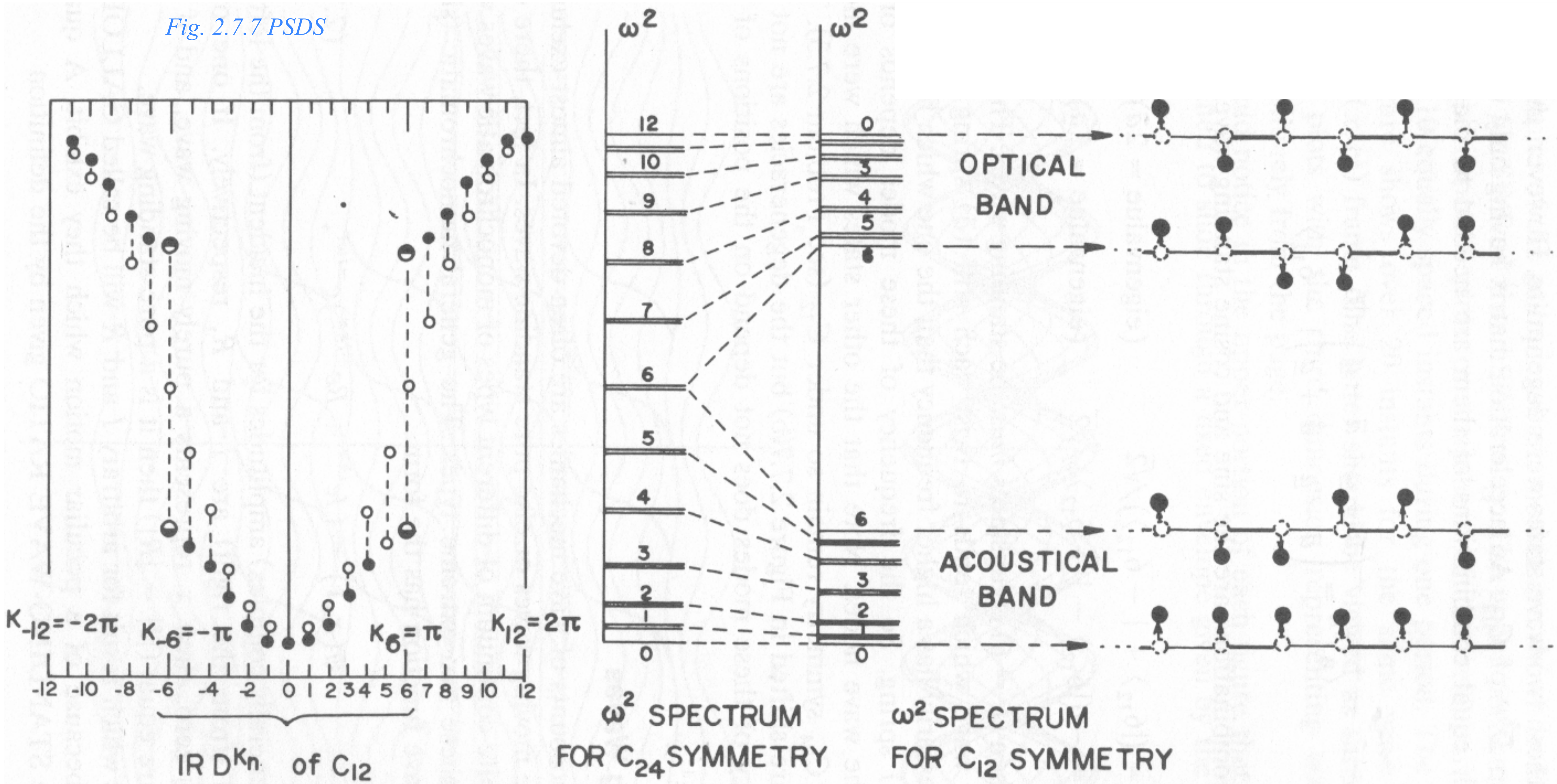


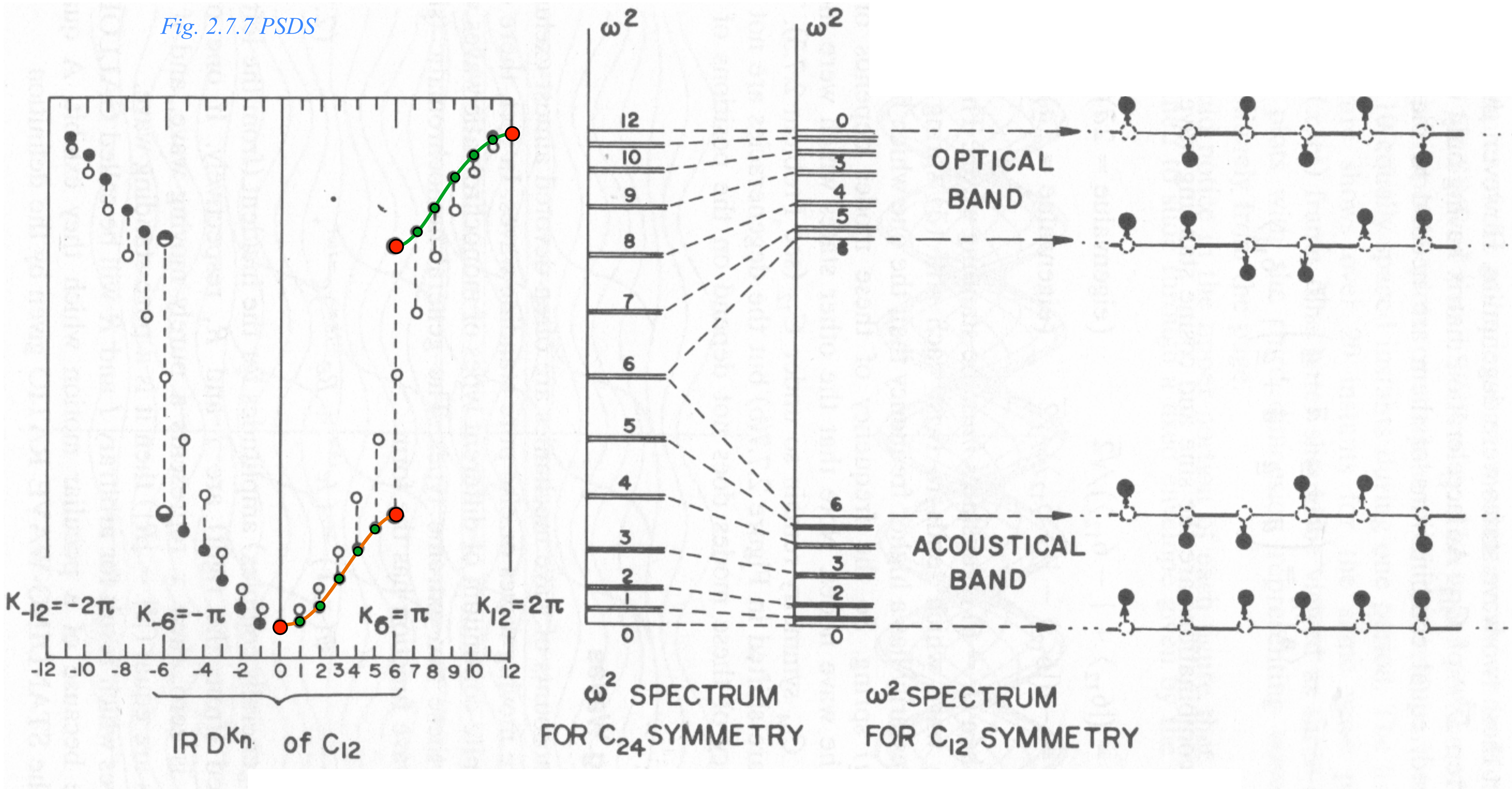
Figure 2.7.7 Band splitting due to C_{24}–C_{12} symmetry breaking.

Eigenvalues:

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

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

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



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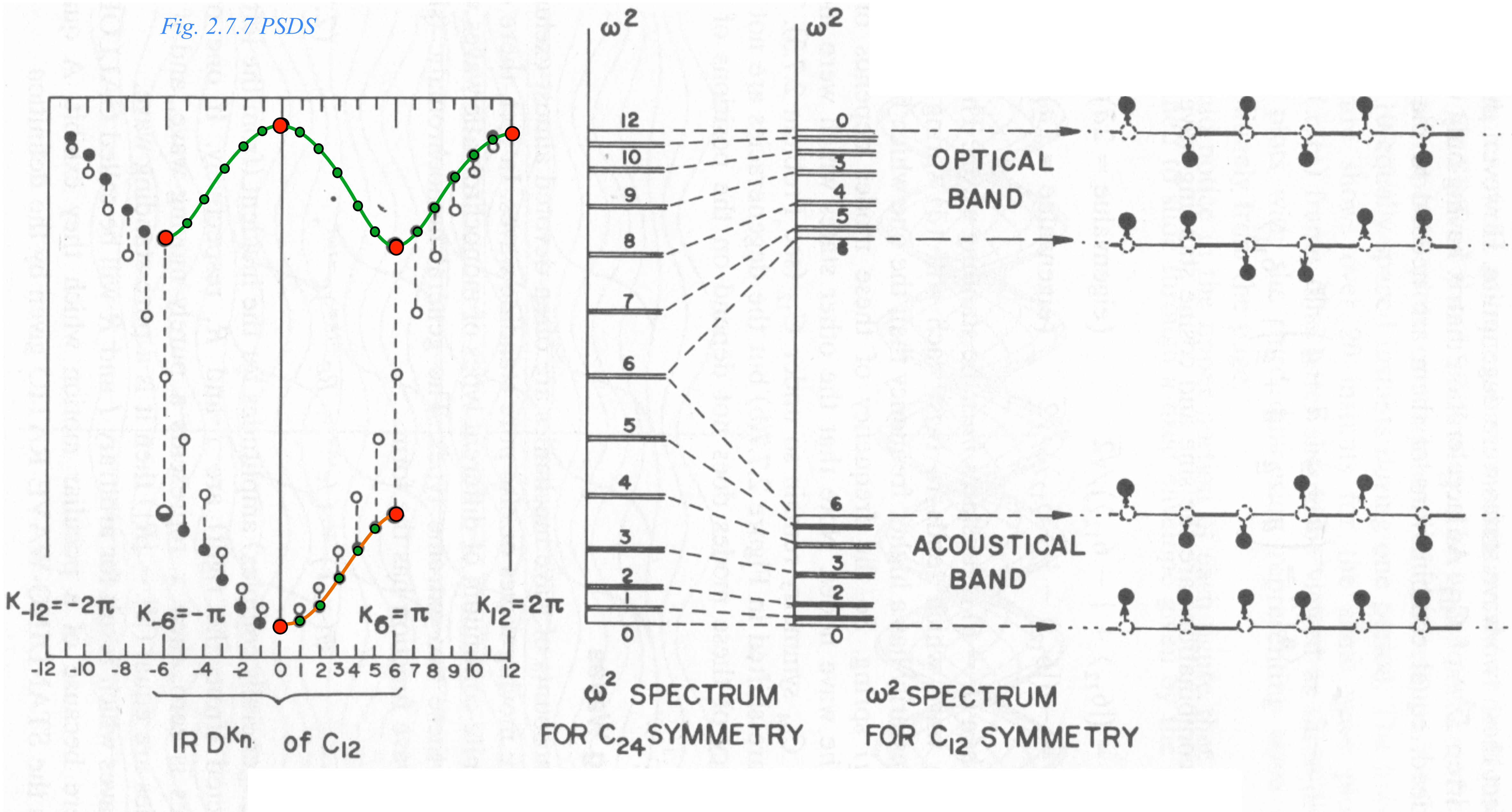
$$\langle \mathbf{K} \rangle^{k_m} = \begin{pmatrix} \langle k_m | \mathbf{K} | k_m \rangle & \langle k_m | \mathbf{K} | k'_m \rangle \\ \langle k'_m | \mathbf{K} | k_m \rangle & \langle k'_m | \mathbf{K} | k'_m \rangle \end{pmatrix}$$

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



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Eigenvalues:

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

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

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

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

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Acoustical modes vs. Optical modes

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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 Group Zoo

Fig. 2.12.1 PSDS

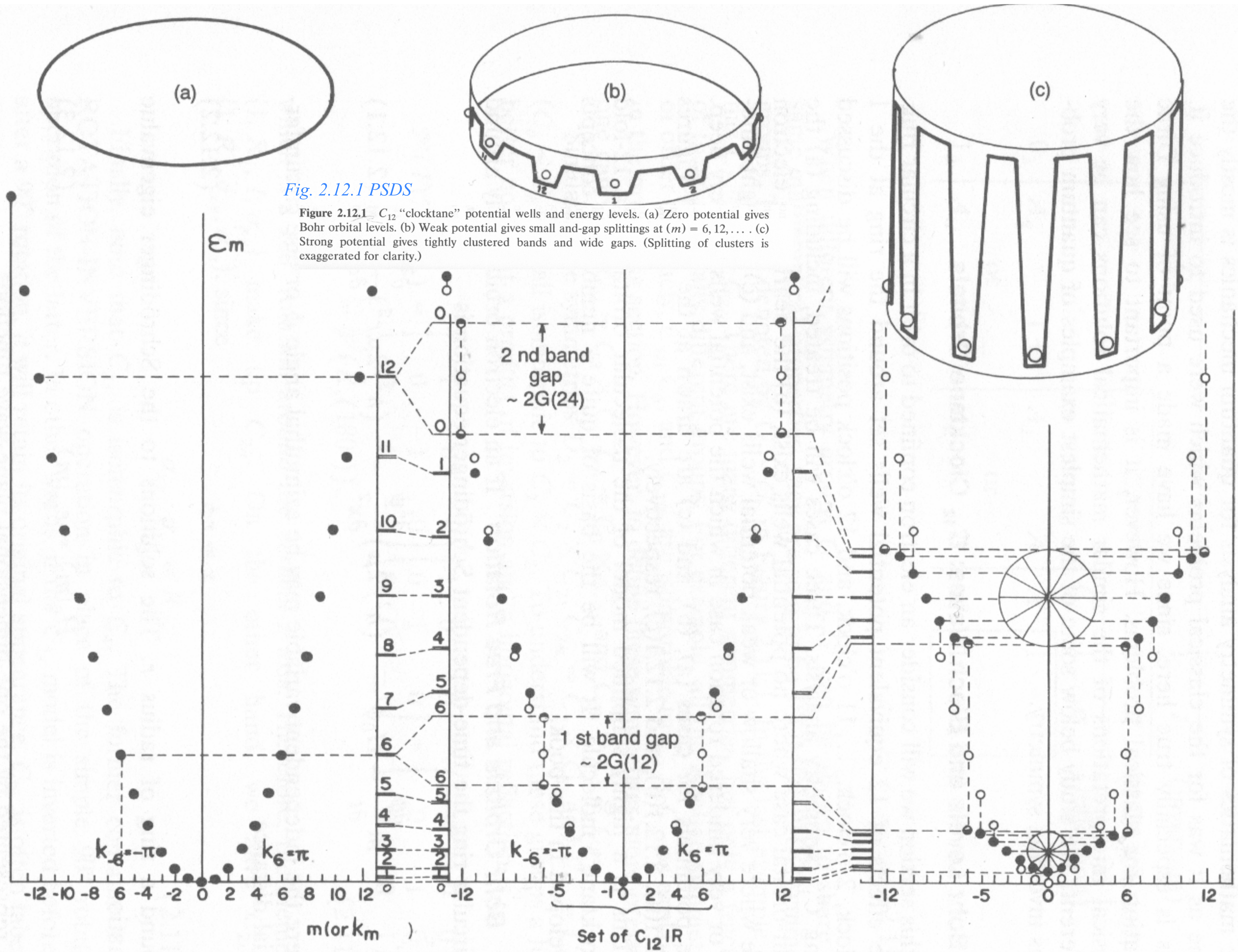
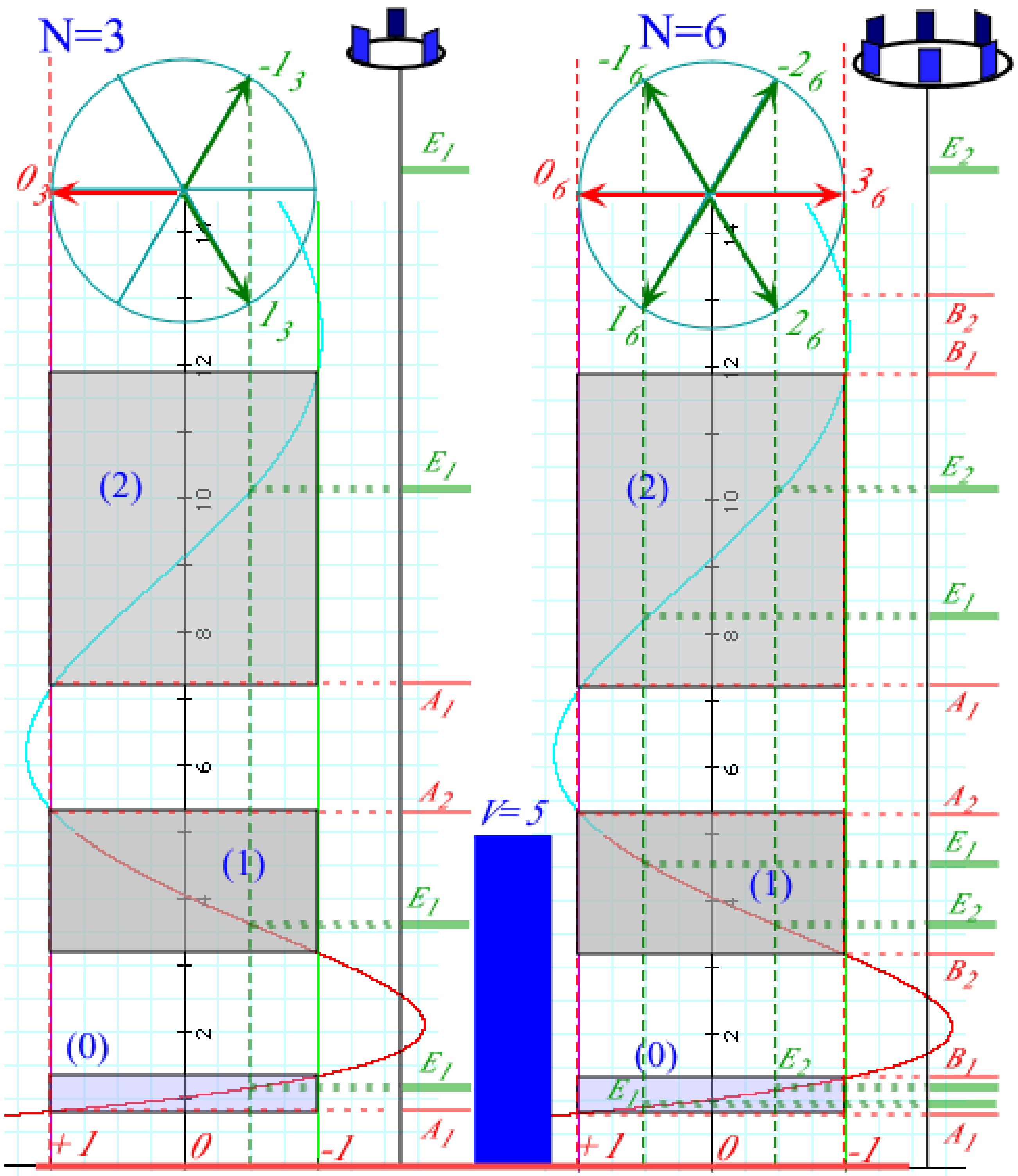


Figure 2.12.1 C_{12} "clocktane" potential wells and energy levels. (a) Zero potential gives Bohr orbital levels. (b) Weak potential gives small and-gap splittings at $(m) = 6, 12, \ldots$. (c) Strong potential gives tightly clustered bands and wide gaps. (Splitting of clusters is exaggerated for clarity.)

Bohr-It simulations assume ring-periodic-boundary conditions



Bohr-It simulations assume ring-periodic-boundary conditions

Band-It simulations line-non-periodic scattering conditions

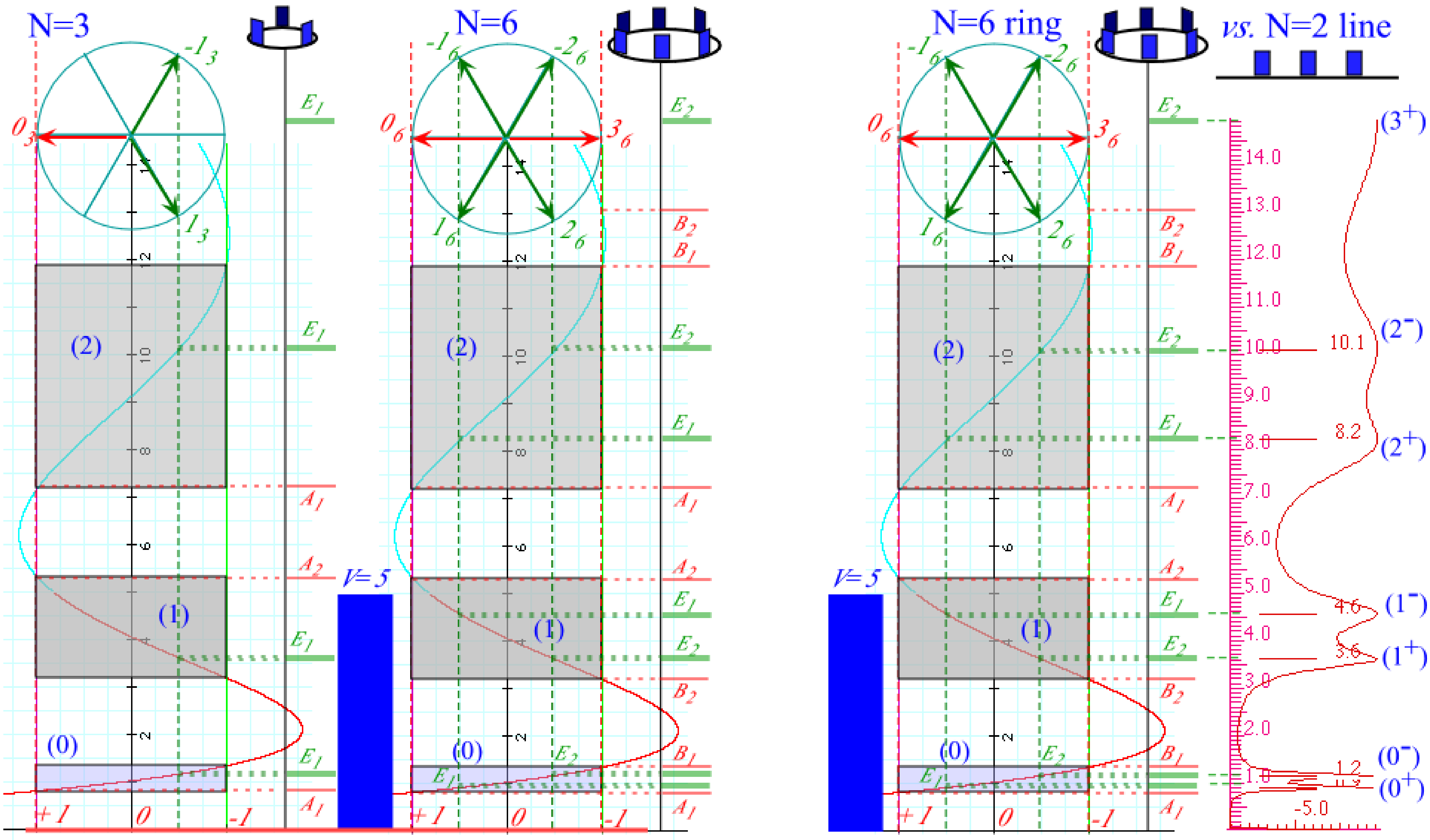


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Fig. 2.12.7 PSDS

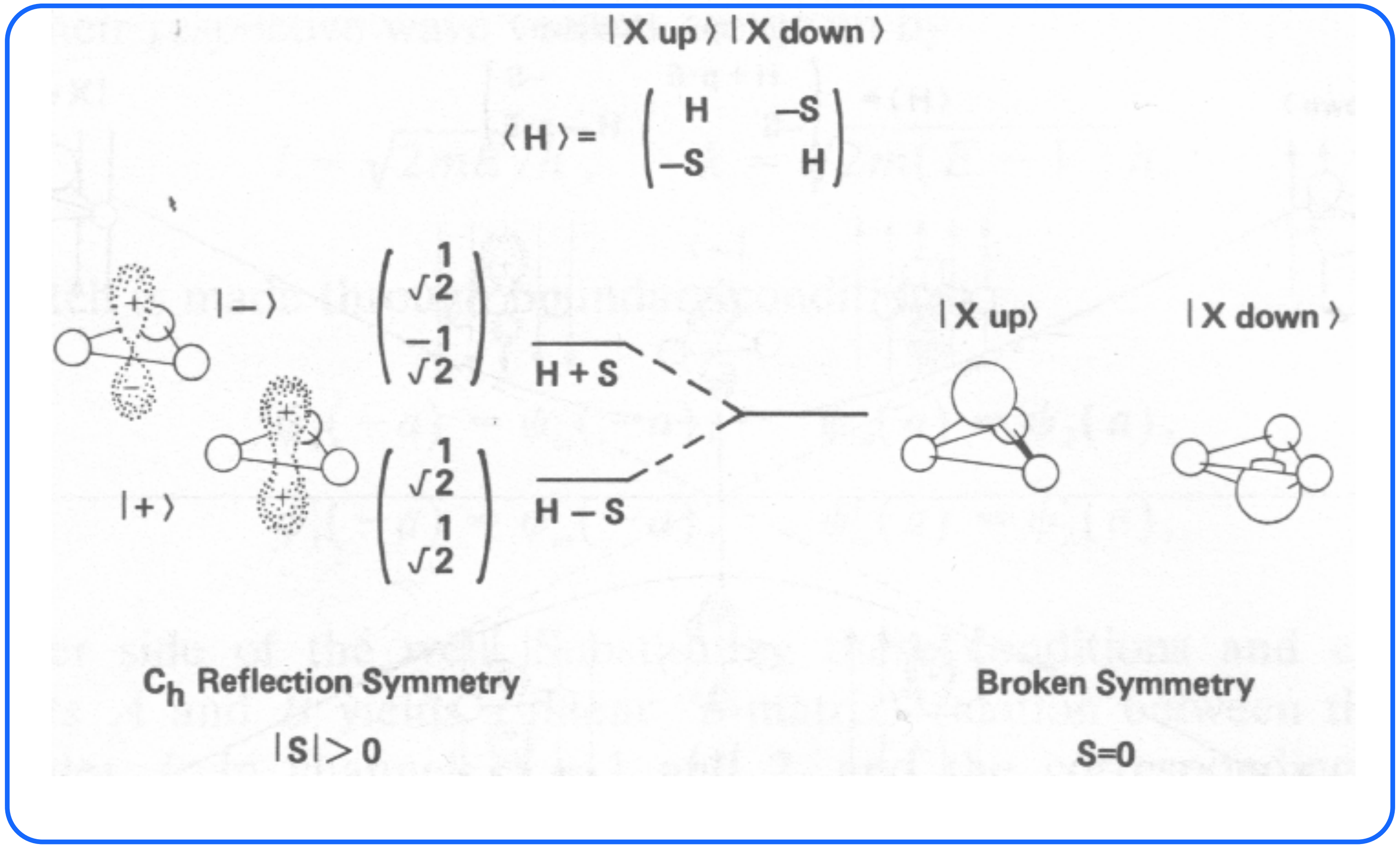


Fig. 2.12.7 PSDS

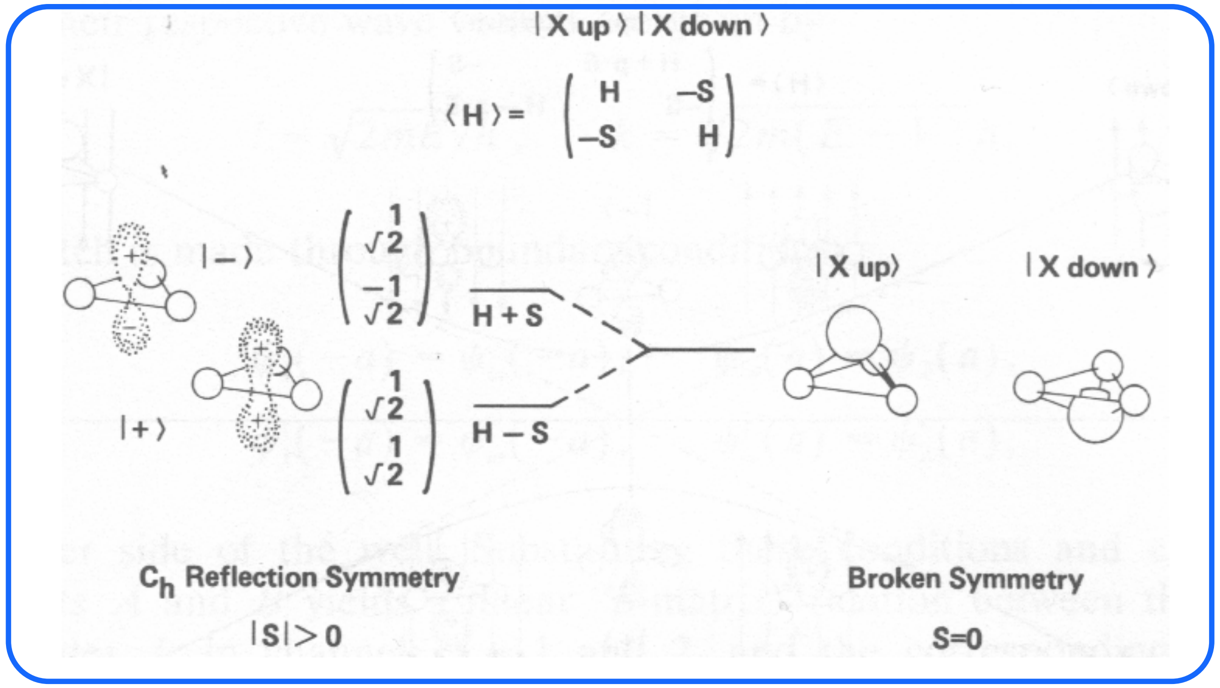
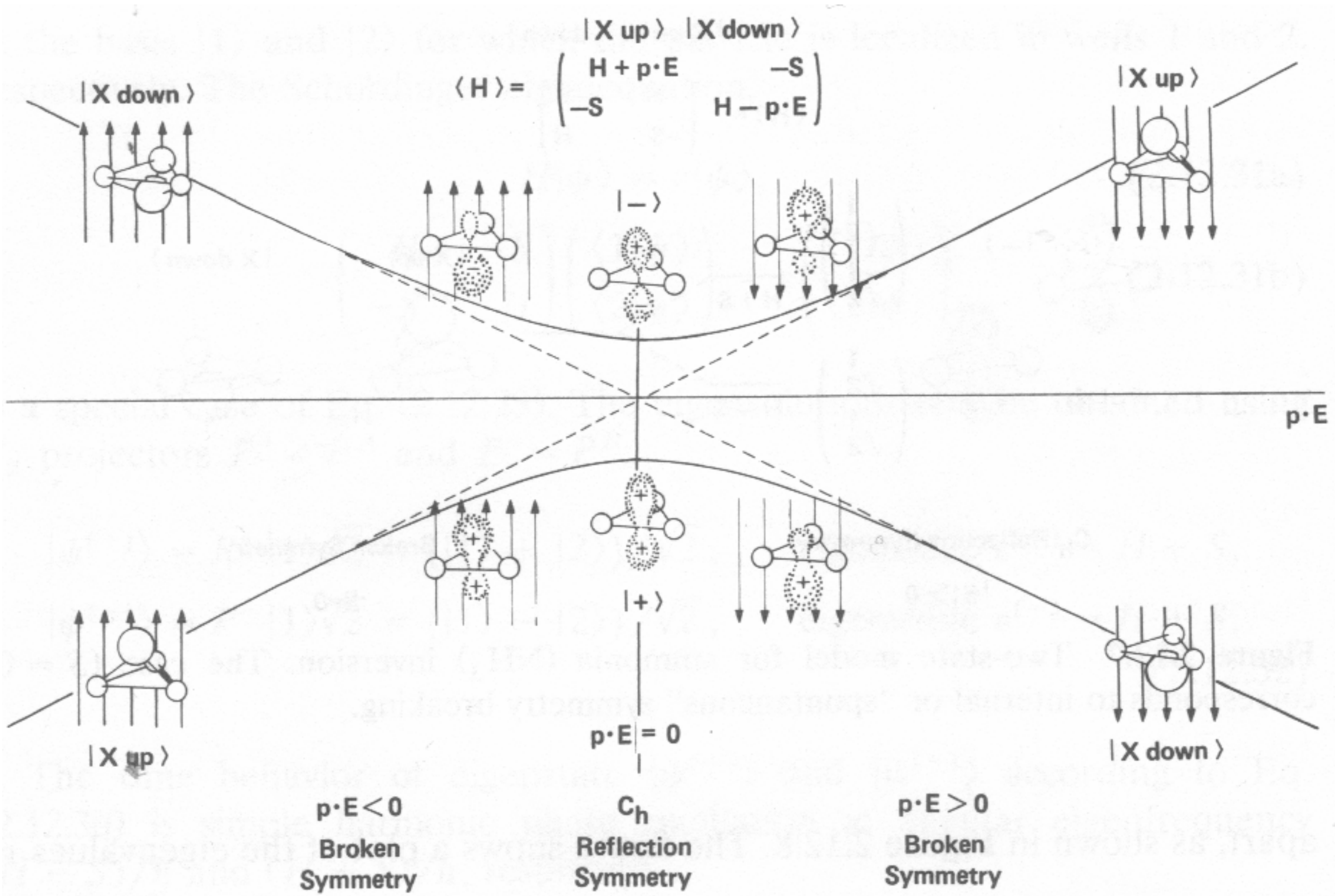


Fig. 2.12.8 PSDS



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Some D_2 modes

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

Fig. 2.11.1 PSDS

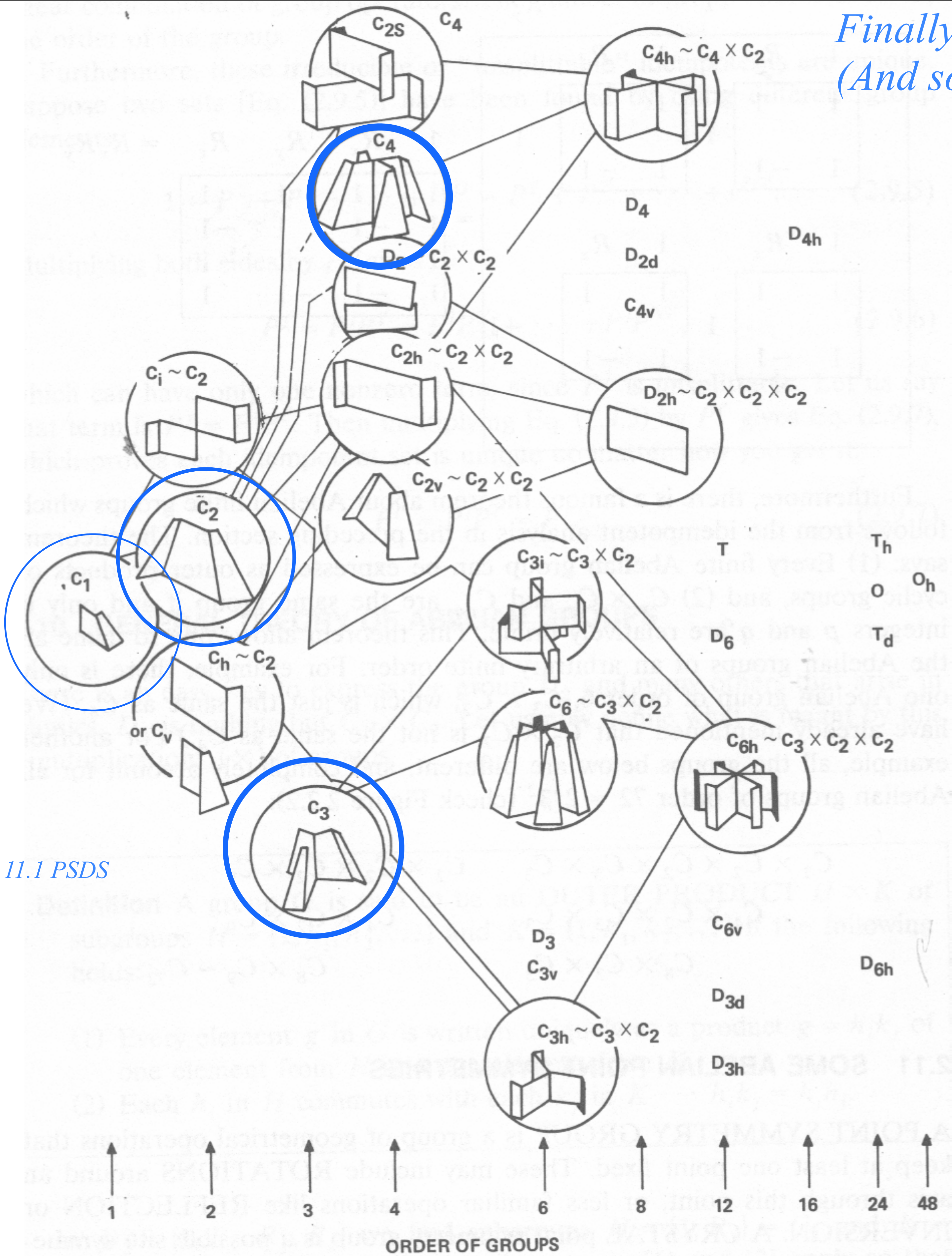


Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

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

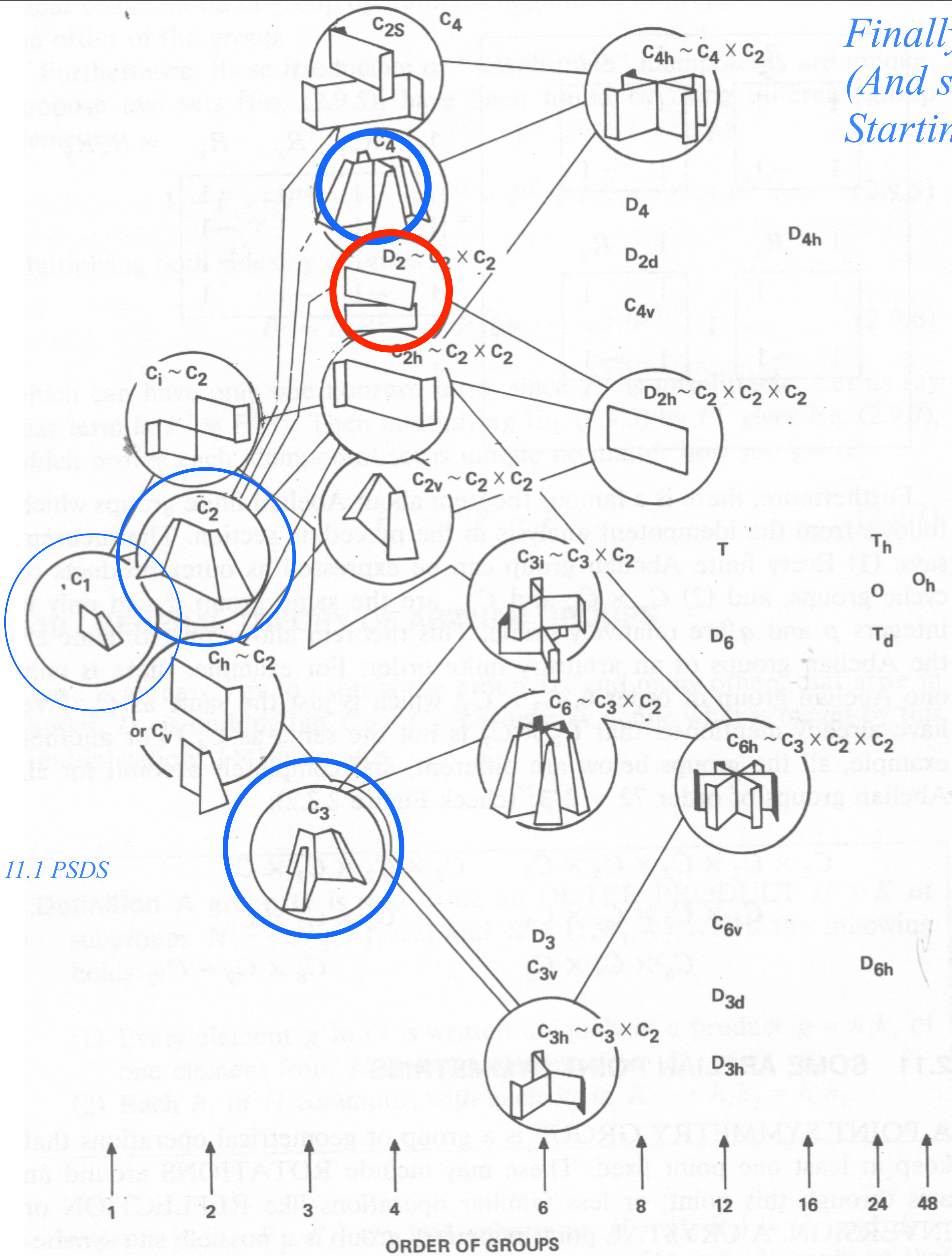


Fig. 2.11.1 PSDS

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 and C_{2h} and C_{2v}

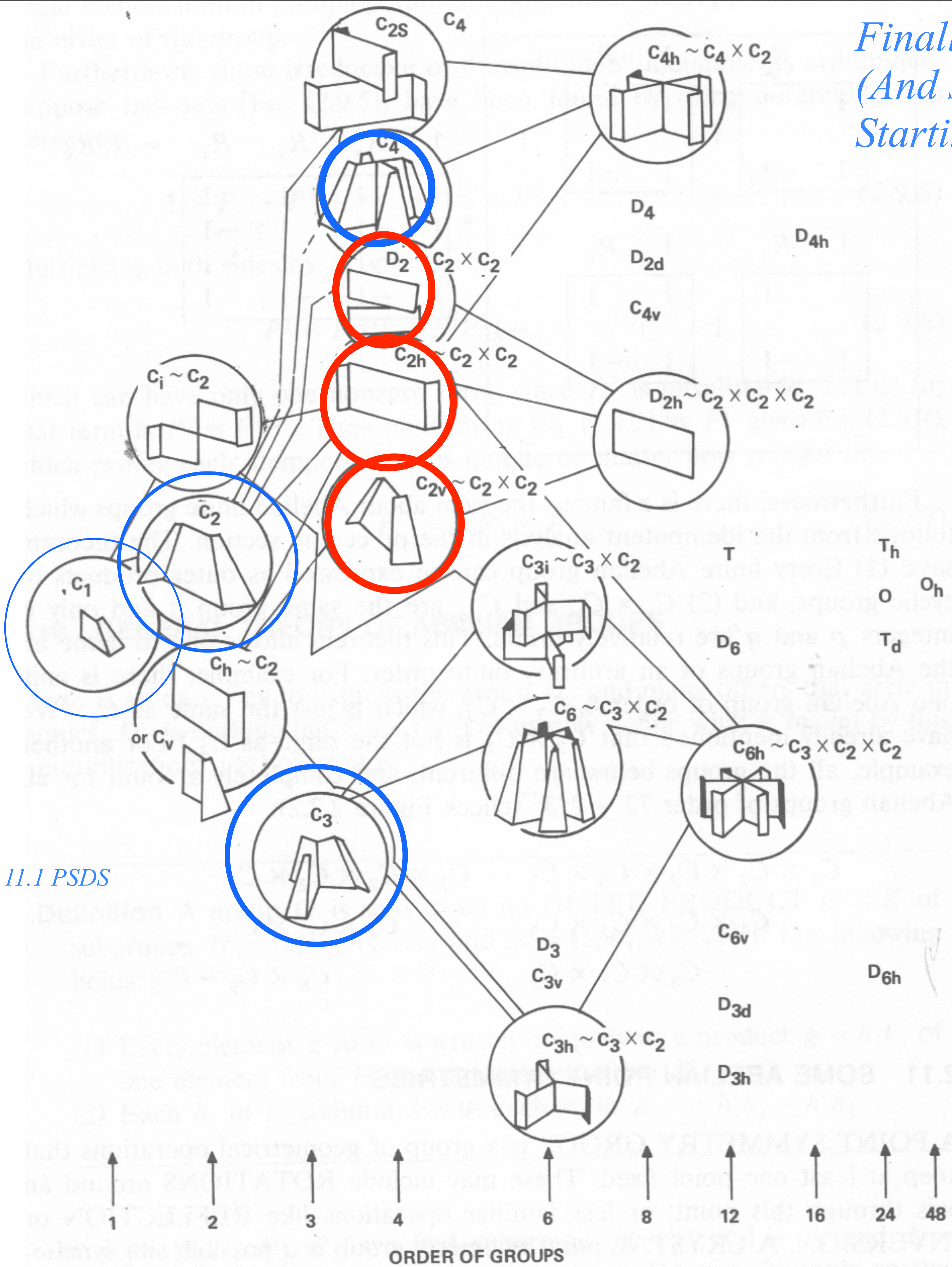
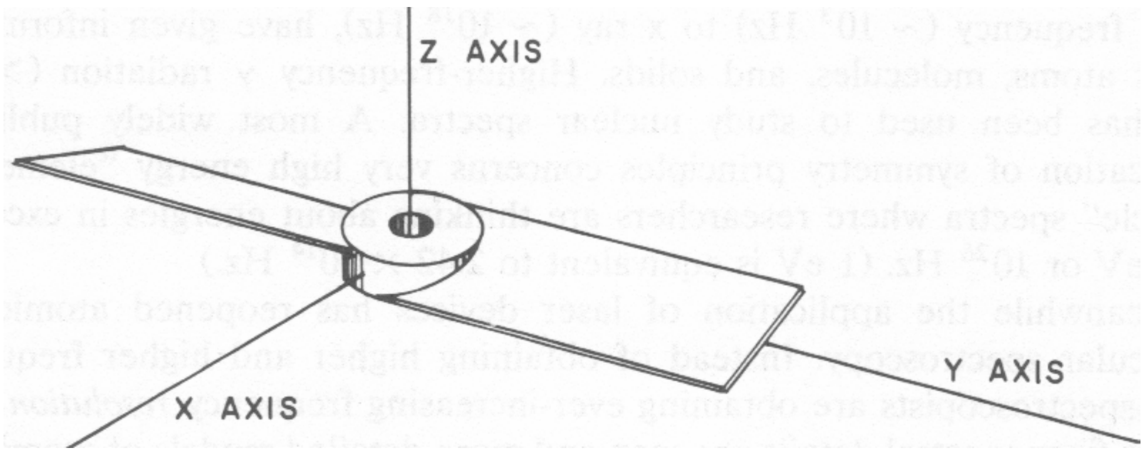


Fig. 2.11.1 PSDS

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.

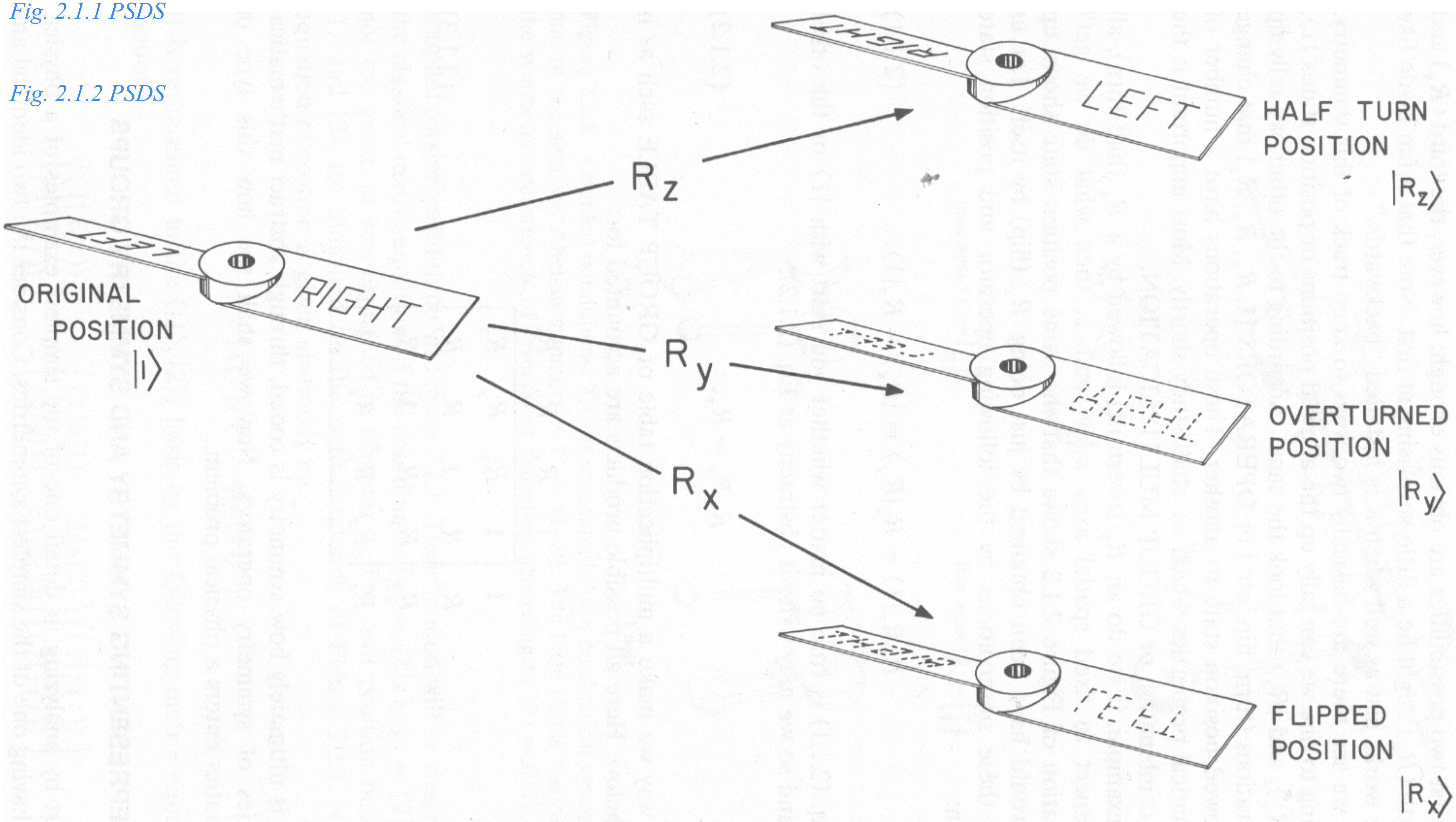
D_2 Symmetry (The 4-Group)



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



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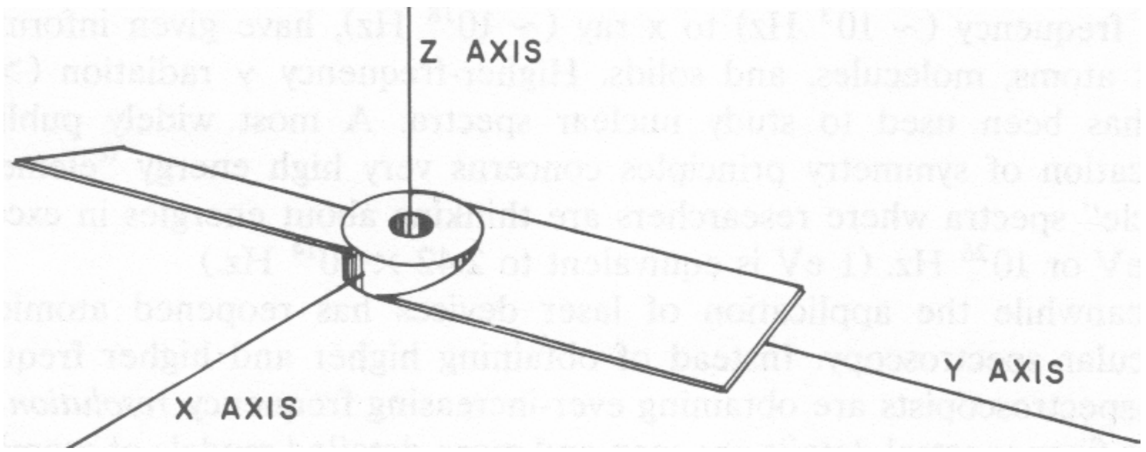

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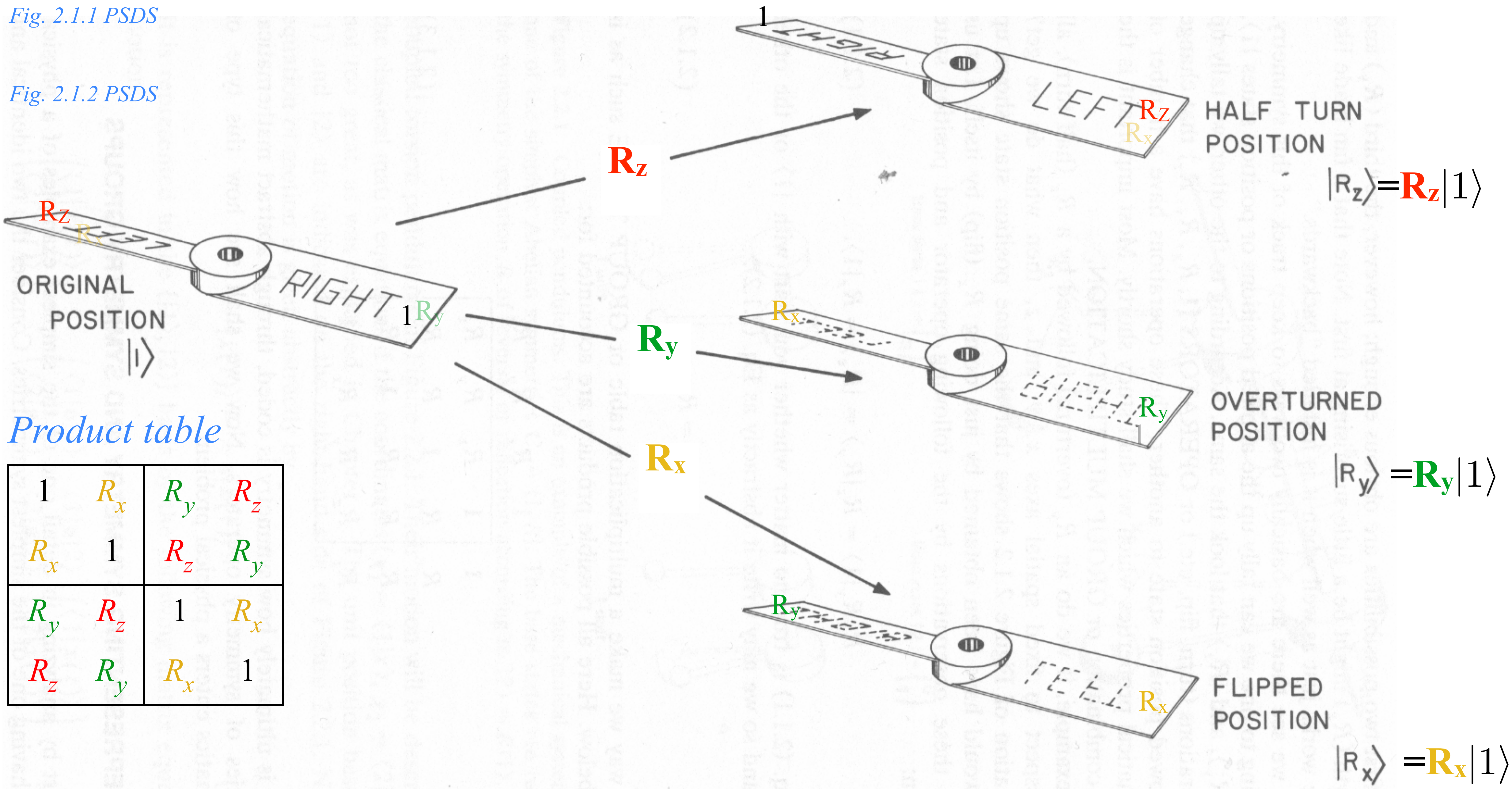
Fig. 2.1.1 PSDS

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

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

Two C_2 subgroup minimal equations:

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

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

Two C_2 subgroup minimal equations and their projectors:

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

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

reducible projectors

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

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

Completeness

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

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

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

$$\mathbf{R}_x = \mathbf{P}_x^+ - \mathbf{P}_x^- \qquad \textit{Spec.decomps} \qquad \mathbf{R}_y = \mathbf{P}_y^+ - \mathbf{P}_y^-$$

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

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

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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*

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

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

reducible projectors

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

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

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

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

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

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

Two C_2 subgroup minimal equations and their projectors:

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

reducible projectors

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

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

Completeness

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

Spec.decomps

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

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*)

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

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

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

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

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

Two C_2 subgroup minimal equations and their projectors:

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

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

reducible projectors

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

Completeness

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

Spec.decomps

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

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

×

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

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

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

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*

$$\mathbf{P}^{++} \equiv \mathbf{P}_x^+\cdot\mathbf{P}_y^+ = \frac{(\mathbf{1}+\mathbf{R}_x)\cdot(\mathbf{1}+\mathbf{R}_y)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x+\mathbf{R}_y+\mathbf{R}_z\right)$$

$$\mathbf{P}^{-+} \equiv \mathbf{P}_x^-\cdot\mathbf{P}_y^+ = \frac{(\mathbf{1}-\mathbf{R}_x)\cdot(\mathbf{1}+\mathbf{R}_y)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x+\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{+-} \equiv \mathbf{P}_x^+\cdot\mathbf{P}_y^- = \frac{(\mathbf{1}+\mathbf{R}_x)\cdot(\mathbf{1}-\mathbf{R}_y)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x-\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{--} \equiv \mathbf{P}_x^-\cdot\mathbf{P}_y^- = \frac{(\mathbf{1}-\mathbf{R}_x)\cdot(\mathbf{1}-\mathbf{R}_y)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x-\mathbf{R}_y+\mathbf{R}_z\right)$$

(*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

$=$

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

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

$=$

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

$=$

D_2	$\mathbf{1}$	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$
$++=A_1$	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

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

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

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

reducible projectors

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

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

Completeness
Spec.decomps

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*

$$\mathbf{P}^{++} \equiv \mathbf{P}_x^+\cdot\mathbf{P}_y^+ = \frac{(\mathbf{1}+\mathbf{R}_x)\cdot(\mathbf{1}+\mathbf{R}_y)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x+\mathbf{R}_y+\mathbf{R}_z\right)$$

$$\mathbf{P}^{-+} \equiv \mathbf{P}_x^-\cdot\mathbf{P}_y^+ = \frac{(\mathbf{1}-\mathbf{R}_x)\cdot(\mathbf{1}+\mathbf{R}_y)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x+\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{+-} \equiv \mathbf{P}_x^+\cdot\mathbf{P}_y^- = \frac{(\mathbf{1}+\mathbf{R}_x)\cdot(\mathbf{1}-\mathbf{R}_y)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x-\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{--} \equiv \mathbf{P}_x^-\cdot\mathbf{P}_y^- = \frac{(\mathbf{1}-\mathbf{R}_x)\cdot(\mathbf{1}-\mathbf{R}_y)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x-\mathbf{R}_y+\mathbf{R}_z\right)$$

$(completeness\ is\ first)$

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

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

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

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

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

$=$

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

Shortcut notation for getting D_2 character table

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 Group Zoo

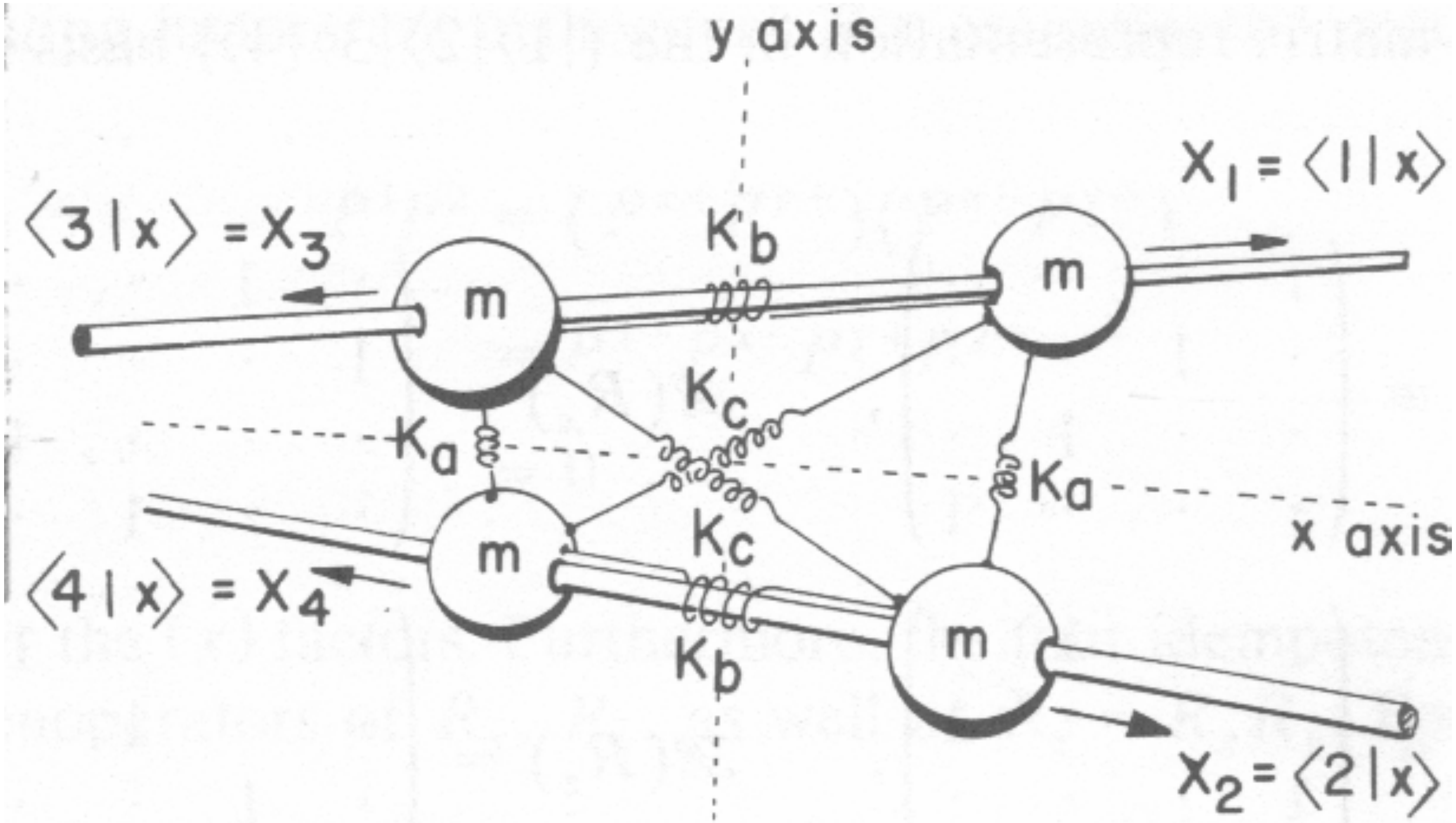


Fig. 2.8.1 PSDS

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

$$A = -\left(k_a \cos^2(a,b) + k_b + k_c \cos^2(b,c)\right)/m,$$
$$a = -k_a \cos^2(a,b)/m,$$
$$b = -k_b/m,$$
$$c = -k_c \cos^2(b,c)/m.$$

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

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

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

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

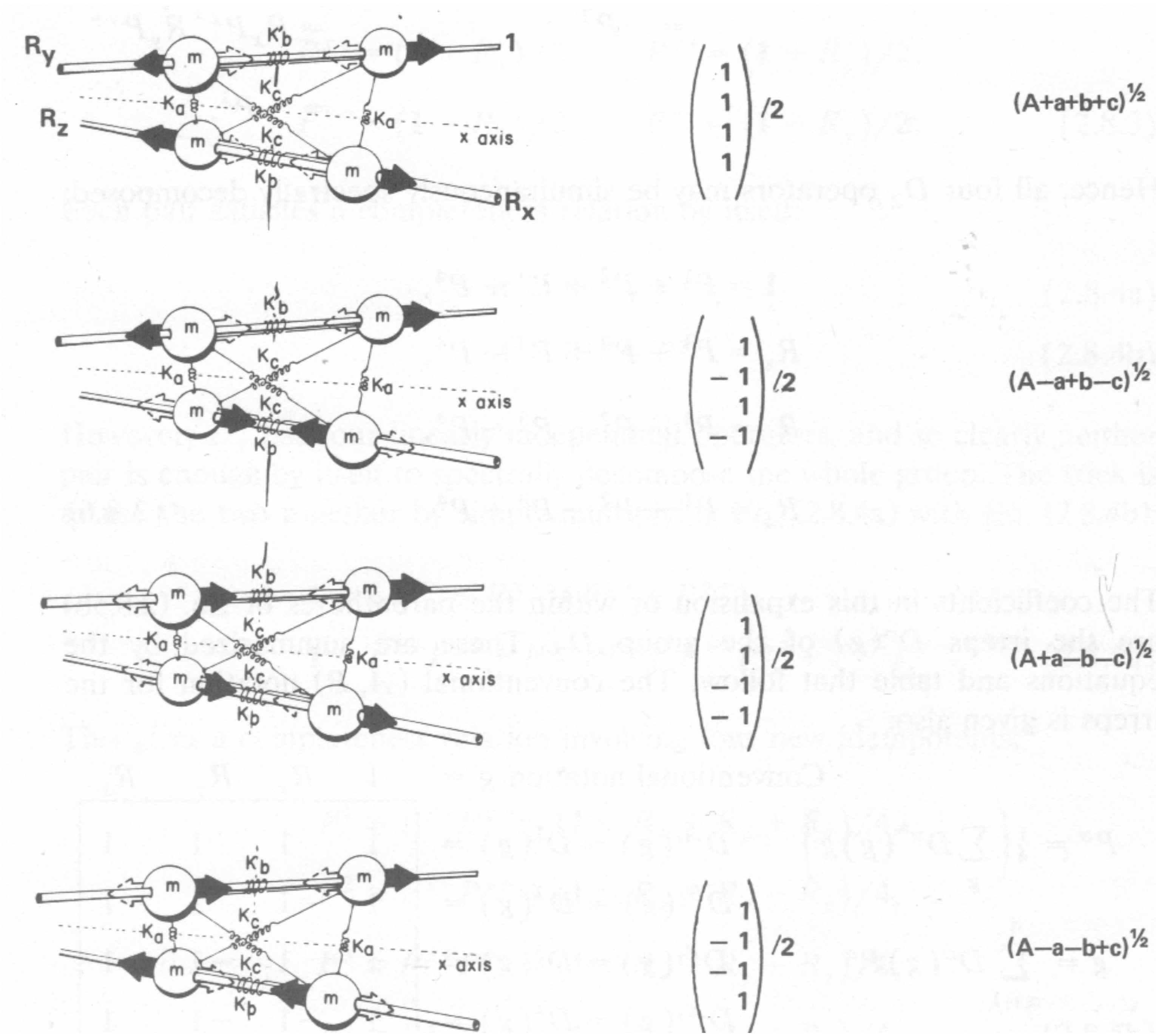


Fig. 2.8.2 PSDS

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 Group Zoo

Fig. 2.11.1 PSDS

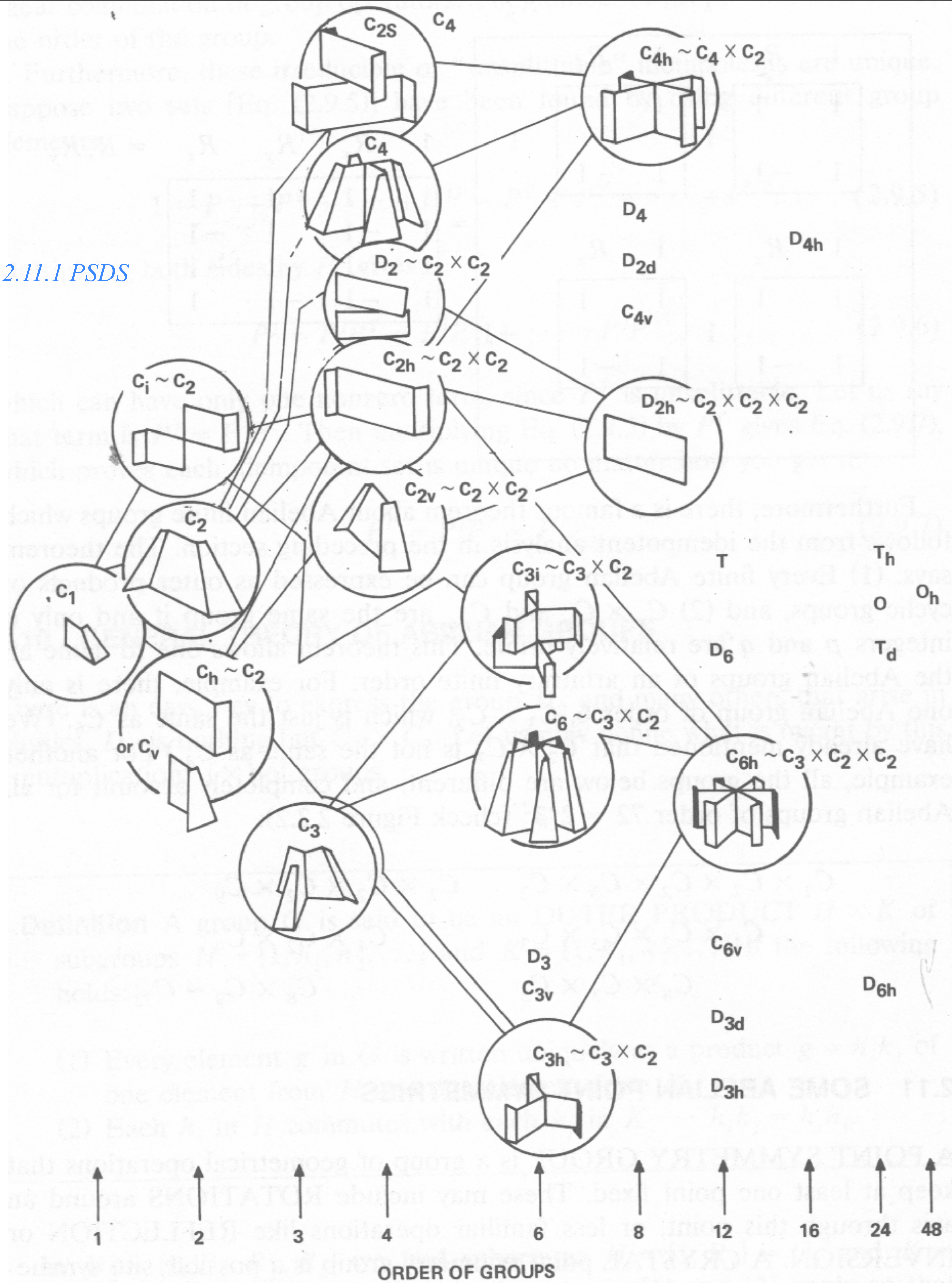


Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

Fig. 2.2.2 PSDS

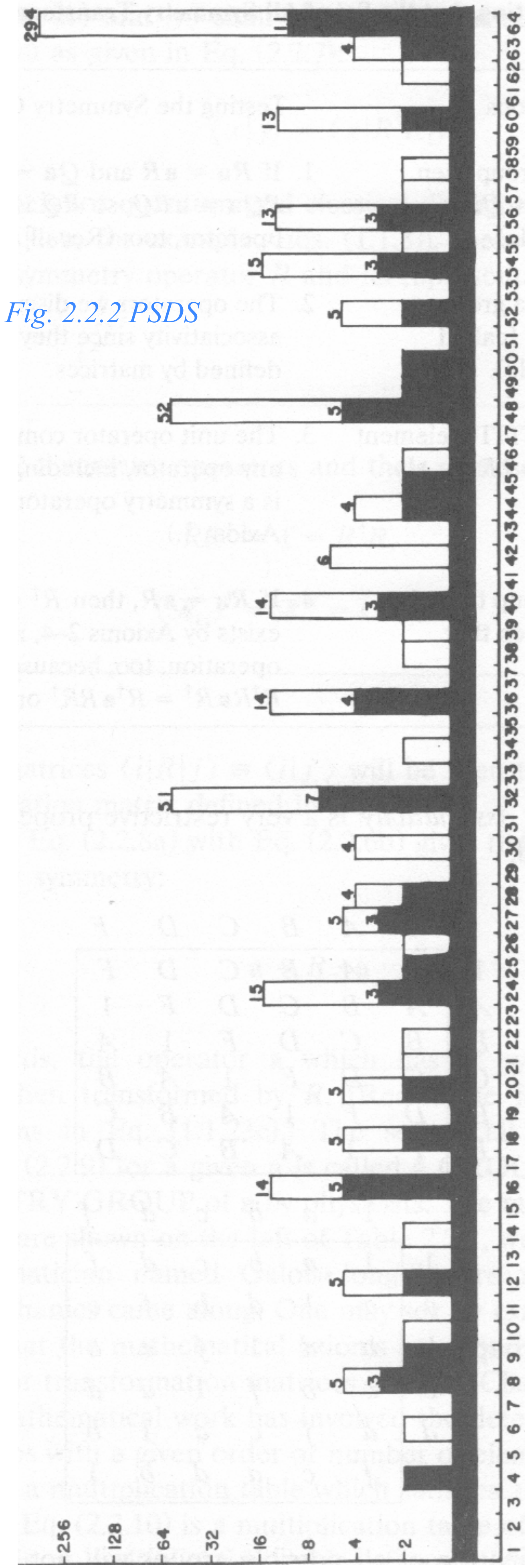


Fig. 3.1.1 PSDS

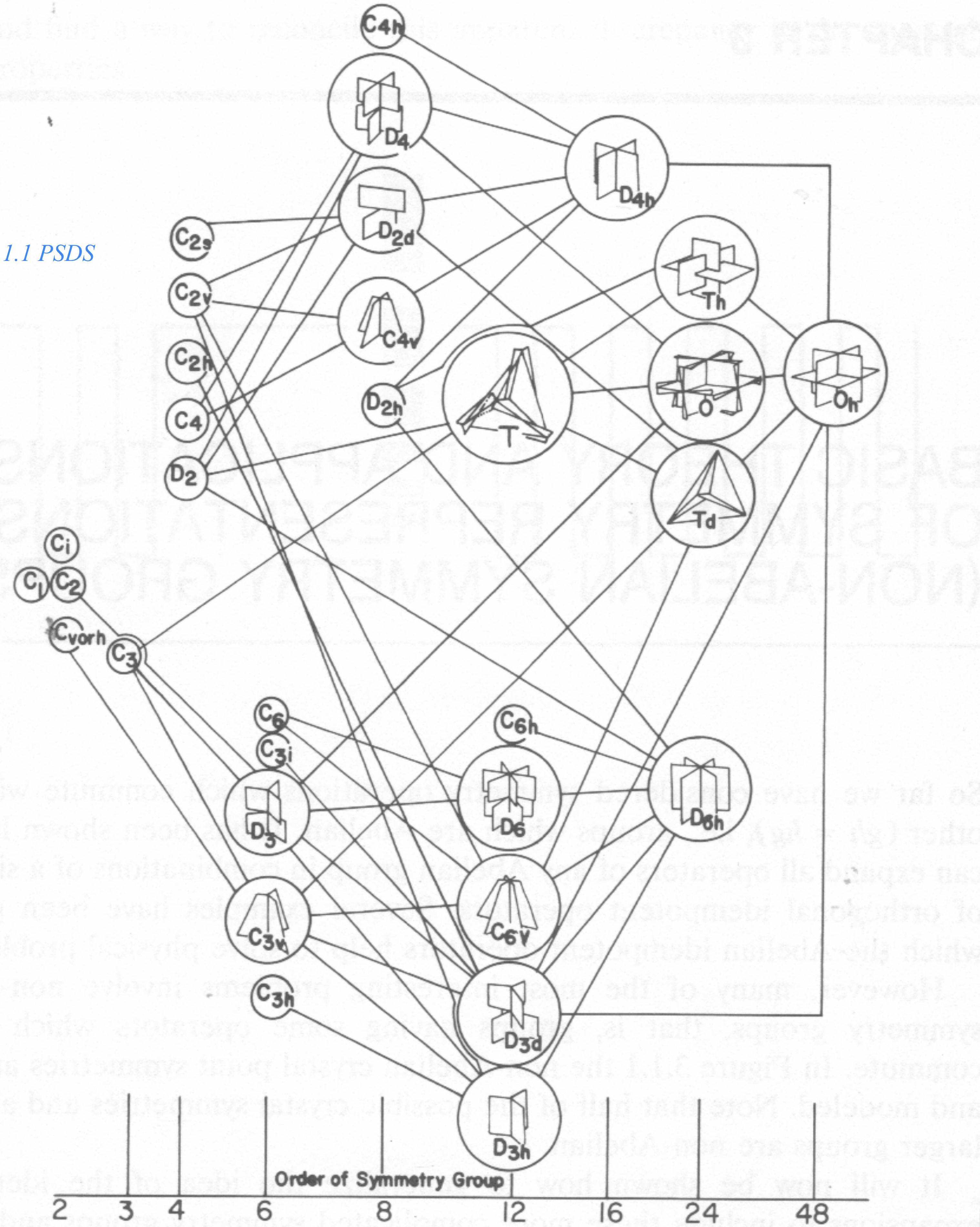
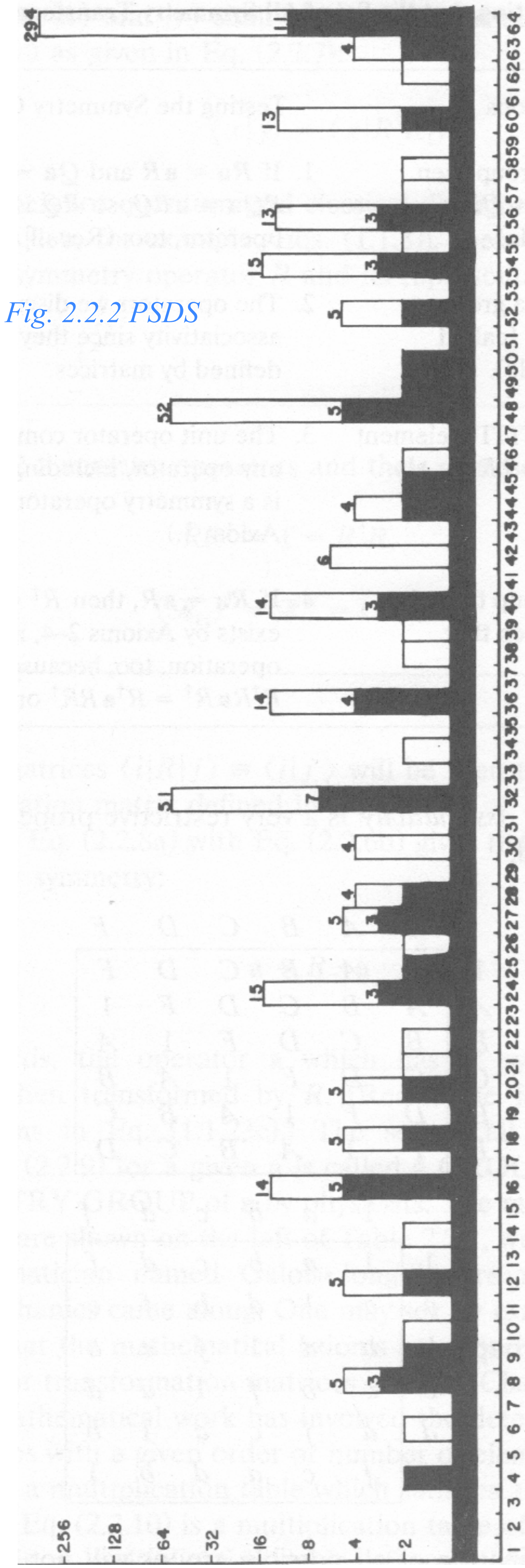


Figure 3.1.1 Crystal point symmetry groups. Models are sketched in circles for the 16 non-Abelian groups. (See also Figure 2.11.1.)

Fig. 2.2.2 PSDS



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* $C_3 \times C_2$ *(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

$=$

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

$=$

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