AMOP reference links on page 2

3.28.18 class 19.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

$S_1 \subset S_2 \subset S_3 \subset S_4 \subset S_5$ …permutation symmetry algebra and spinor-rotor correlations

Substitution Group products: S_n cycle notation
- Cyclic product algebra: bicycles tricycles quadricycles
  - Permutation unraveling
  - Product arrays shortcuts
- S_n class transformation algebra
- S_n class cycle labeling
- S_n class cycle counting

S_n tableaus spin-symmetry and characters: X_n and XY_n molecules
- Tableau dimension formulae
- Methane-like XY_4 Introducing rovibrational spectral nomogram
  - Large molecule character and correlation formulae
- Hexafluoride-like:XY_6.
  - How does level clustering affect nuclear hyperfine?

AMOP reference links *(Updated list given on 2nd page of each class presentation)*

Web Resources - front page
UAF Physics UTube channel

Quantum Theory for the Computer Age
Principles of Symmetry, Dynamics, and Spectroscopy
Classical Mechanics with a Bang!
Modern Physics and its Classical Foundations

2014 AMOP
2017 Group Theory for QM
2018 AMOP

Frame Transformation Relations And Multipole Transitions In Symmetric Polyatomic Molecules - RMP-1978
Rotational energy surfaces and high- J eigenvalue structure of polyatomic molecules - Harter - Patterson - 1984
Galloping waves and their relativistic properties - ajp-1985-Harter
Asymptotic eigensolutions of fourth and sixth rank octahedral tensor operators - Harter-Patterson-JMP-1979
Nuclear spin weights and gas phase spectral structure of 12C60 and 13C60 buckminsterfullerene -Harter-Reimer-Cpl-1992 - (Alt1, Alt2 Erratum)

Theory of hyperfine and superfine levels in symmetric polyatomic molecules.

I) Trigonal and tetrahedral molecules: Elementary spin-1/2 cases in vibronic ground states - PRA-1979-Harter-Patterson (Alt scan)
II) Elementary cases in octahedral hexafluoride molecules - Harter-PRA-1981 (Alt scan)

Rotation-vibration scalar coupling zeta coefficients and spectroscopic band shapes of buckminsterfullerene - Weeks-Harter-CPL-1991 (Alt scan)
Fullerene symmetry reduction and rotational level fine structure/ the Buckyball isotopomer 12C 13C59 - jcp-Reimer-Harter-1997 (HiRez)
Molecular Eigensolution Symmetry Analysis and Fine Structure - IJMS-harter-mitchell-2013

Rotation–vibration spectra of icosahedral molecules.

I) Icosahedral symmetry analysis and fine structure - harter-weeks-jcp-1989
II) Icosahedral symmetry, vibrational eigenfrequencies, and normal modes of buckminsterfullerene - weeks-harter-jcp-1989
III) Half-integral angular momentum - harter-reimer-jcp-1991

QTCA Unit 10 Ch 30 - 2013
Molecular Symmetry and Dynamics - Ch32-Springer Handbooks of Atomic, Molecular, and Optical Physics - Harter-2006
AMOP Ch 0 Space-Time Symmetry - 2019

RESONANCE AND REVIVALS

I) QUANTUM ROTOR AND INFINITE-WELL DYNAMICS - ISMSLi2012 (Talk) OSU knowledge Bank
II) Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 (Talks)
III) Quantum Resonant Beats and Revivals in the Morse Oscillators and Rotors - (2013-Li-Diss)

Rovibrational Spectral Fine Structure Of Icosahedral Molecules - Cpl 1986 (Alt Scan)
Gas Phase Level Structure of C60 Buckyball and Derivatives Exhibiting Broken Icosahedral Symmetry - reimer-diss-1996
Resonance and Revivals in Quantum Rotors - Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 (Talk)
Quantum Revivals of Morse Oscillators and Farey-Ford Geometry - Li-Harter-cpl-2013
Wave Node Dynamics and Revival Symmetry in Quantum Rotors - harter - jms - 2001

**In development - a web based A.M.O.P. oriented reference page, with thumbnail/previews, greater control over the information display, and eventually full on* Apache-SOLR *Index and search for* nuanced, whole-site content/metadata level *searching. This bad boy will be a sure force multiplier.*

(Int.J.Mol.Sci, 14, 714(2013) p.755-774 , QTCA Unit 7 Ch. 23-26)
(PSDS - Ch. 5, 7)

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How does level clustering affect nuclear hyperfine?

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Let players return them in a permuted order, say: $\{4,2,8,6,3,7,1,5\}$.
Suppose your job to reorder them. With two hands it's natural to switch two at a time.
You find the **1**-ball and switch it with the **4**-ball (that was in the number-***1*** position).

$$(\mathbf{14})\left|4,2,8,6,3,7,1,5\right\rangle = \left|\mathbf{1},2,8,6,3,7,\mathbf{4},5\right\rangle$$

Such a "2-flip" operation **(14)** is called a *transposition* or a *bicycle* operation.

Substitution Group products: S_n cycle notation

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Next you see the **2**-ball already in the number-***2*** position so you leave it alone.

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Such a "no-flip" operation **(2)** is called an *identity* or a *unicycle* (non)-operation.

Substitution Group products: S_n cycle notation

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Next you see **3**-ball has to switch **8**-ball out of **3**'s rightful position-***3*** and into position-***5***.

$$(\mathbf{38})(\mathbf{2})(\mathbf{14})\left|4,2,8,6,3,7,1,5\right\rangle = (\mathbf{38})\left|1,\mathbf{2},8,6,3,7,4,5\right\rangle = \left|1,2,\mathbf{3},6,\mathbf{8},7,4,5\right\rangle$$

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$$(\mathbf{38})(\mathbf{2})(\mathbf{14})|4,2,8,6,3,7,1,5\rangle = (\mathbf{38})|1,\mathbf{2},8,6,3,7,4,5\rangle = |1,2,\mathbf{3},6,\mathbf{8},7,4,5\rangle$$

Next bicycle **(46)** puts **4**-ball into *4th* spot where **6**-ball was sitting (but now dropped to *7th*).

$$(\mathbf{46})(\mathbf{38})(\mathbf{2})(\mathbf{14})|4,2,8,6,3,7,1,5\rangle = (\mathbf{46})|1,2,\mathbf{3},6,\mathbf{8},7,4,5\rangle = |1,2,3,\mathbf{4},8,7,\mathbf{6},5\rangle$$

Substitution Group products: S_n cycle notation

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Next bicycle **(46)** puts **4**-ball into *4th* spot where **6**-ball was sitting (but now dropped in *7th*).

$$(\mathbf{46})(\mathbf{38})(\mathbf{2})(\mathbf{14})\left|4,2,8,6,3,7,1,5\right\rangle = (\mathbf{46})\left|1,2,\mathbf{3},6,\mathbf{8},7,4,5\right\rangle = \left|1,2,3,\mathbf{4},8,7,\mathbf{6},5\right\rangle$$

Then bicycle **(58)** puts **5**-ball into *5th* spot where **8**-ball was sitting (but now dropped to *8th*).

$$(\mathbf{58})(\mathbf{46})(\mathbf{38})(\mathbf{2})(\mathbf{14})\left|4,2,8,6,3,7,1,5\right\rangle = (\mathbf{58})\left|1,2,3,\mathbf{4},8,7,\mathbf{6},5\right\rangle = \left|1,2,3,4,\mathbf{5},7,6,\mathbf{8}\right\rangle$$

Substitution Group products: S_n cycle notation

Suppose pool balls are stored in numerical order: $\{1,2,3,4,5,6,7,8\}$.
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$$(\mathbf{67})(58)(46)(38)(2)(14)|4,2,8,6,3,7,1,5\rangle = |1,2,3,4,5,\mathbf{6},\mathbf{7},8\rangle$$

(67) finishes the job.

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Substitution Group products: S_n cycle notation and algebra

Suppose pool balls are stored in numerical order: $\{1,2,3,4,5,6,7,8\}$.
Let players return them in a permuted order, say: $\{4,2,8,6,3,7,1,5\}$.
Suppose your job to reorder them. With two hands it's natural to switch two at a time.

This permutation has 5 *bicycle* **(ab)** operations so it is an ODD-permutation.

$$\overset{1}{(\mathbf{67})}\overset{2}{(58)}\overset{3}{(46)}\overset{4}{(38)}(2)\overset{5}{(14)}\left|4,2,8,6,3,7,1,5\right\rangle = \left|1,2,3,4,5,\mathbf{6},\mathbf{7},8\right\rangle$$

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Substitution Group products: S_n cycle notation and algebra

Suppose pool balls are stored in numerical order: $\{1,2,3,4,5,6,7,8\}$.
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$$\overset{1}{\downarrow}\ \overset{2}{\downarrow}\ \overset{3}{\downarrow}\ \overset{4}{\downarrow}\ \overset{5}{\downarrow}$$

$$(\mathbf{67})(58)(46)(38)(2)(14)|4,2,8,6,3,7,1,5\rangle = |1,2,3,4,5,\mathbf{6},\mathbf{7},8\rangle$$

(67) finishes the job.

Flip any single pair and it becomes EVEN.

This permutation has 6 *bicycle* **(ab)** operations so it is an EVEN-permutation.

$$\overset{1}{\downarrow}\ \overset{2}{\downarrow}\ \overset{3}{\downarrow}\ \overset{4}{\downarrow}\ \overset{5}{\downarrow}\ \overset{6}{\downarrow}$$

$$(67)(58)(46)(38)(2)(14)(67)|4,2,8,7,3,6,1,5\rangle = |1,2,3,4,5,6,7,8\rangle$$

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1 2 3 4 5

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$$(67)(58)(46)(38)(2)(14)(67)\left|4,2,8,7,3,6,1,5\right\rangle=\left|1,2,3,4,5,6,7,8\right\rangle$$

or: $$(67)(58)(46)(38)(2)(14)(84)\left|8,2,4,7,3,6,1,5\right\rangle=\left|1,2,3,4,5,6,7,8\right\rangle$$

Substitution Group products: S_n cycle notation and algebra

Suppose pool balls are stored in numerical order: $\{1,2,3,4,5,6,7,8\}$.
Let players return them in a permuted order, say: $\{4,2,8,6,3,7,1,5\}$.
Suppose your job to reorder them. With two hands it's natural to switch two at a time.

The *inverse* of our permutation operation… $(67)(58)(46)(38)(2)(14)|4,2,8,6,3,7,1,5\rangle = |1,2,3,4,5,6,7,8\rangle$

…is simply reverse-ordered products: $|4,2,8,6,3,7,1,5\rangle = (14)(2)(38)(46)(58)(67)|1,2,3,4,5,6,7,8\rangle$

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Note all *bicycle* **(ab)** operations have flip-order symmetry **(ab)≡(ba)=(ab)**$^{-1}$

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Note all *bicycle* **(ab)** operations have flip-order symmetry $(\mathbf{ab})\equiv(\mathbf{ba})=(\mathbf{ab})^{-1}$

…minimal equation $(\mathbf{ab})^2=\mathbf{1}\equiv(\mathbf{a})(\mathbf{b})$ i.e., $(\mathbf{ab})^2-\mathbf{1}=\mathbf{0}$

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…minimal equation $\mathbf{(ab)}^2=\mathbf{1}\equiv\mathbf{(a)(b)}$ i.e., $\mathbf{(ab)}^2-\mathbf{1}=\mathbf{0}=(\mathbf{(ab)}-\mathbf{1})(\mathbf{(ab)}+\mathbf{1})$

…eigenvalues of ± 1.

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3.28.18 class 19.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

$S_1 \subset S_2 \subset S_3 \subset S_4 \subset S_5$ …permutation symmetry algebra and spinor-rotor correlations

Substitution Group products: S_n cycle notation
- Cyclic product algebra: bicycles → tricycles quadricycles
  - Permutation unraveling
  - Product arrays shortcuts
- S_n class transformation algebra
- S_n class cycle labeling
- S_n class cycle counting

S_n tableaus spin-symmetry and characters: X_n and XY_n molecules
- Tableau dimension formulae
- Methane-like XY_4 Introducing rovibrational spectral nomogram
  - Large molecule character and correlation formulae
- Hexafluoride-like: XY_6.
  - How does level clustering affect nuclear hyperfine?

Substitution Group products: S_n cycle notation and cyclic algebra

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Let players return them in a permuted order, say: $\{4,2,8,6,3,7,1,5\}$.
Suppose your job: reorder them. With two hands it's natural (but *slower*) to switch two at a time.
Much faster with *multi-cycles (tricycles, quadricycles, etc.)*

Rewriting permutation operation… $(67)(58)(46)(38)(2)(14)\left|4,2,8,6,3,7,1,5\right\rangle = \left|1,2,3,4,5,6,7,8\right\rangle$

Permutation operations **(ab)** and **(cd)** commute if and *only* if *neither* **a** *nor* **b** *equals* **c** *or* **d**.

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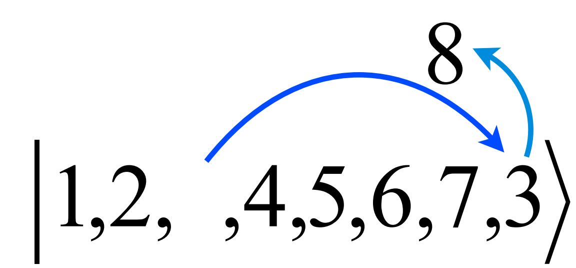

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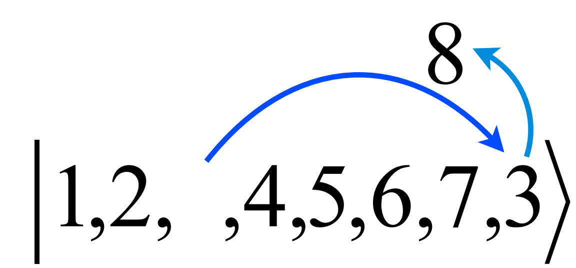

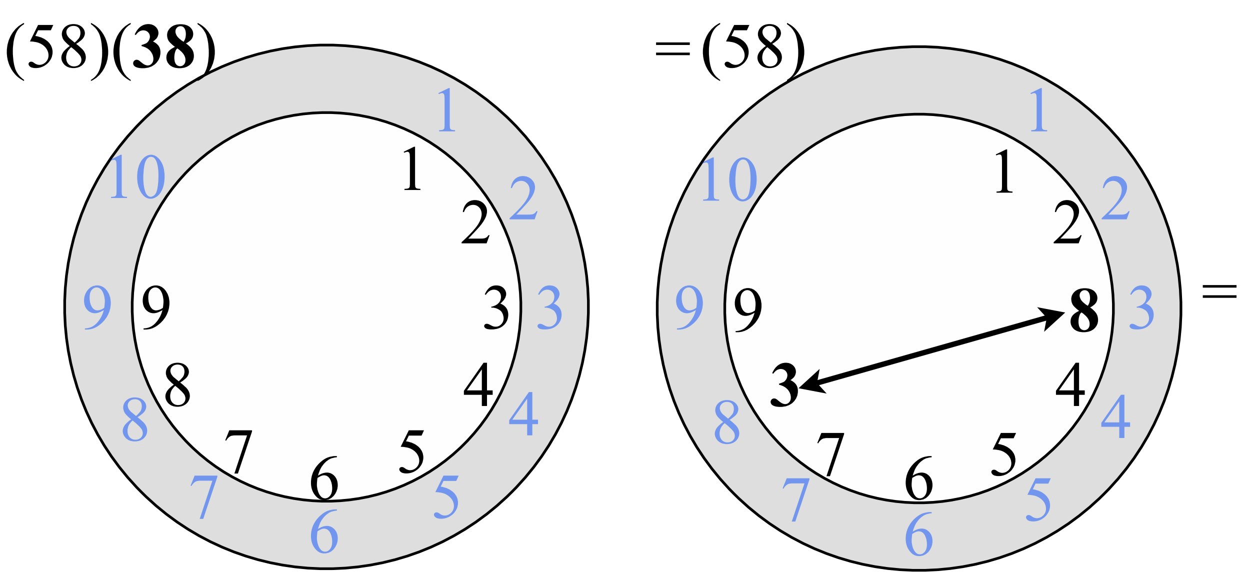

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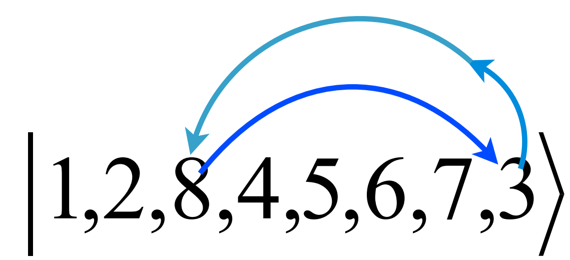

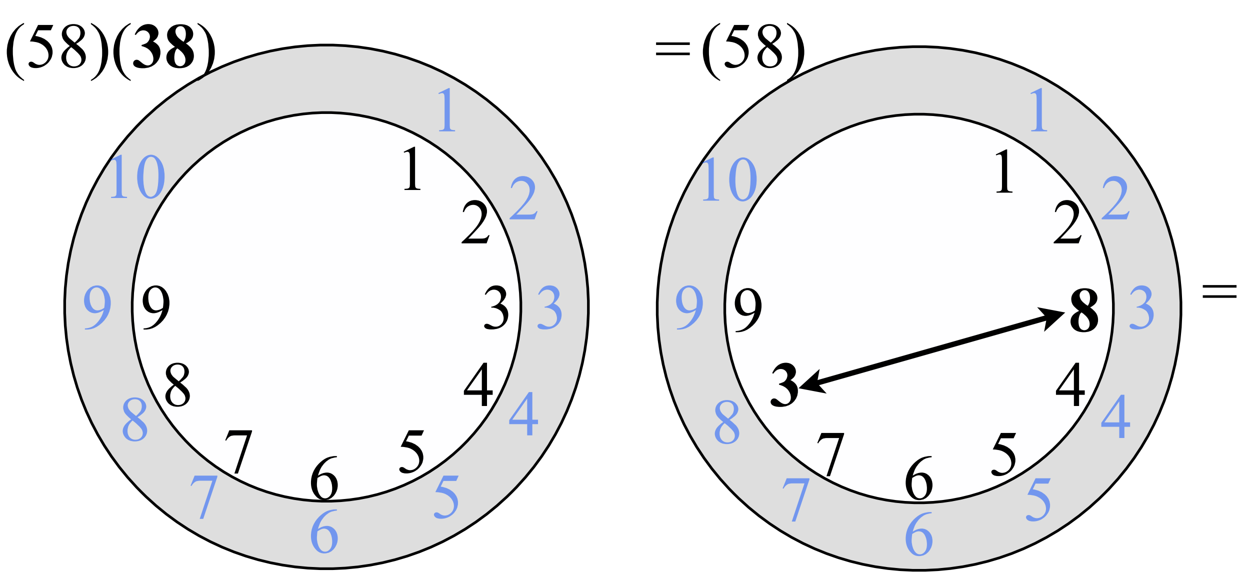

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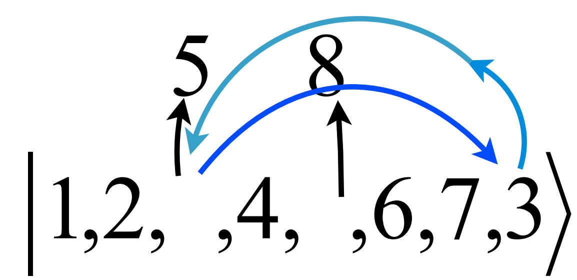

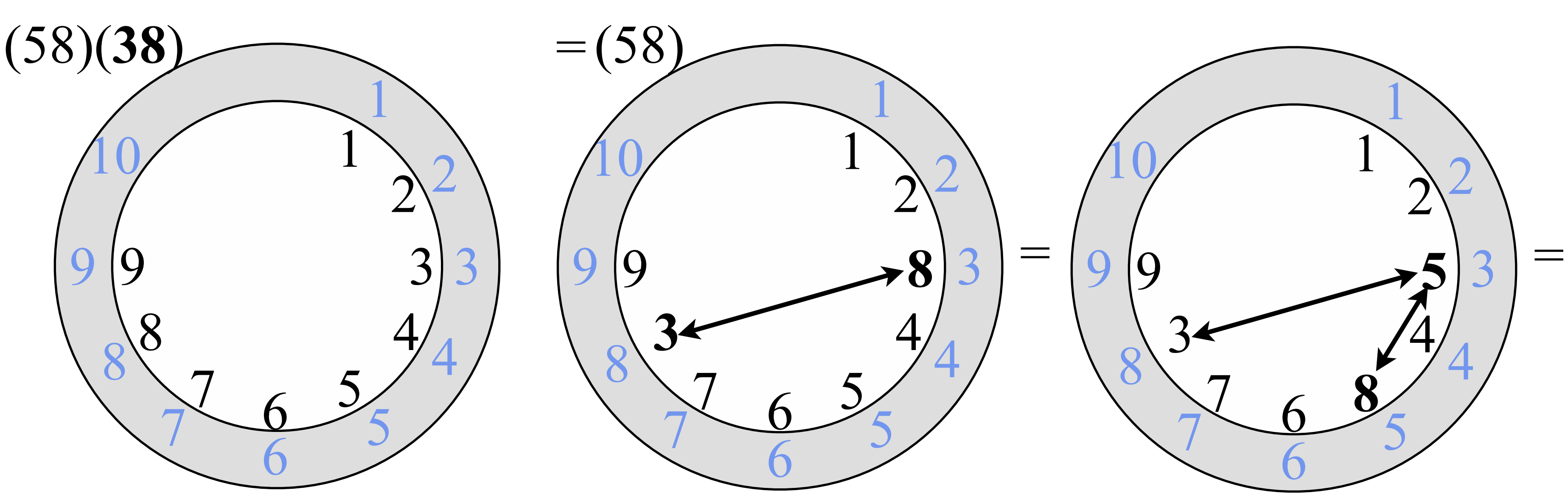

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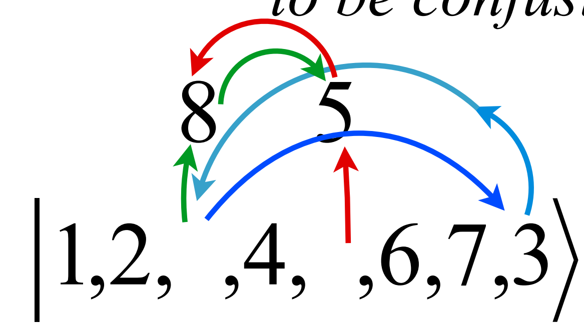

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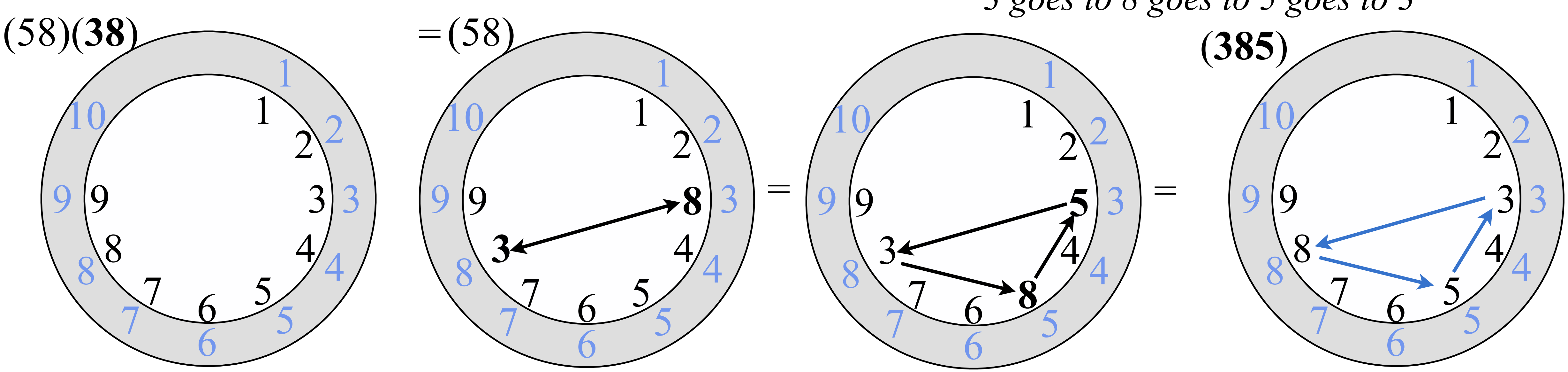

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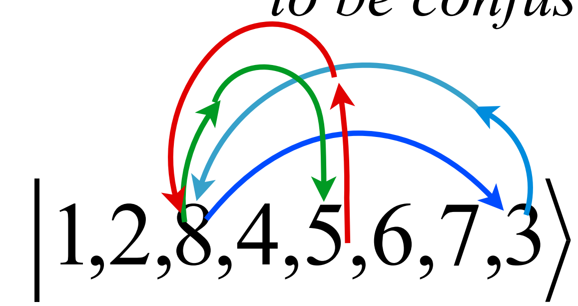

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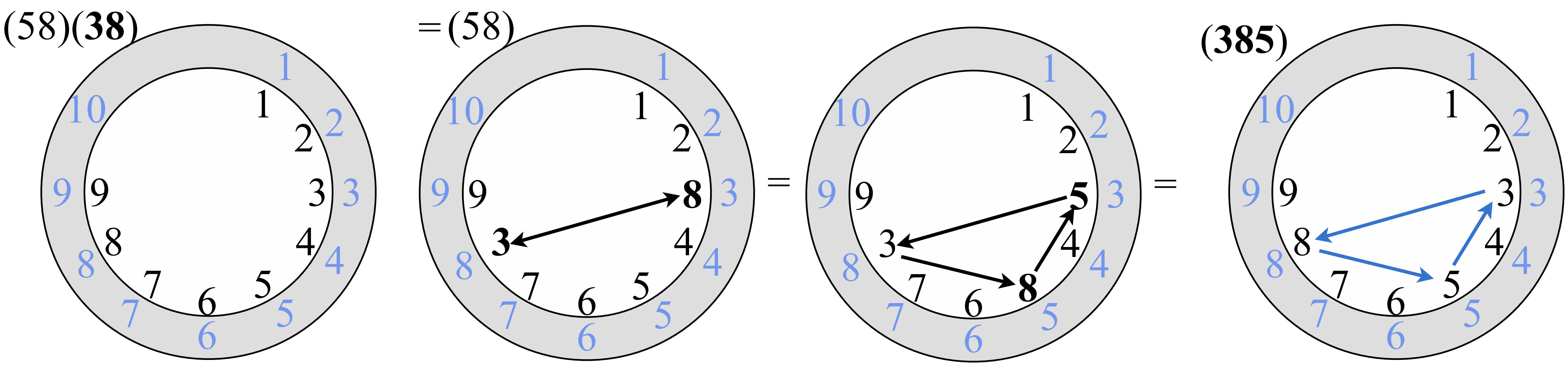
…that may be written *three different ways*.



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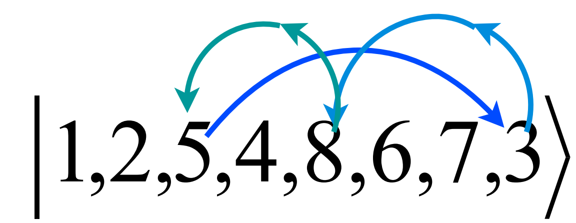

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Here is *inverse* of (58)(38):…(38)(58)=(358)=(583)=(835) …also written *three different ways*.

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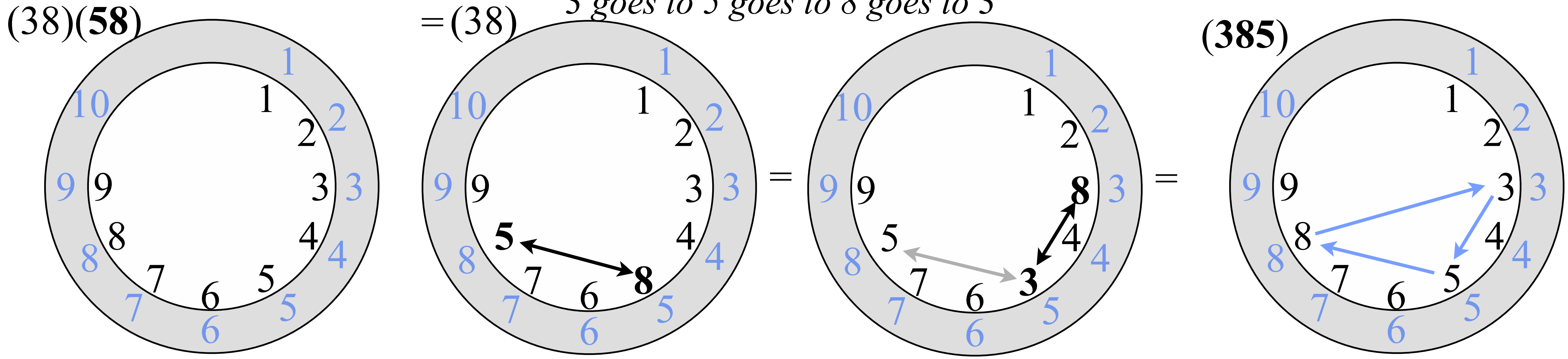

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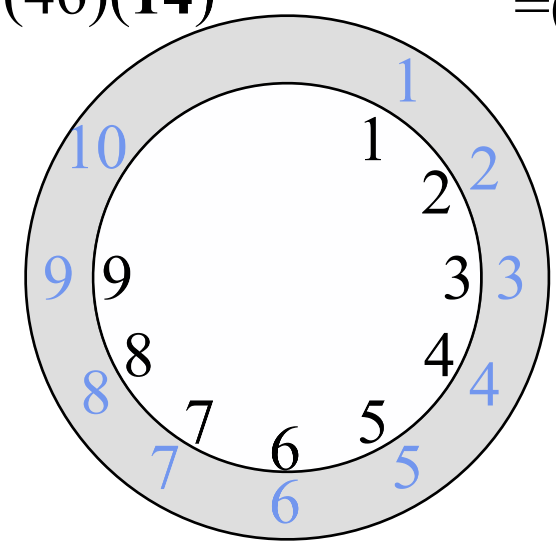

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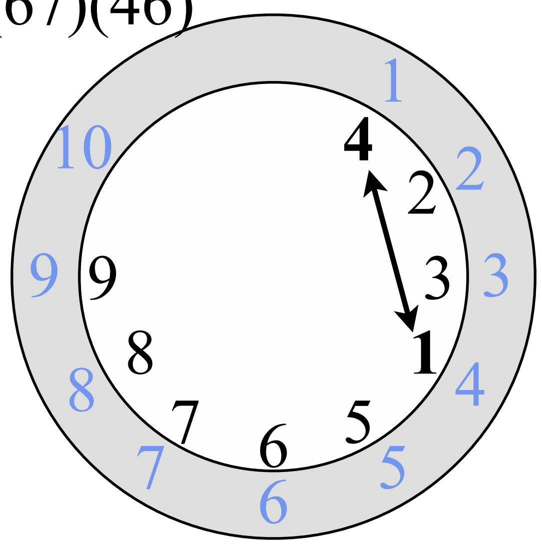

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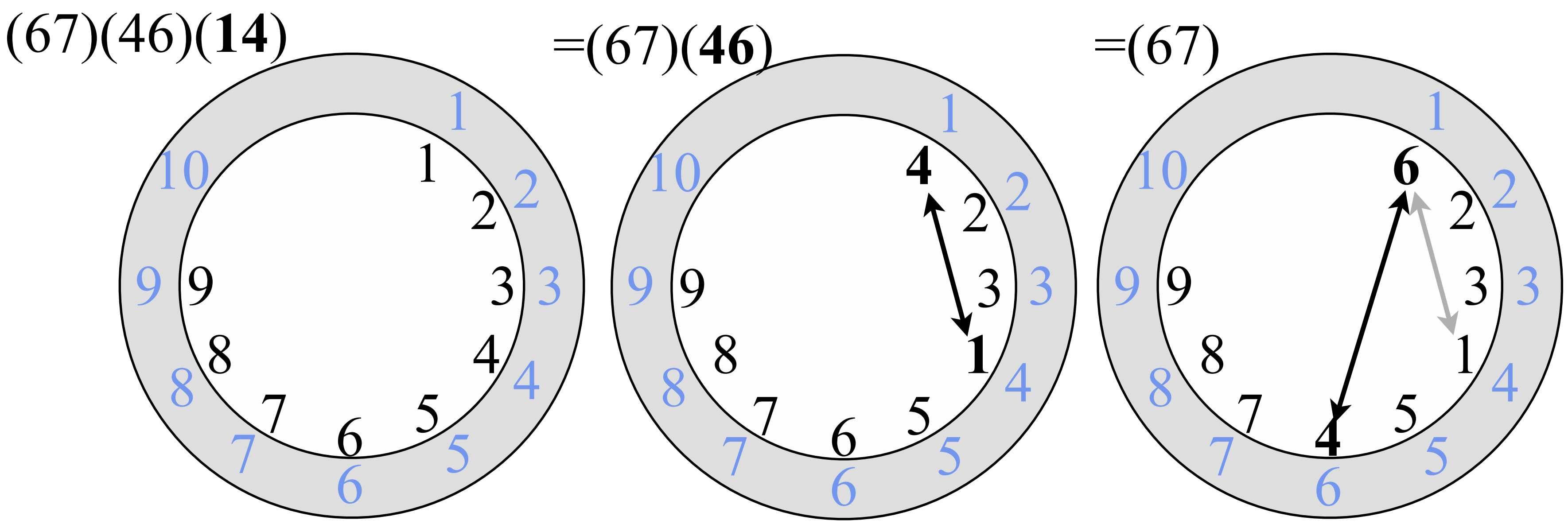

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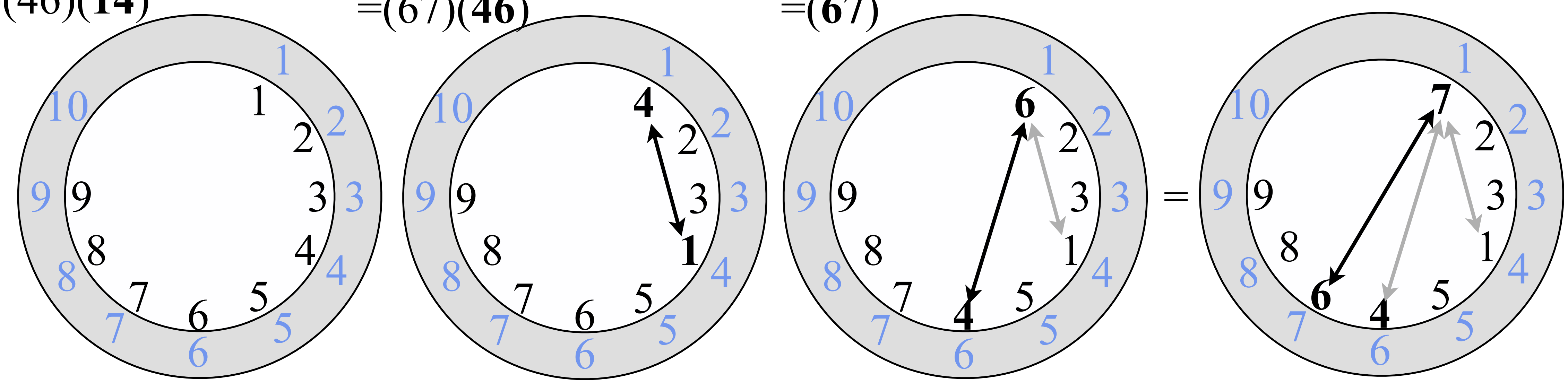

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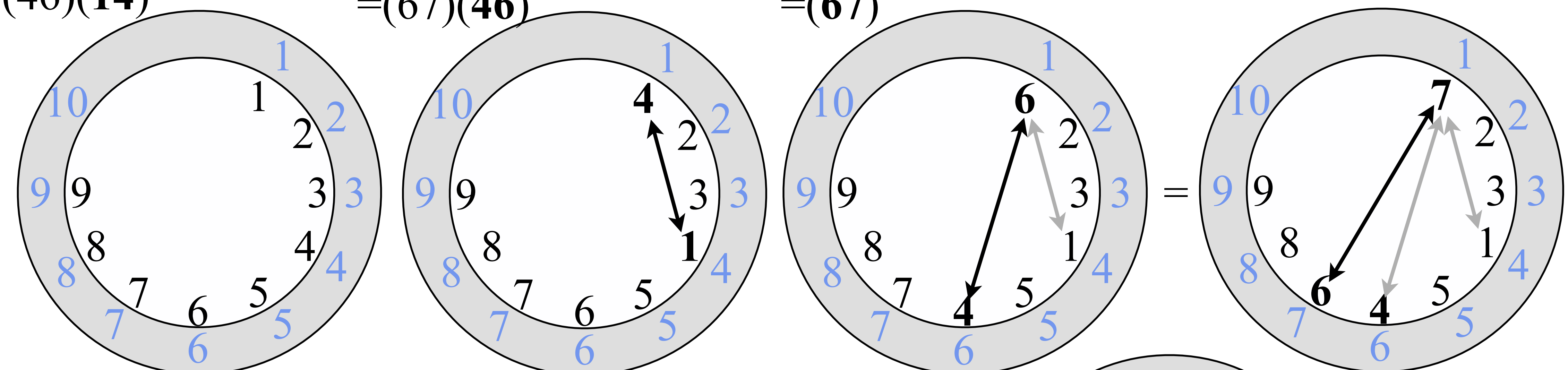

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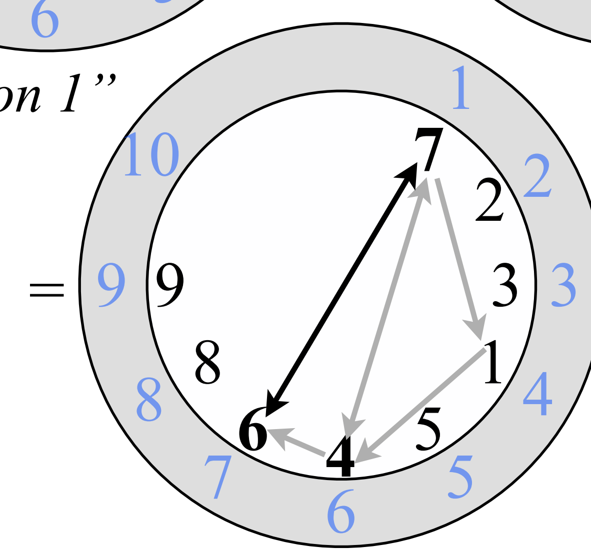

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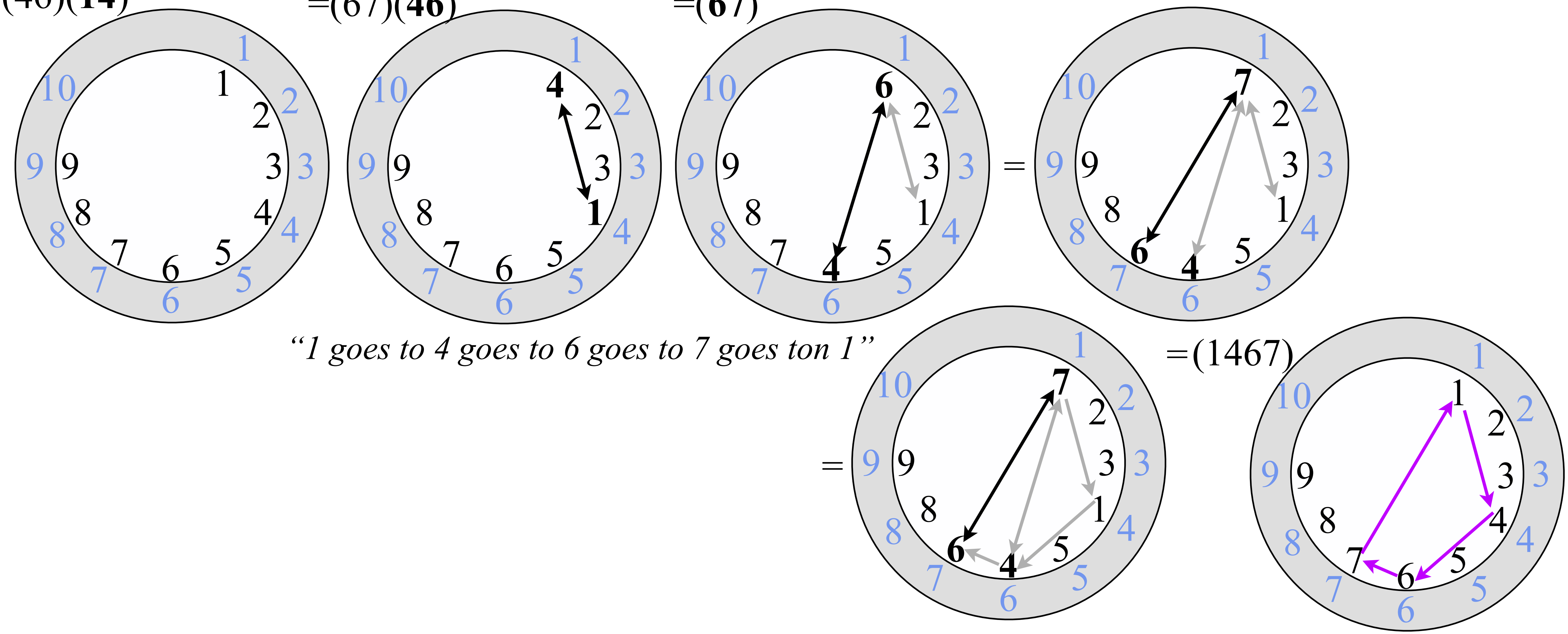

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Suppose pool balls are stored in numerical order: {1,2,3,4,5,6,7,8}.
Let players return them in a permuted order, say: {4,2,8,6,3,7,1,5}.
Suppose your job: reorder them. With two hands it's natural (but *slower*) to switch two at a time.
Much faster with *multi-cycles (tricycles, quadricycles, etc.)*

Rewriting permutation operation… $(67)(58)(46)(38)(2)(14)\left|4,2,8,6,3,7,1,5\right\rangle = \left|1,2,3,4,5,6,7,8\right\rangle$

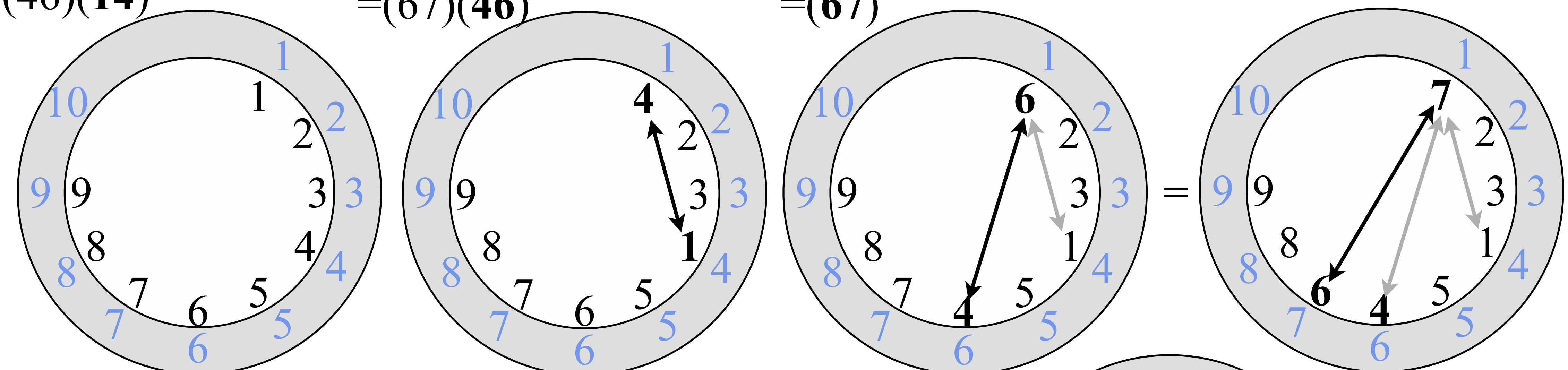
Permutation operations **(ab)** and **(cd)** commute if and *only* if *neither* **a** *nor* **b** *equals* **c** *or* **d**.

So: $(67)(58)(46)(38)(2)(14)$ since: $(58)(46)=(46)(58)$ *etc*

$=(67)(46)(14)\cdot(58)(38)\cdot(2)$. and: $(58)(14)=(14)(58)$ *etc.*

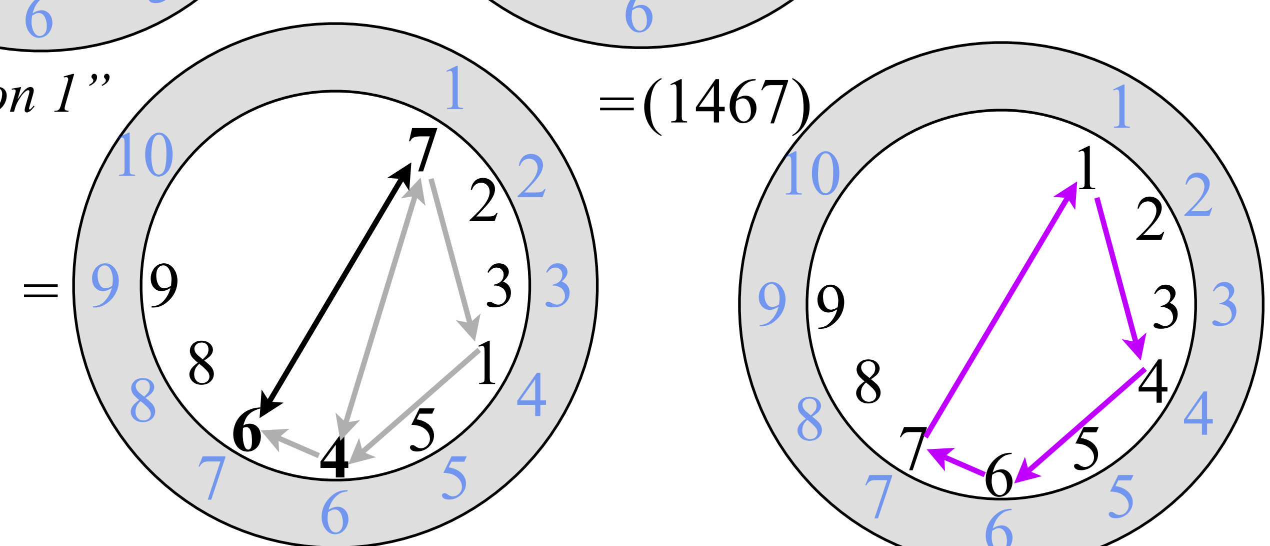
Consider three bicycles (67)(46)(14) sharing **6**-ball and **4**-ball:

(67)(46)(**14**) =(67)(**46**) =(**67**)



"*1 goes to 4 goes to 6 goes to 7 goes ton 1*"

=(1467)



So three bicycles (67)(46)(14)
give a *quadricycle* (1467)
that may be written four ways…

(67)(46)(14) = (1467) = (7146) = (6714) = (4671)

Substitution Group products: S_n cycle notation and cyclic algebra

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So: $(67)(58)(46)(38)(2)(14)$ since: $(58)(46)=(46)(58)$ *etc*

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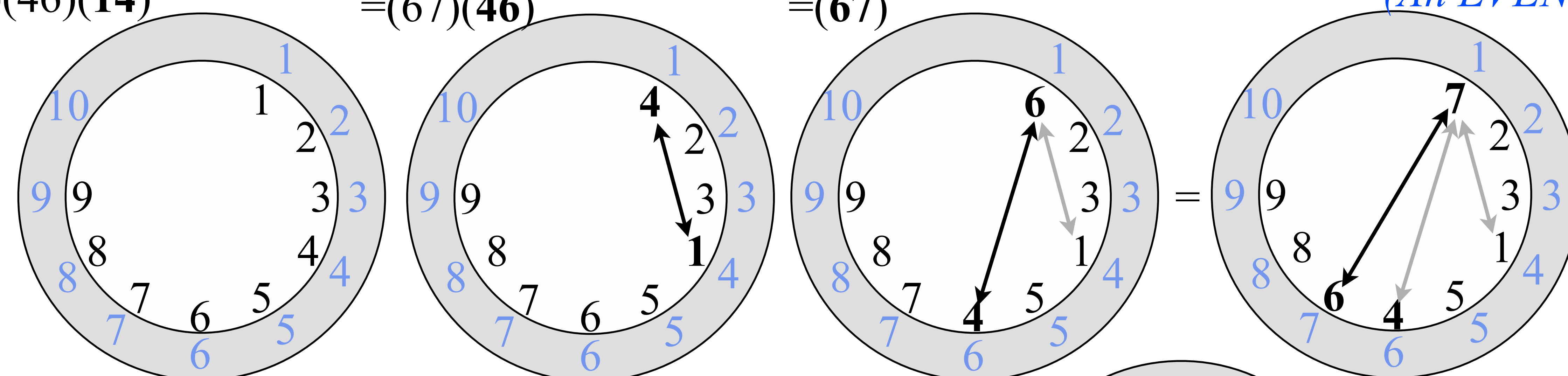
…with *tricycle* (58)(38)
=(385)=(538)=(853)
(An EVEN permutation)

Consider three bicycles (67)(46)(14) sharing **6**-ball and **4**-ball:

(67)(46)(**14**) =(67)(**46**) =(**67**)



(An ODD permutation)

So three bicycles (67)(46)(14)
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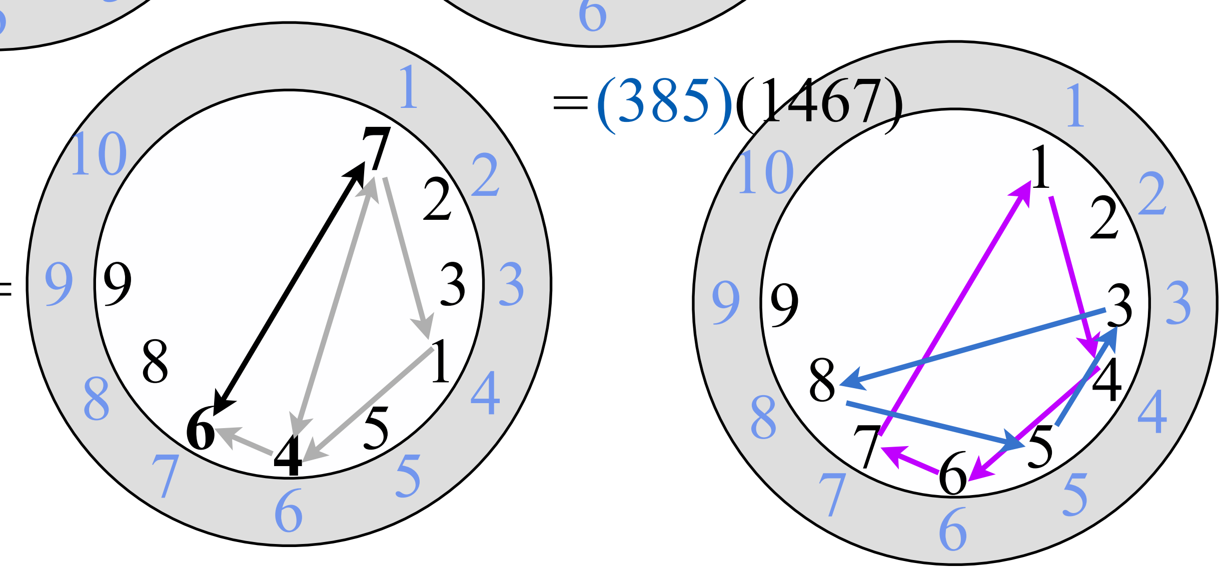
that may be written four ways…

$(67)(46)(14) = (1467) = (7146) = (6714) = (4671)$

=



=(385)(1467)

AMOP reference links on page 2

3.28.18 class 19.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

$S_1 \subset S_2 \subset S_3 \subset S_4 \subset S_5$ …permutation symmetry algebra and spinor-rotor correlations

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- Cyclic product algebra: bicycles tricycles quadricycles
  - Permutation unraveling
  - Product arrays shortcuts
- S_n class transformation algebra
- S_n class cycle labeling
- S_n class cycle counting

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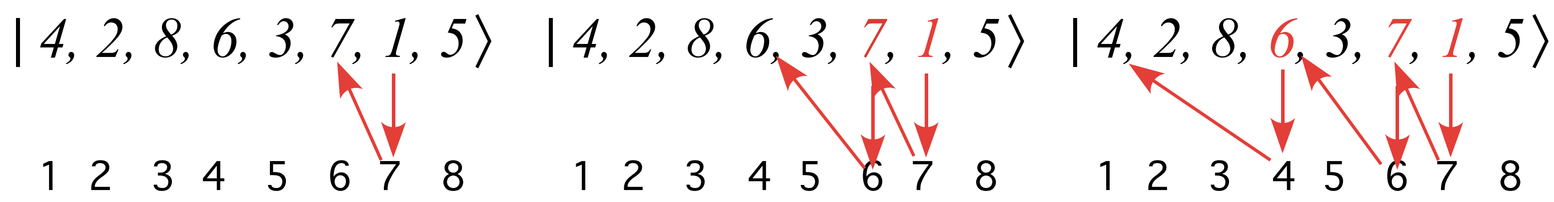
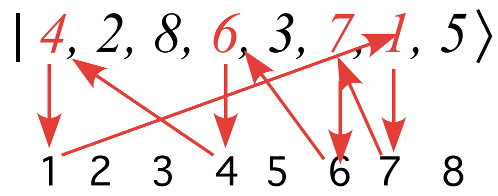
Unraveling a permutation (Starting with "1")

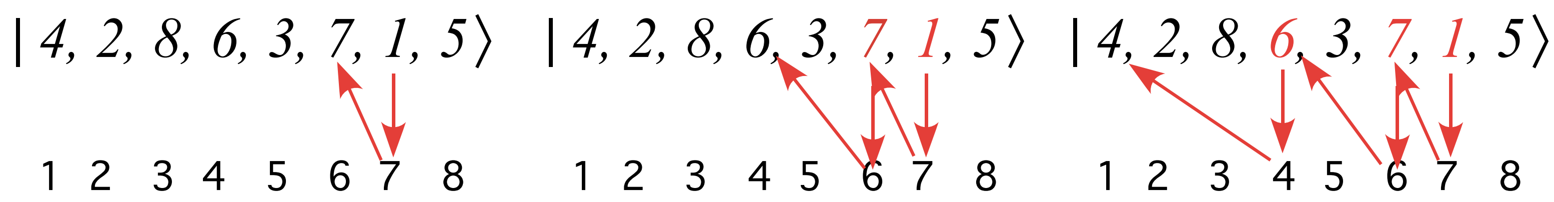


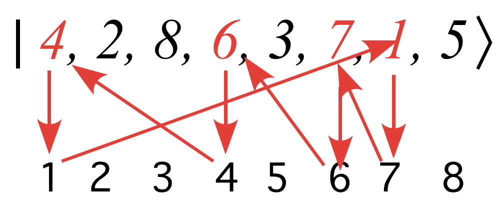


Closes on a permutation quadracycle

(1764)=(4176)=etc.

Unraveling a permutation (Starting with "1")





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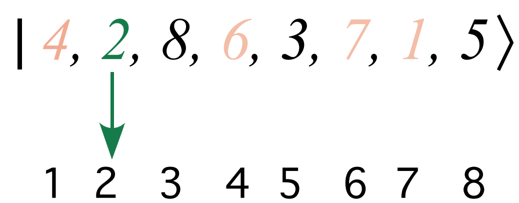
(1764)=(4176)=etc.

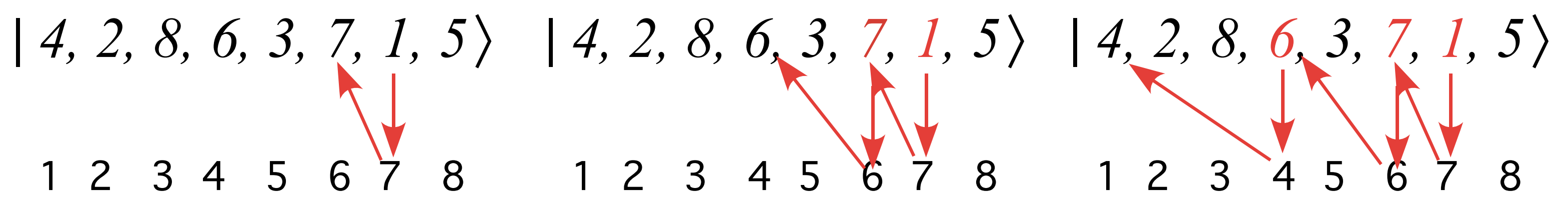
(Next higher number that has not been used is a "2")

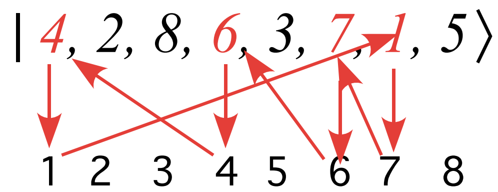


Closes on a permutation unicycle

(2)

Unraveling a permutation (Starting with "1")





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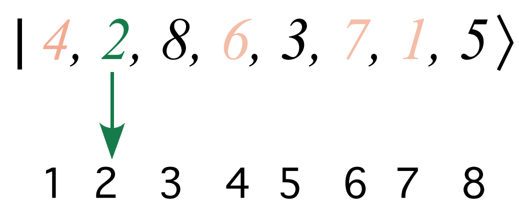
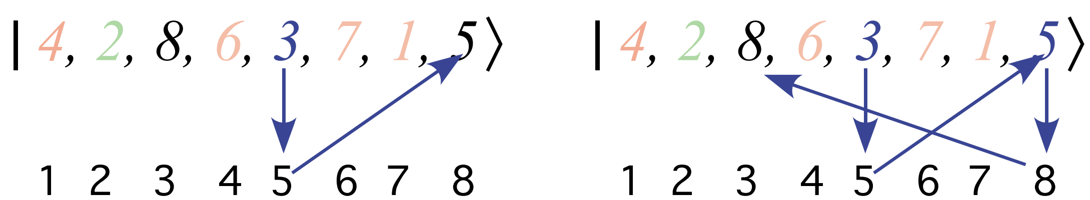
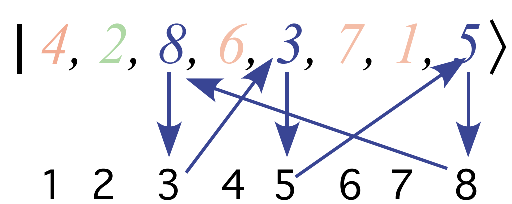


Closes on a permutation unicycle

(2)

(Next higher number that has not been used is a "3")





Closes on a permutation tricycle

(358)=(835)=etc.

"OK , but its the ***inverse*** *of the pool ball operation"*

Final result: *(1764)(2)(358)=(358)(1764)*

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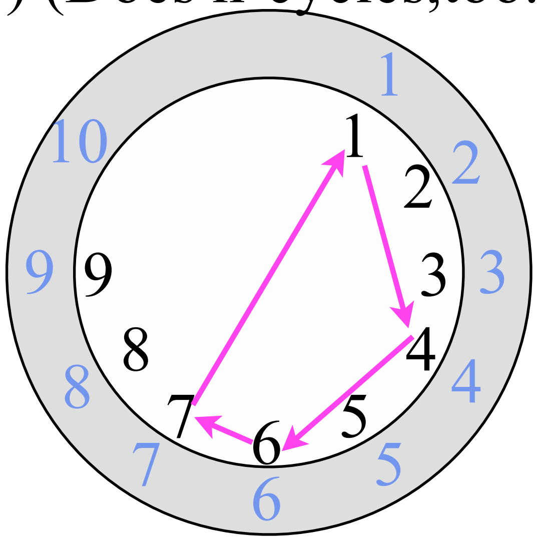
A (nearly) foolproof table method to find cycle products like:(67)(58)(46)(38)(14) (Does n-cycles,too.)

(1) Apply *n*-cycle (right-most 1st) to each row starting on <1>=1,2,3,4,5,…,n_{max}

1	2	3	4	5	6	7	8	$\langle 1 \rangle$
								(14)
								(38)
								(46)
								(58)
								(67)
1	2	3	4	5	6	7	8	$\langle 1 \rangle$



(67)(58)(46)(38)(14)=? (1467)

Substitution Group products: S_n cycle notation and cyclic algebra

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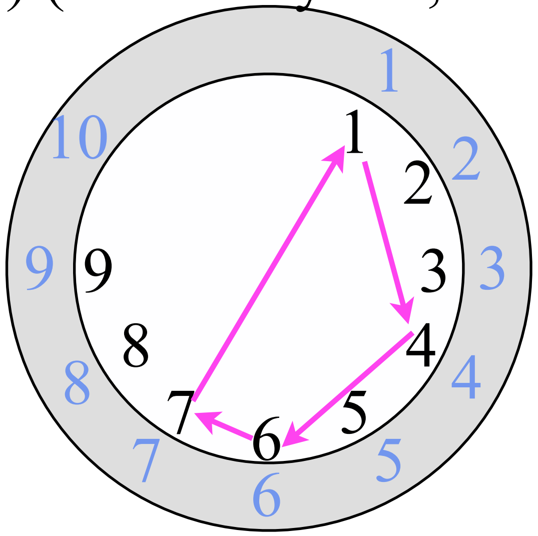

1	2	3	4	5	6	7	8	$\langle 1 \rangle$
4	2	3	**1**	5	6	7	8	(14)
								(38)
								(46)
								(58)
								(67)
1	2	3	4	5	6	7	8	$\langle 1 \rangle$

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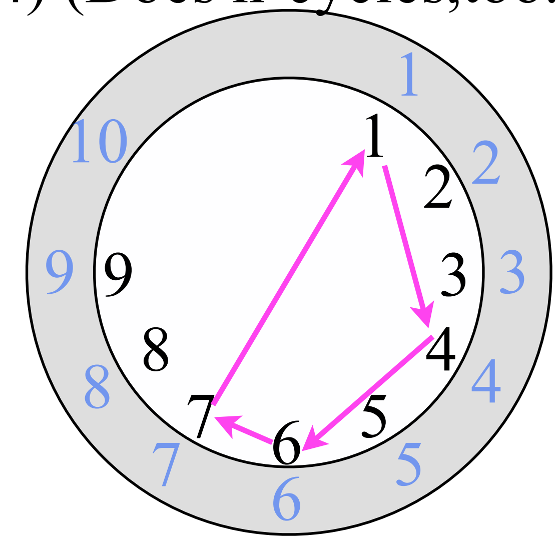

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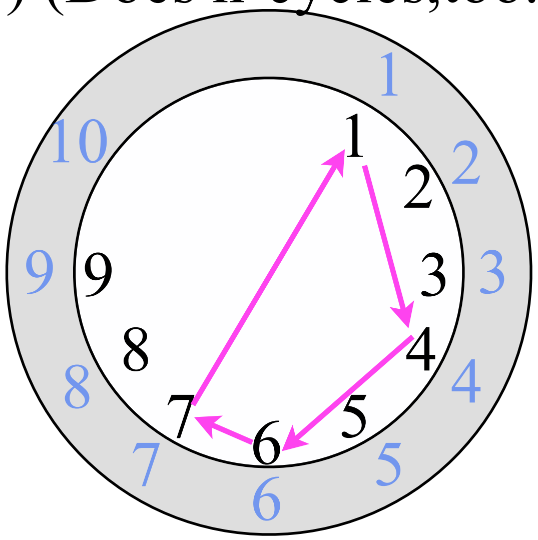
1	2	3	4	5	6	7	8	⟨1⟩



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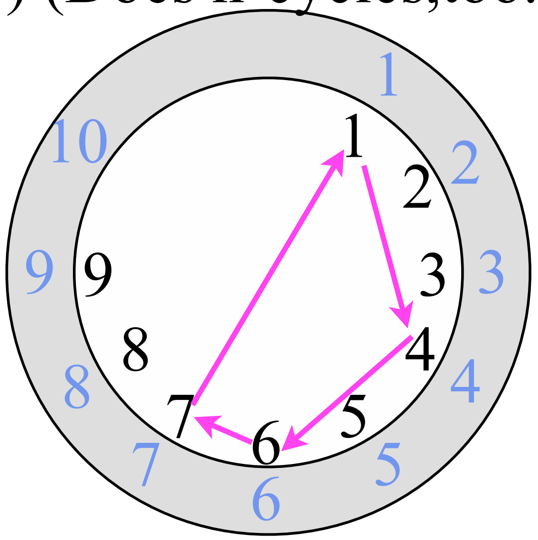

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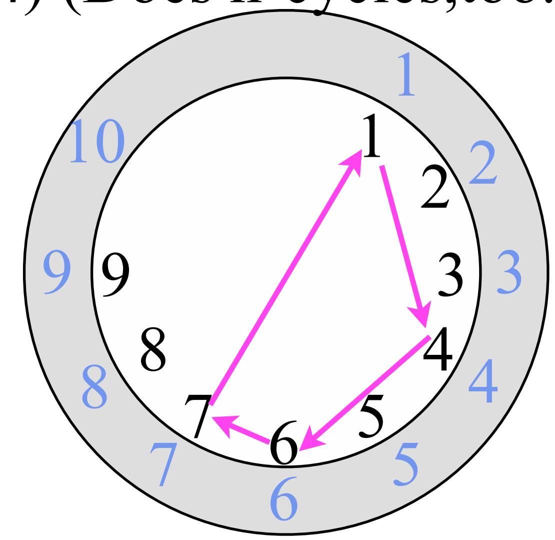

1	2	3	4	5	6	7	8	$\langle 1 \rangle$
4	2	3	**1**	5	6	7	8	(14)
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6	2	**5**	1	**8**	4	7	3	(58)
7	2	5	1	8	4	**6**	3	(67)
1	2	3	4	5	6	7	8	$\langle 1 \rangle$

(67)(58)(46)(38)(14)=? (14

(14

(2) Sort into ***distinct*** ordered (abc..e)-cycles

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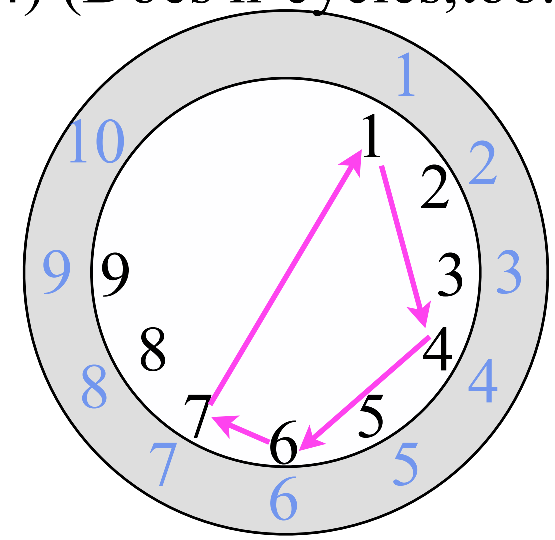
1	2	3	4	5	6	7	8	⟨1⟩



(67)(58)(46)(38)(14)=? (146

(146

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Substitution Group products: S_n cycle notation and cyclic algebra

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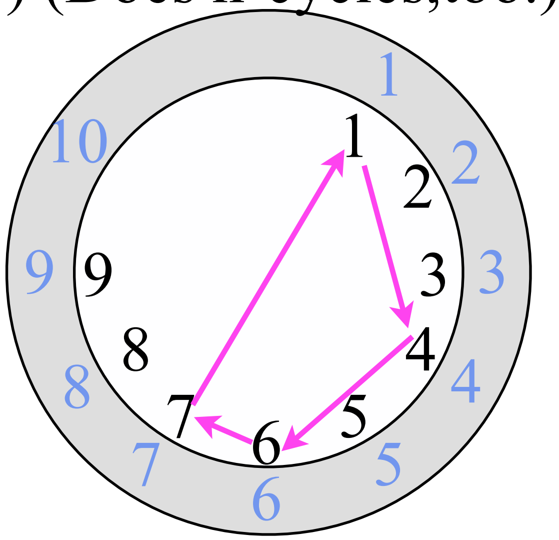

(67)(58)(46)(38)(14)=? (1467

(1467

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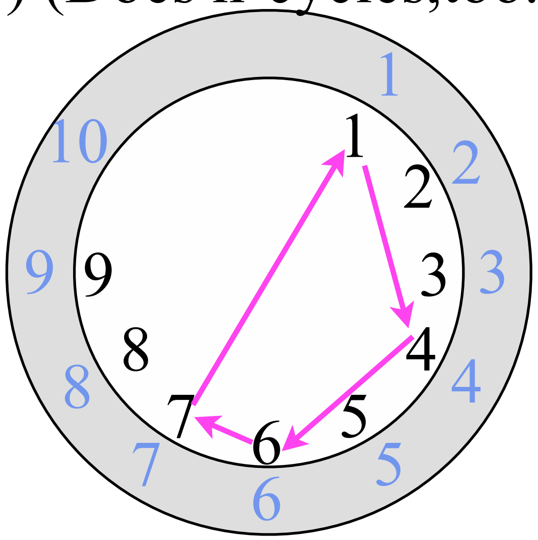
1	2	3	4	5	6	7	8	⟨1⟩

(1467)



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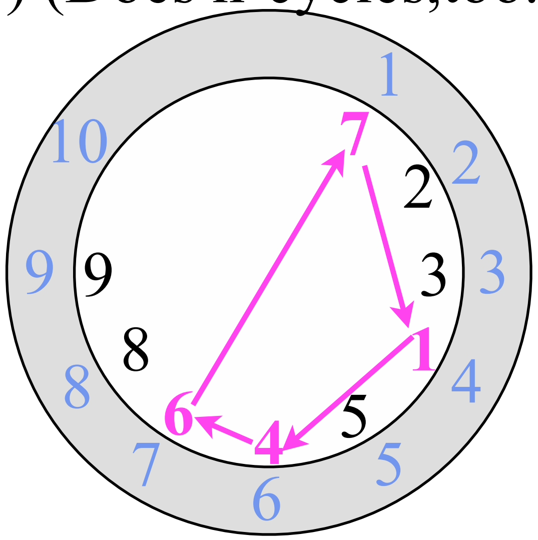

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$\frac{N_{new}}{N_{old}}$ tells which new number $\underline{N_{new}}$ now sits in the space that started with old number N_{old}

(1467)

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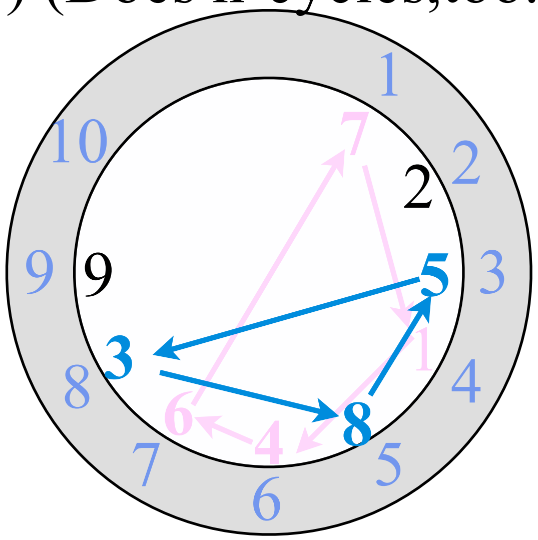

1	2	3	4	5	6	7	8	⟨1⟩
4	2	3	**1**	5	6	7	8	(14)
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7	2	5	1	8	4	**6**	3	(67)
1	2	3	4	5	6	7	8	⟨1⟩

(1467) (385)

(67)(58)(46)(38)(14)= (385)(1467)

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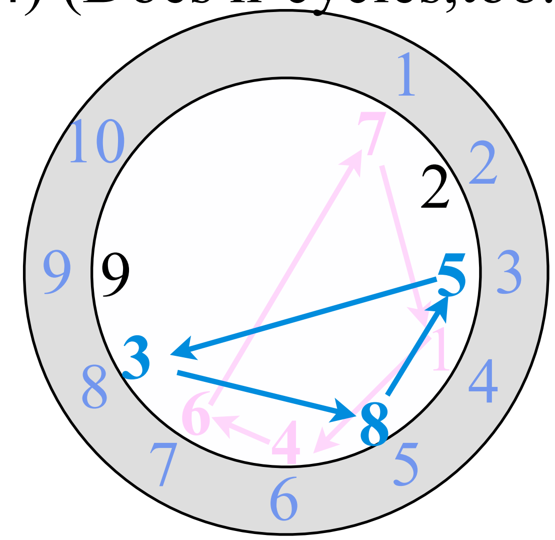

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(1467) (385)

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$\frac{N_{new}}{N_{old}}$ tells which new number $\underline{N_{new}}$ now sits in the space that started with old number N_{old}

(2) Sort into *distinct* ordered (abc..e)-cycles

A shortcut method to reduce cycle products like : (67)(46)(14) (58)(38)

Last op (67) moves 6 to 7.	6→7	This implies (67
But whence came 7?	7→6→4→1	This implies (671
But whence came 1?	1→4	This implies (6714
But whence came 4?	4→6	This implies (6714) that is (1467)
Last op (58) moves 5 to 8.	5→8→3	This implies (53
3?	3→8	This implies (538
8?	8→5	This implies (538) that is (385)

Shortcut method reduces cycle products like : (12)(13)(14)(15)

(12 implied by last op involving 2: 1→2

(123 implied by last op involving 3: 2→1→3

(1234 implied by last op involving 4: 3→1→4

(12345 implied by last op involving 5: 4→1→5

(12345) implied by last op involving 5: 5→1

Shortcut method reduces cycle products like : (12)(13)(14)(15) Start with any number (say 3)

(34 implied by last op involving 3: 3→1→4

(345 implied by last op involving 4: 4→1→5

(3451 implied by last op involving 5: 5→1

(34512 implied by last op involving 1: 1→2

(34512) implied by last op involving 2: 2→1→3

Shortcut: (1234)(456)

(12 1→2

(123 2→3

(1235 3→4→5

(12356 5→6

(123564 6→4

(123564) 4→1

Test:

1	2	3	4	5	6	$\langle 1 \rangle$
1	2	3	**6**	**4**	**5**	(456)
4	**1**	**2**	6	**3**	5	(1234)
1	2	3	4	5	6	$\langle 1 \rangle$

=(123564)

Shortcut: (456)(1234)

(12 1→2

(123 2→3

(1234 3→4

(12345 4→5

(123456 5→6

(123456) 6→4→1

Test:

1	2	3	4	5	6	$\langle 1 \rangle$
4	**1**	**2**	**3**	5	6	(1234)
6	1	2	3	**4**	**5**	(456)
1	2	3	4	5	6	$\langle 1 \rangle$

=(123456)

AMOP reference links on page 2

3.28.18 class 19.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

$S_1 \subset S_2 \subset S_3 \subset S_4 \subset S_5$ …permutation symmetry algebra and spinor-rotor correlations

Substitution Group products: S_n cycle notation
- Cyclic product algebra: bicycles tricycles quadricycles
  - Permutation unraveling
  - Product arrays shortcuts
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- S_n class cycle counting

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- Tableau dimension formulae
- Methane-like XY_4 Introducing rovibrational spectral nomogram
  - Large molecule character and correlation formulae
- Hexafluoride-like: XY_6.
  - How does level clustering affect nuclear hyperfine?

Substitution Group products: S_n class transformation algebra

Similarity transform $\mathbf{y} = \mathbf{t} \cdot \mathbf{x} \cdot \mathbf{t}^{-1}$ = (15)(2738496) · (5678)(19)(234) · (51)(2694837)

= (1923)(45)(678)

(15)(2738496) · (5678)(19)(234) · (51)(2694837)

(19	1→5→6→9
(192	9→6→7→2
(1923	2→7→8→3
(1923)	3→8→5→1
(45	4→9→1→5
(45)	5→1→9→4
(67	6→2→3→7
(678	7→3→4→8
(678)	8→4→2→6

1	2	3	4	5	6	7	8	9	$\langle 1 \rangle$
5	7	8	9	1	2	3	4	6	(15)(2694837)
8	6	7	1	9	4	2	3	5	(5678)(19)(234)
3	9	2	5	4	8	6	7	1	(51)(2738496)
1	2	3	4	5	6	7	8	9	$\langle 1 \rangle$

(5678)(19)(234) = **x**

= (1923)(45)(678) = $\mathbf{t} \cdot \mathbf{x} \cdot \mathbf{t}^{-1}$

Substitution Group products: S_n class transformation algebra

Similarity transform **y**= **t**·**x**·**t**$^{-1}$ =(15)(2738496) · (5678)(19)(234) · (51)(2694837)

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(15)(2738496) · (5678)(19)(234) · (51)(2694837)

(19 — 1→5→6→9

(192 — 9→6→7→2

(1923 — 2→7→8→3

(1923) — 3→8→5→1

(45 — 4→9→1→5

(45) — 5→1→9→4

(67 — 6→2→3→7

(678 — 7→3→4→8

(678) — 8→4→2→6

1	2	3	4	5	6	7	8	9	⟨1⟩
5	7	8	9	1	2	3	4	6	(15)(2694837)
8	6	7	1	9	4	2	3	5	(5678)(19)(234)
3	9	2	5	4	8	6	7	1	(51)(2738496)
1	2	3	4	5	6	7	8	9	⟨1⟩

(5678)(19)(234) = **x**

= (1923)(54)(678) = **t**·**x**·**t**$^{-1}$

t·=(15)(2738496)

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Substitution Group products: S_n class cycle labeling

Permutations are classified by the numbers of ν_1 of unicycles, ν_2 of bicycles, ν_3 of tricycles, *etc.*

Ball-numbers can’t be repeated after cycle reduction. So cycle length sum is number N of balls.

$$\nu_1 + 2\,\nu_2 + 3\,\nu_3 + 4\,\nu_4 + 5\,\nu_5 + \ldots + N\nu_N = N$$

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S_4 example

$\nu_1 = 1 \quad \nu_2 = 0 \quad \nu_3 = 1$

(4) (321)

Number of classes of S_n equals the number of *partitions* of integer $N=n$.

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$\nu_1 = 5$ $\nu_2 = 3$ $\nu_3 = 1$

(14)(13)(12)(11)(10) (98)(76)(54) (321)

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For $N=2$ there are just two classes of two permutations.

Class $\{\nu_1 = 2, \nu_2 = 0\}$ *corresponding to partition :* $2 = 1 + 1$ ⊙ ⊙

One permutation : *(1)(2)*

Class $\{\nu_1 = 0, \nu_2 = 1\}$ *corresponding to partition :* $2 = 2$ ⊙ ⊙

One permutation : *(12)*

Substitution Group products: S_n class cycle labeling

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⊙
⊙

One permutation : *(1)(2)*

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⊙ ⊙

One permutation : *(12)*

For $N=3$ there are three classes of six permutations.

Class $\{\nu_1 = 3, \nu_2 = 0, \nu_3 = 0\}$ *corresponding to partition* : $3 = 1 + 1 + 1$

⊙
⊙
⊙

One permutation :: *(1)(2)(3)*

Class $\{\nu_1 = 1, \nu_2 = 1, \nu_3 = 0\}$ *corresponding to partition* : $3 = 2 + 1$

⊙ ⊙
⊙

Three permutations : *(12)(3), (13)(2), (23)(1)*

Class $\{\nu_1 = 0, \nu_2 = 0, \nu_3 = 1\}$ *corresponding to partition* : $3 = 3$

⊙ ⊙ ⊙

Two permutations : *(123), (132)*

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The number of permutations in each partition class depends on the redundancy of cycle labeling

Each m-cycle can be written m ways by cycling the numbers:

(123… m) = (m 12… m-1) = (m-1 m 123… m-2)=… *Example:* (123)=(312)=(231)

Substitution Group products: S_n class cycle counting

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If there are ν_m such m-cycles in a permutation then there are $(m)^{\nu_m}$ such reorderings.

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Example: (123)(456)=(456)(231)

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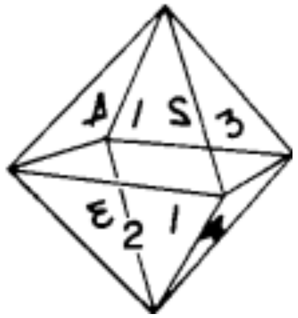
$$\textit{Number in partition class } \nu_1\nu_2\nu_3\nu_4\cdots = \frac{N!}{\nu_1!1^{\nu_1}\,\nu_2!2^{\nu_2}\,\nu_3!3^{\nu_3}\nu_4!4^{\nu_4}\cdots}$$

where: $$N = \nu_1 + 2\nu_2 + 3\nu_3 + 4\nu_4\cdots$$

Example:Order of Octahedral O classes: (1)(2)(3)(4) , (1)(123), (12)(34). (1234), (12)(3)(4)



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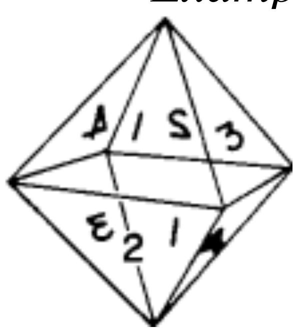
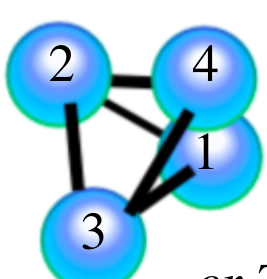


$$\nu_1\nu_2\nu_3\nu_4\cdots = \quad 4\,0\,0\,0,\quad 1\,0\,1\,0,\quad 0\,2\,0\,0,\quad 0\,0\,0\,1,\quad 2\,1\,0\,0,$$

$$\frac{N!}{\nu_1!1^{\nu_1}\,\nu_2!2^{\nu_2}\,\nu_3!3^{\nu_3}\nu_4!4^{\nu_4}\ldots} = \quad \frac{4!}{4!}=1,\quad \frac{4!}{1!3^1}=8,\quad \frac{4!}{2!2^2}=3,\quad \frac{4!}{1!4^1}=6,\quad \frac{4!}{2!1^2 1!2^1}=6.$$



…or Tetrahedral T_d classes

$$S_4 \sim T_d$$

Substitution Group products: S_n class cycle counting

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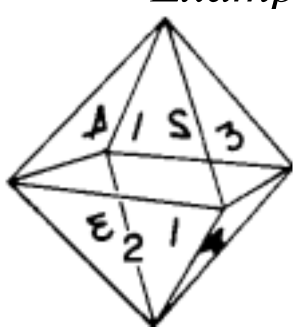

$$\nu_1\nu_2\nu_3\nu_4\cdots = \quad 4\,0\,0\,0,\quad 1\,0\,1\,0,\quad 0\,2\,0\,0,\quad 0\,0\,0\,1,\quad 2\,1\,0\,0,$$

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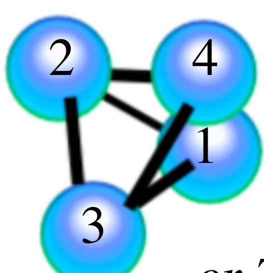
(1)(2)(3)(4)	(1)(234)	(13)(24)	(1432)	(14)(3)(2)
	(2)(143)	(14)(23)	(1243)	(23)(1)(4)
	(3)(124)	(13)(24)	(1324)	(23)(1)(4)
	(4)(132)		(1234)	(12)(3)(4)
	(1)(243)		(1423)	(24)(1)(3)
	(2)(134)		(1342)	(13)(2)(4)
	(3)(142)			
	(4)(123)			



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Permutation group S_n is equivalent to **Point group $\mathscr{G}$**

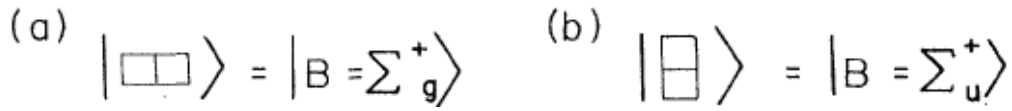
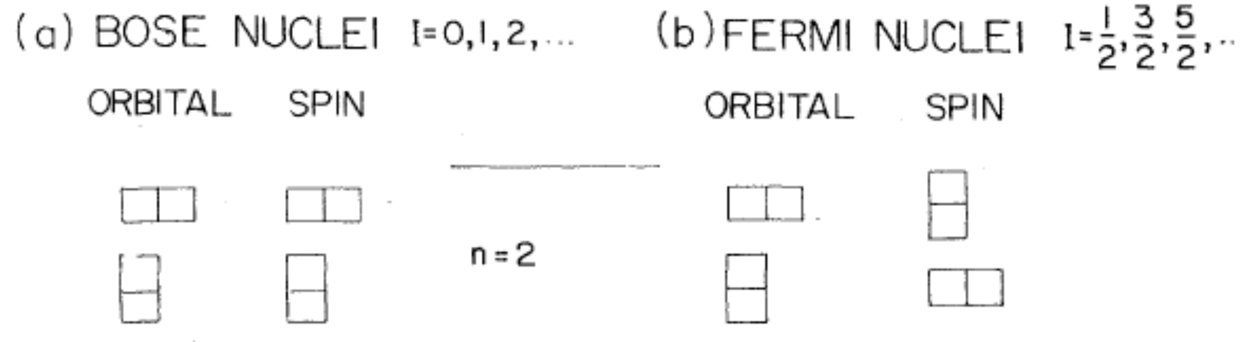
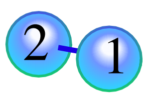


FIG. 25. Orbital tableau labeling of a homonuclear diatomic

FIG. 26. Orbital and spin tableaus used to label homonuclear n-atomic molecules ($n = 2, 3, 4, \ldots$).





$S_2 \sim C_2$

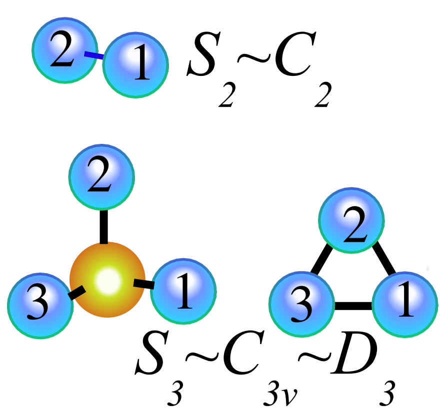
S_2

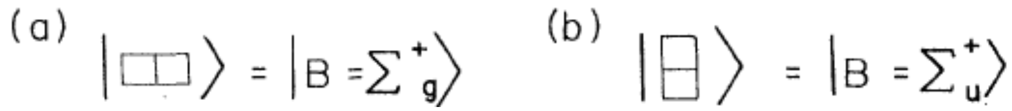
S_2	(1)(2)	(12)
A_1 [1 2]	1	1
A_2 [1 / 2]	1	-1

C_2	**1**	**σ**
A_1	1	1
A_2	1	-1

S_n tableaus spin-symmetry and characters: X_n and XY_n molecules

Permutation group S_n is equivalent to Point group $\mathscr{G}$





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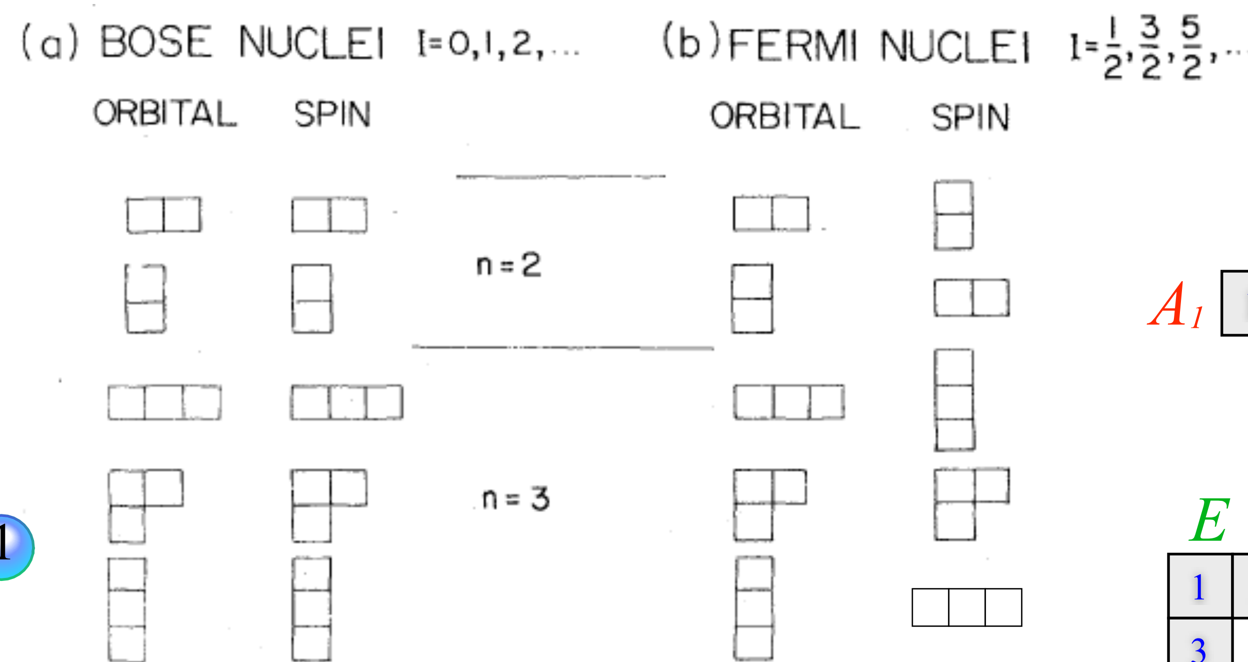
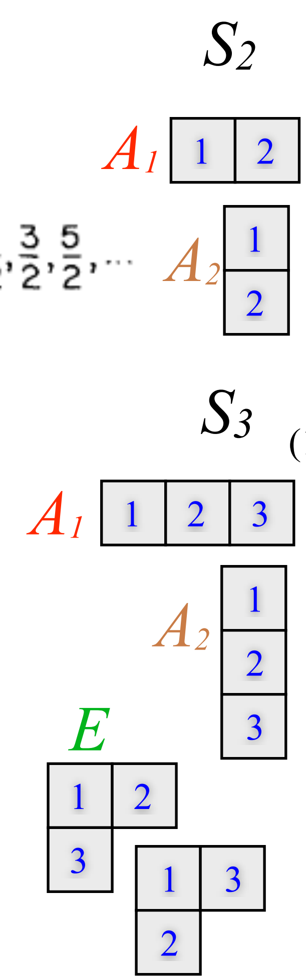




S_2	(1)(2)	(12)
A_1	1	1
A_2	1	-1

C_2	**1**	**σ**
A_1	1	1
A_2	1	-1

S_3	(1)(2)(3)	(123) (132)	(12) (13) (23)
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

C_{3v}	**1**	$\mathbf{r}^1$ $\mathbf{r}^2$	$\boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2 \boldsymbol{\sigma}_3$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Rev. Mod. Phys. 50,1,1 (1978)

S_n tableaus spin-symmetry and characters: X_n and XY_n molecules

Permutation group S_n is equivalent to Point group $\mathscr{G}$

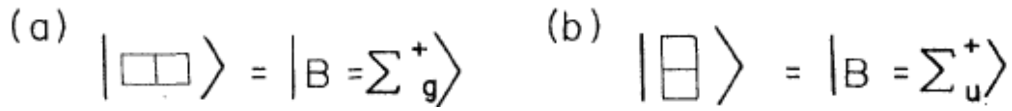
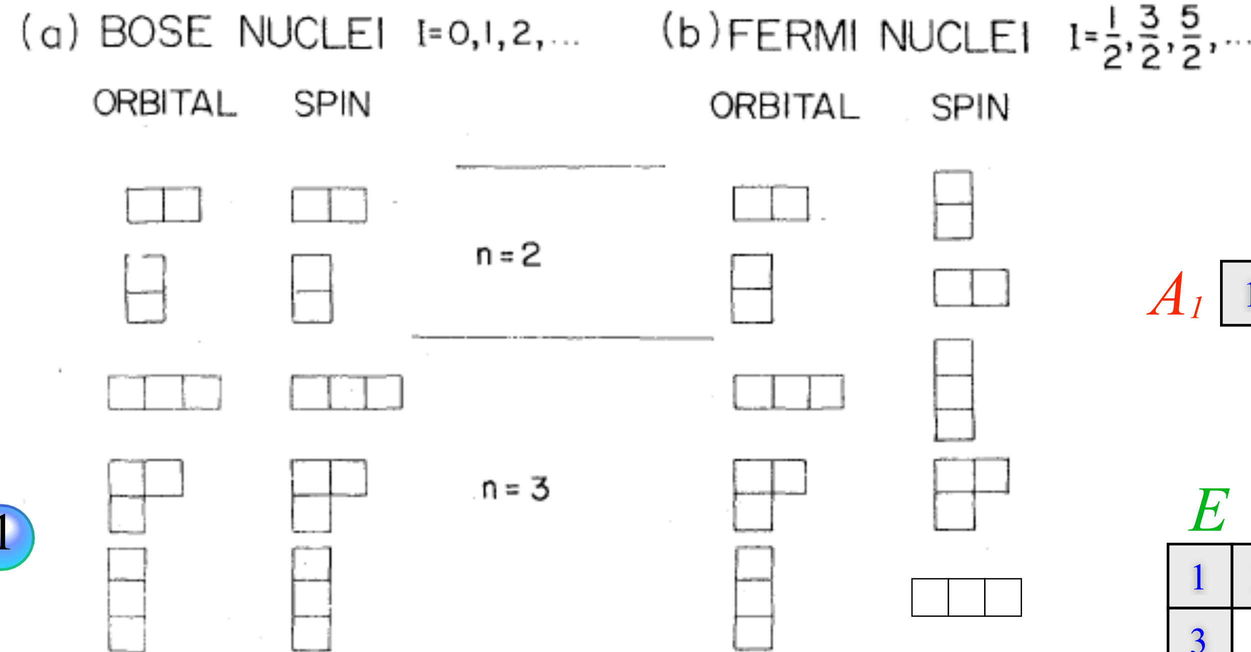
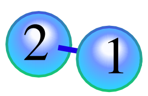


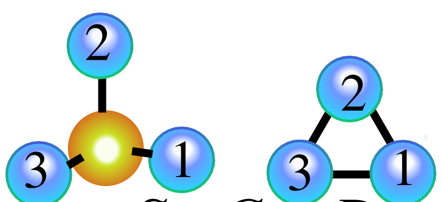
FIG. 25. Orbital tableau labeling of a homonuclear diatomic

FIG. 26. Orbital and spin tableaus used to label homonuclear n-atomic molecules (n=2.3.4....).

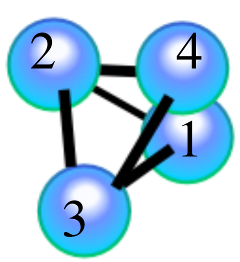




$S_2 \sim C_2$

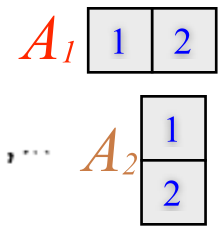


$S_3 \sim C_{3v} \sim D_3$



$S_4 \sim T_d$

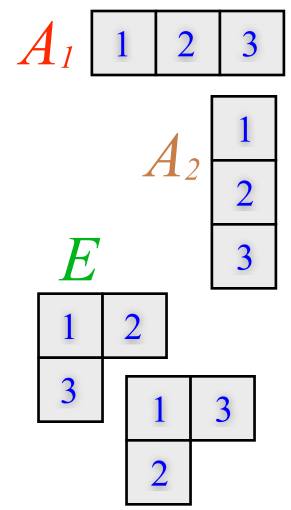
S_2



S_2	(1)(2)	(12)
A_1	1	1
A_2	1	-1

C_2	**1**	**σ**
A_1	1	1
A_2	1	-1

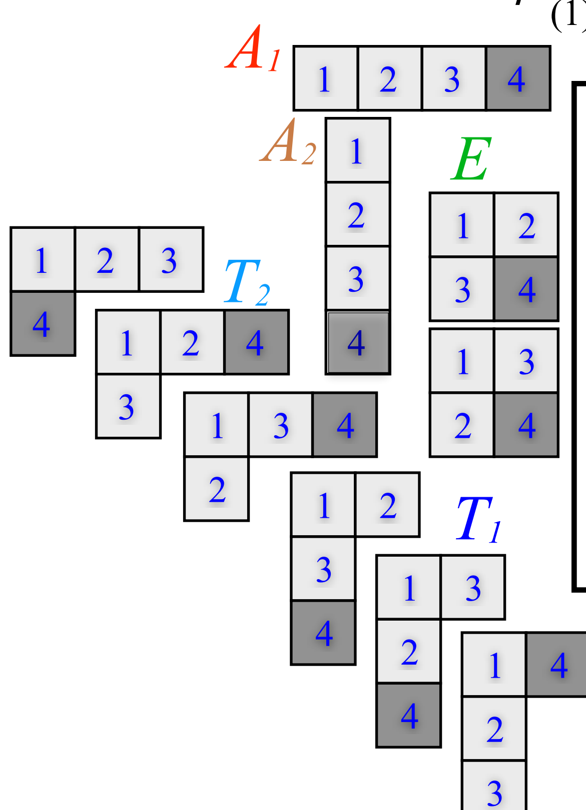
S_3



S_3	(1)(2)(3)	(123) (132)	(12) (13) (23)
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

C_{3v}	**1**	$\mathbf{r}^1$ $\mathbf{r}^2$	$\boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2 \boldsymbol{\sigma}_3$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

S_4



S_4	(1)(2)(3)(4)	(123)(4)	(12)(34)	(1234)	(12)(3)(4)
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_2	3	0	-1	1	-1
T_1	3	0	-1	-1	1

Tetrahedral: $\mathscr{G} = T_d$

T_d	**1**	$\mathbf{r}_{1...4}$	180° $\boldsymbol{\rho}_{xyz}$	$\mathbf{I}\cdot$90° $\mathbf{R}_{xyz}$	$\mathbf{I}\cdot$180° $\boldsymbol{\sigma}_{1...6}$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_2	3	0	-1	-1	1
T_1	3	0	-1	1	-1

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S_n tableaus spin-symmetry and characters: X_n and XY_n molecules

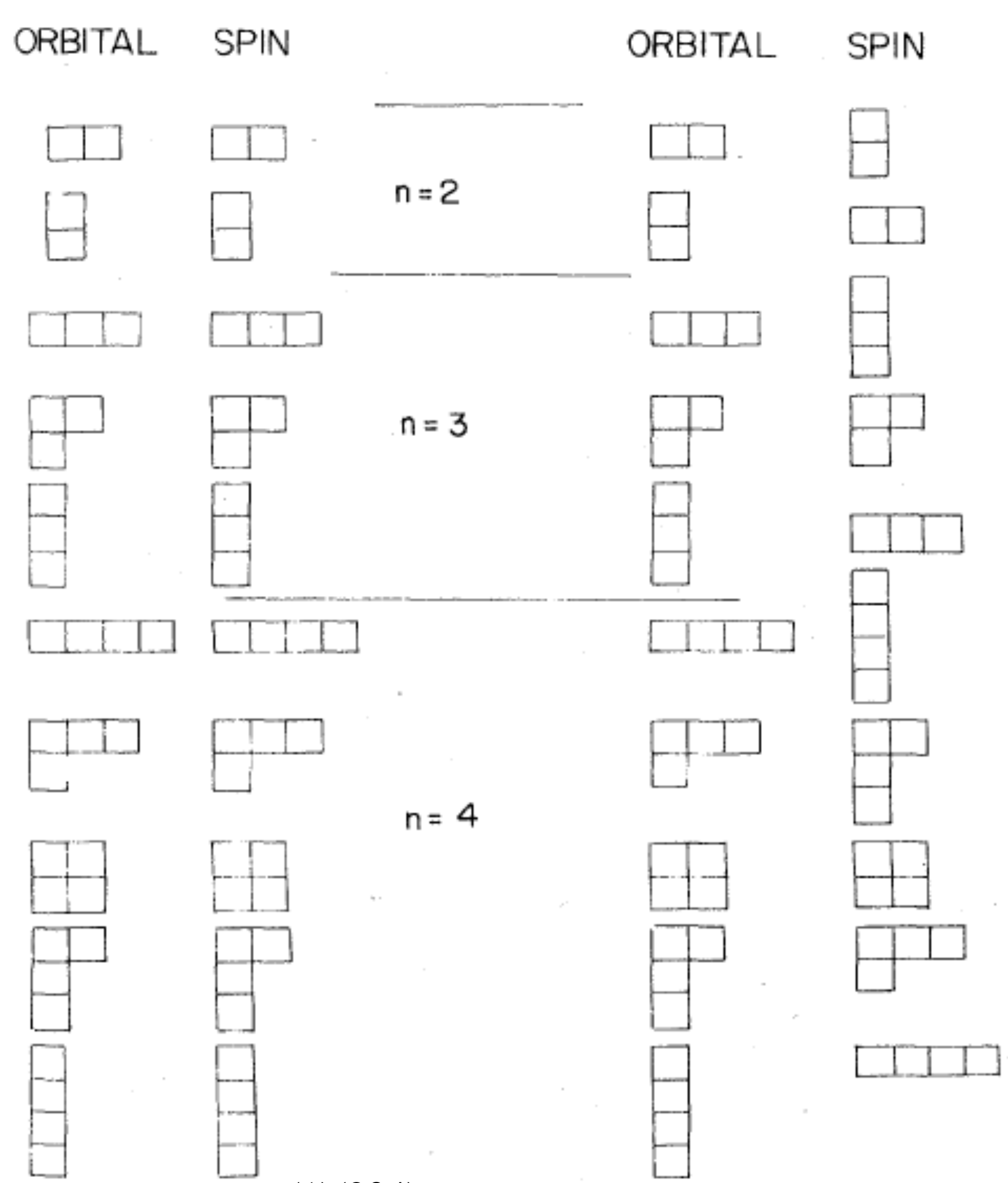
Permutation group S_n is equivalent to Point group $\mathscr{G}$

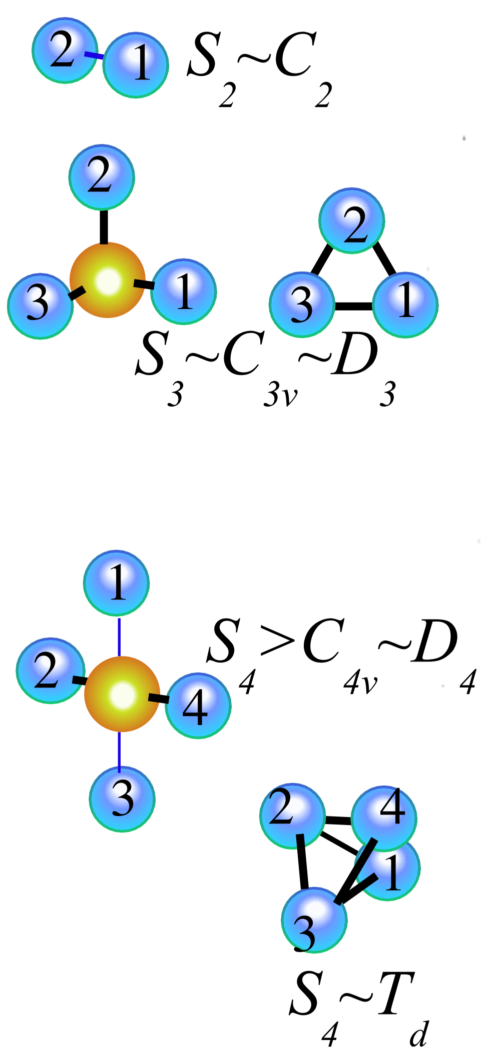
(a) $|\square\square\rangle = |B = \Sigma_g^+\rangle$ (b) $|\,\boxminus\,\rangle = |B = \Sigma_u^+\rangle$

FIG. 25. Orbital tableau labeling of a homonuclear diatomic

FIG. 26. Orbital and spin tableaus used to label homonuclear n-atomic molecules ($n=2,3,4,\ldots$).

(a) BOSE NUCLEI $I=0,1,2,\ldots$ (b) FERMI NUCLEI $I=\frac{1}{2},\frac{3}{2},\frac{5}{2},\ldots$





(1)(2)(3)(4)

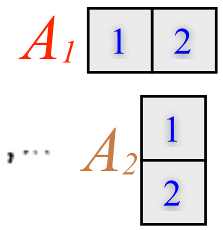
(1)(234)
(2)(143)
(3)(124)
(4)(132)
(1)(243)
(2)(134)
(3)(142)
(4)(123)

(13)(24)
(14)(23)
(13)(24)

(1432)
(1243)
(1324)
(1234)
(1423)
(1342)

(14)(3)(2)
(23)(1)(4)
(23)(1)(4)
(12)(3)(4)
(24)(1)(3)
(13)(2)(4)

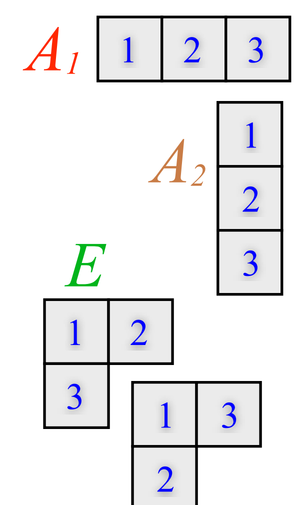
S_2



	(1)(2)	(12)
A_1	1	1
A_2	1	-1

C_2	**1**	**σ**
A_1	1	1
A_2	1	-1

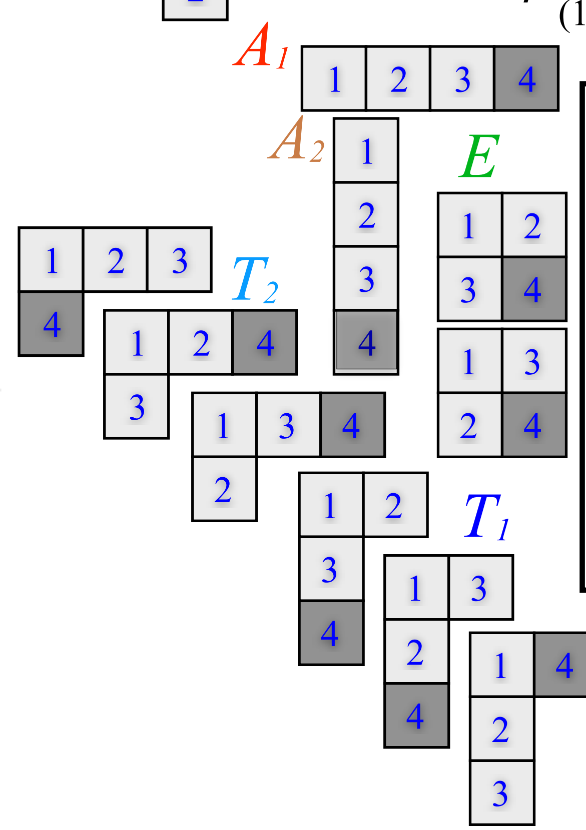
S_3



	(1)(2)(3)	(123) (132)	(12) (13) (23)
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

C_{3v}	**1**	$\mathbf{r}^1$ $\mathbf{r}^2$	$\sigma_1\sigma_2\sigma_3$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

S_4



	(1)(2)(3)(4)	(123)(4)	(12)(34)	(1234)	(12)(3)(4)
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_2	3	0	-1	1	-1
T_1	3	0	-1	-1	1

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S_n tableaus spin-symmetry and characters: X_n and XY_n molecules

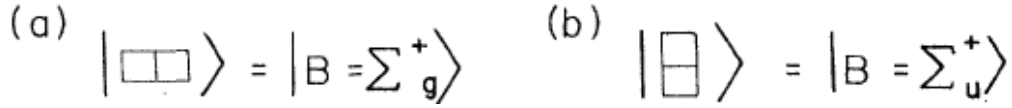
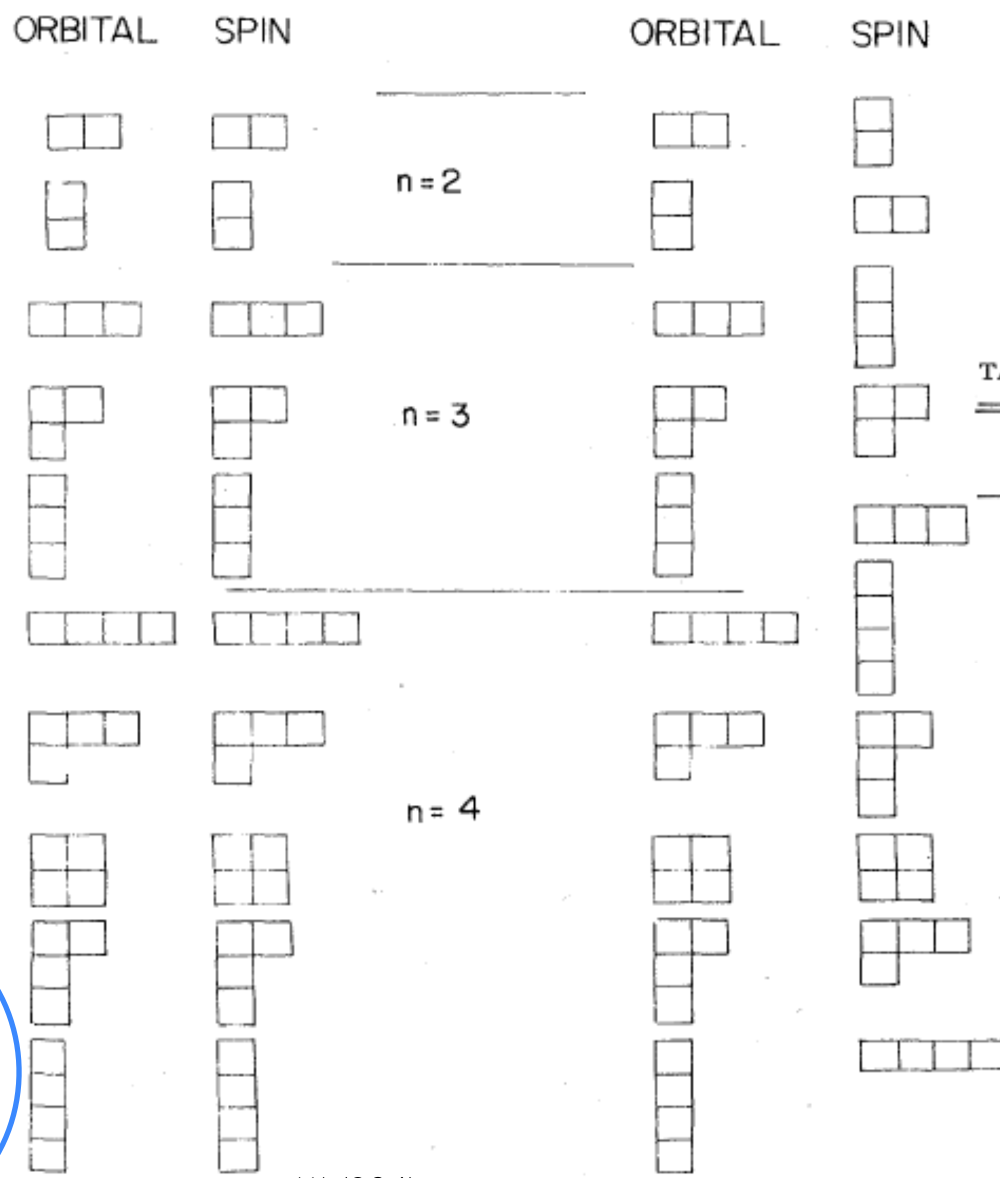
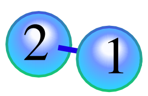


FIG. 25. Orbital tableau labeling of a homonuclear diatomic

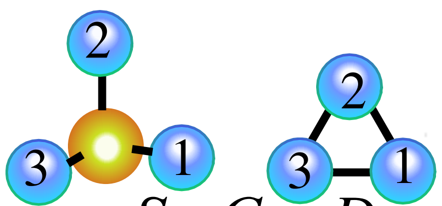
FIG. 26. Orbital and spin tableaus used to label homonuclear n-atomic molecules ($n = 2, 3, 4, \ldots$).

(a) BOSE NUCLEI $I = 0, 1, 2, \ldots$ (b) FERMI NUCLEI $I = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$

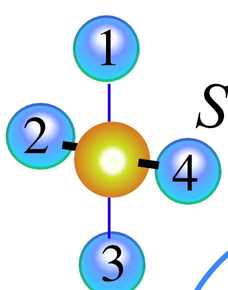




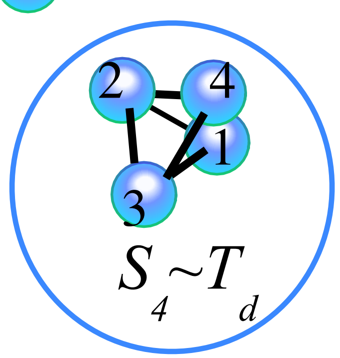
$S_2 \sim C_2$



$S_3 \sim C_{3v} \sim D_3$



$S_4 > C_{4v} \sim D_4$



$S_4 \sim T_d$

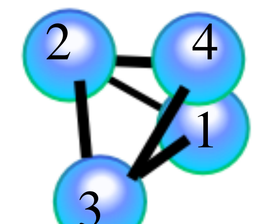
(1)(2)(3)(4)

(1)(234)
(2)(143)
(3)(124)
(4)(132)
(1)(243)
(2)(134)
(3)(142)
(4)(123)

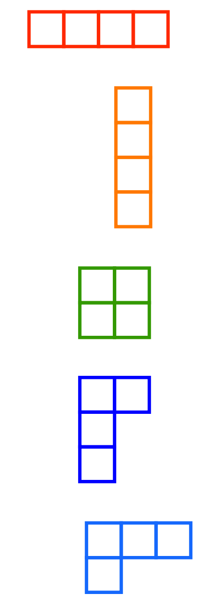
(13)(24)
(14)(23)
(13)(24)

(1432)
(1243)
(1324)
(1234)
(1423)
(1342)

(14)(3)(2)
(23)(1)(4)
(23)(1)(4)
(12)(3)(4)
(24)(1)(3)
(13)(2)(4)



$S_4 \sim T_d$



Methane-like:XY_4

TABLE XIII. T_d characters and symmetry.

T_d	1	$R\left(\frac{2\pi}{3}\right)$	$R(\pi 00)$	$IR\left(\frac{\pi}{2}00\right)$	$IR\left(\frac{\pi}{2}\frac{\pi}{2}\frac{\pi}{2}\right)$	Boson $\{\mu_s\}$	Fermion $\{\mu_s\}$
A_1	1	1	1	1	1	{4}	{1}{1}{1}{1}
A_2	1	1	1	−1	−1	{1}{1}{1}{1}	{4}
E	2	−1	2	0	0	{2}{2}	{2}{2}
$(L_xL_yL_z)\,F_1$	3	0	−1	1	−1	{2}{1}{1}	{3}{1}
$(xyz)\,F_2$	3	0	−1	−1	1	{3}{1}	{2}{1}{1}{1}

TABLE XIV. $O_3 \downarrow T_d$ correlation.

	A_1	A_2	E	F_1	F_2		A_2	A_1	E	F_2	F_1
$J^p = 0^+$	1	...	...	...	...	0^-	1	...	...	...	...
1^+	...	...	...	1	...	1^-	...	...	...	1	...
2^+	...	...	1	...	1	2^-	...	...	1	...	1
3^+	...	1	...	1	1	3^-	...	1	...	1	1
4^+	1	...	1	1	1	4^-	1	...	1	1	1
5^+	...	...	1	2	1	5^-	...	...	1	2	1
6^+	1	1	1	1	2	6^-	1	1	1	1	2
7^+	...	1	1	2	2	7^-	...	1	1	2	2

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3.28.18 class 19.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

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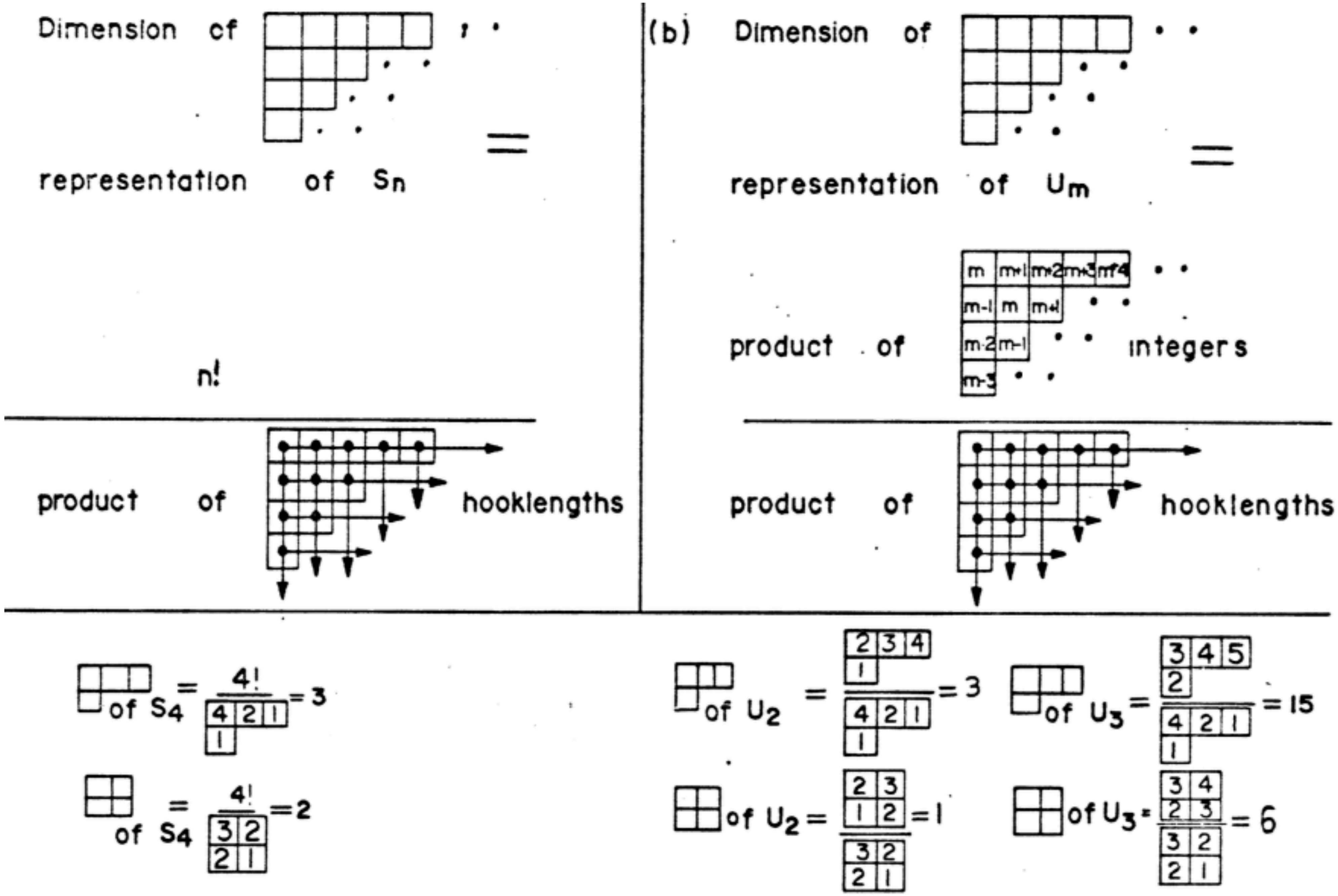
Methane-like XY_4 Introducing rovibrational spectral nomogram

Large molecule character and correlation formulae

Hexafluoride-like:XY_6.

How does level clustering affect nuclear hyperfine?

Tableau dimension formulae



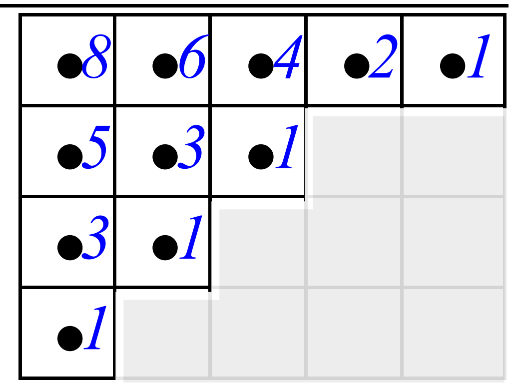
From unpublished Ch.10 for
Principles of Symmetry, Dynamics & Spectroscopy

Fig. 10.1.5 Hall - Robinson Hooklength Formulas
Dimension of representations of (a) S_n and (b) U_m labeled by a single tableau are given by the formulas. A hooklength of a tableau box is simply the number of boxes in a "hook" consisting of all the boxes below it, to the right of it, and itself.

S_n Young Tableaus and spin-symmetry for X_n and XY_n molecules

Tableau dimension formulae

$$\ell^{[\mu_s]}(S_n) = \text{Dimension of } S_n \text{ Tableau } [\mu_1][\mu_2]\cdots[\mu_n] = \frac{n! = n\cdot(n-1)\cdot(n-2)\cdots 3\cdot 2\cdot 1}{\text{hook-length product}}$$



Examples:

$$\ell^{A_1} = \ell^{[3,0,0]}(S_3) = \frac{3\cdot 2\cdot 1}{3 \cdot 2 \cdot 1} = 1$$

$$\ell^{A_2} = \ell^{[1,1,1]}(S_3) = \frac{3\cdot 2\cdot 1}{3 \cdot 2 \cdot 1} = 1$$

$$\ell^{E} = \ell^{[2,1,0]}(S_3) = \frac{3\cdot 2\cdot 1}{3 \cdot 1 \cdot 1} = 2$$

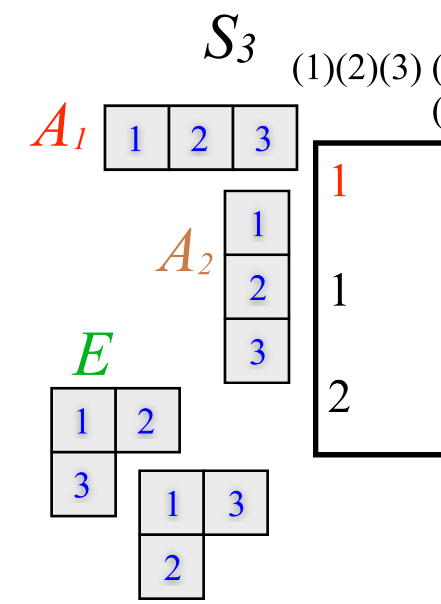
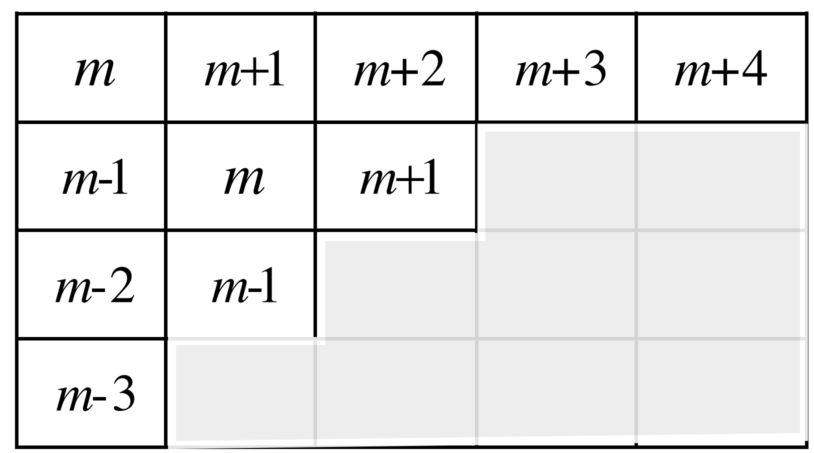
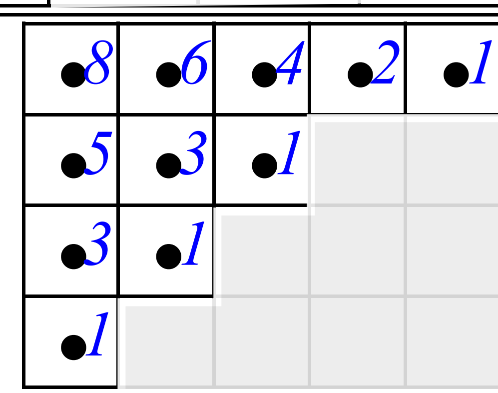


FIG. 28. Robinson formula for statistical weights. The "hook-length" of a box in the tableau is the number of boxes in a "hook" which includes that box and all boxes in the line to the right and in the column below it.

$$\ell^{[\mu_s]}(U_m) = \text{Dimension of } S_n{*}U_m \text{ Tableau } [\mu_1][\mu_2]\cdots[\mu_m] = \frac{m\text{-dimension product}}{\text{hook-length product}}$$





Examples:

$$\ell^{[2,1,0]}(S_3{*}U(3)) = \frac{3\cdot 4\cdot 2}{3\cdot 1\cdot 1} = 8$$

$$\ell^{[3,0,0]}(S_3{*}U(3)) = \frac{3\cdot 4\cdot 5}{3\cdot 2\cdot 1} = 10$$

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  - Product arrays shortcuts
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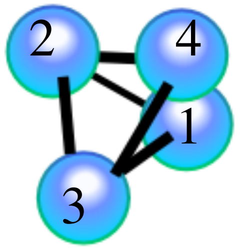
  - How does level clustering affect nuclear hyperfine?

S_4 and spin-symmetry for XY_4 molecules (Introducing hook-length formulae)



$S_4 \sim T_d$

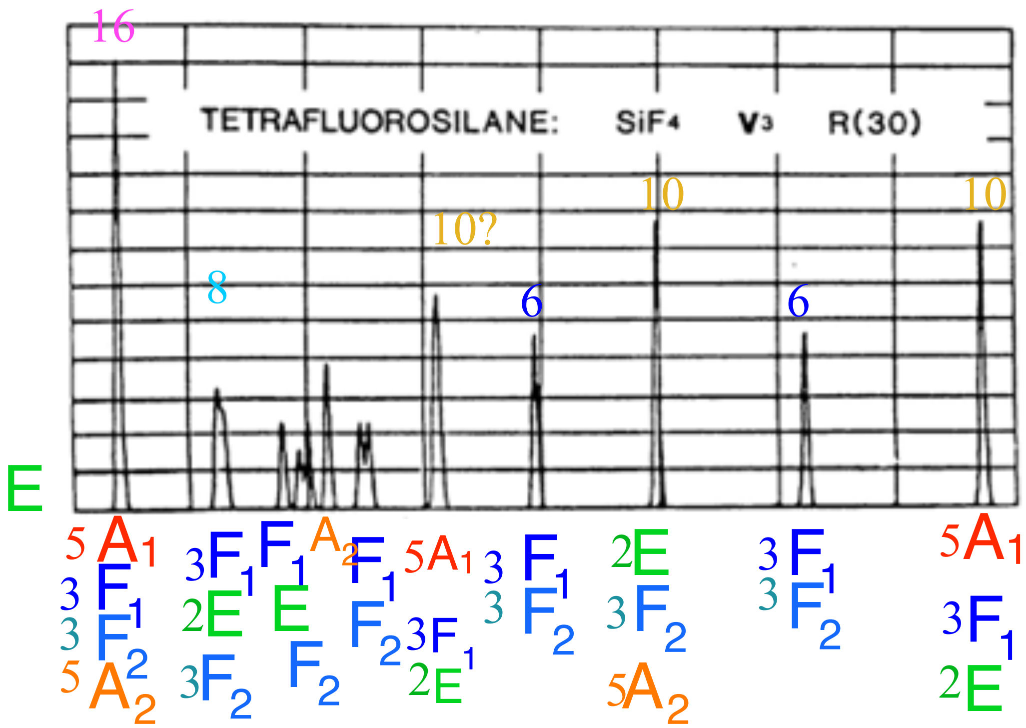
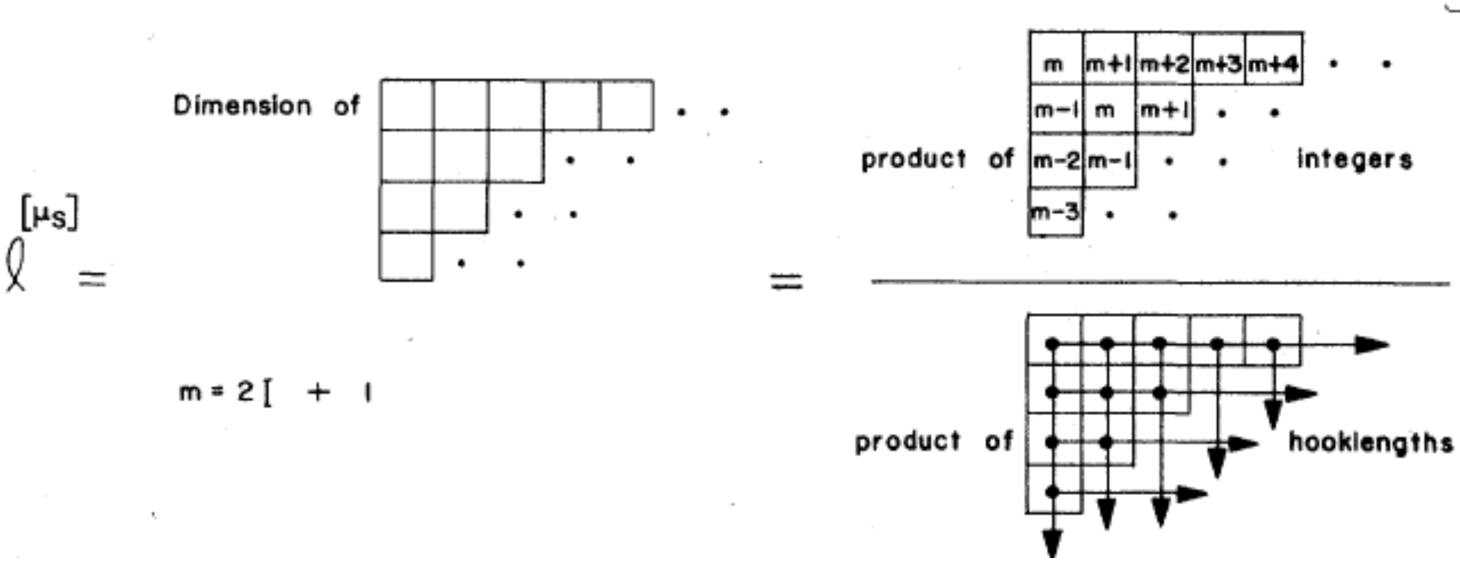


FIG. 28. Robinson formula for statistical weights. The "hook-length" of a box in the tableau is the number of boxes in a "hook" which includes that box and all boxes in the line to the right and in the column below it.



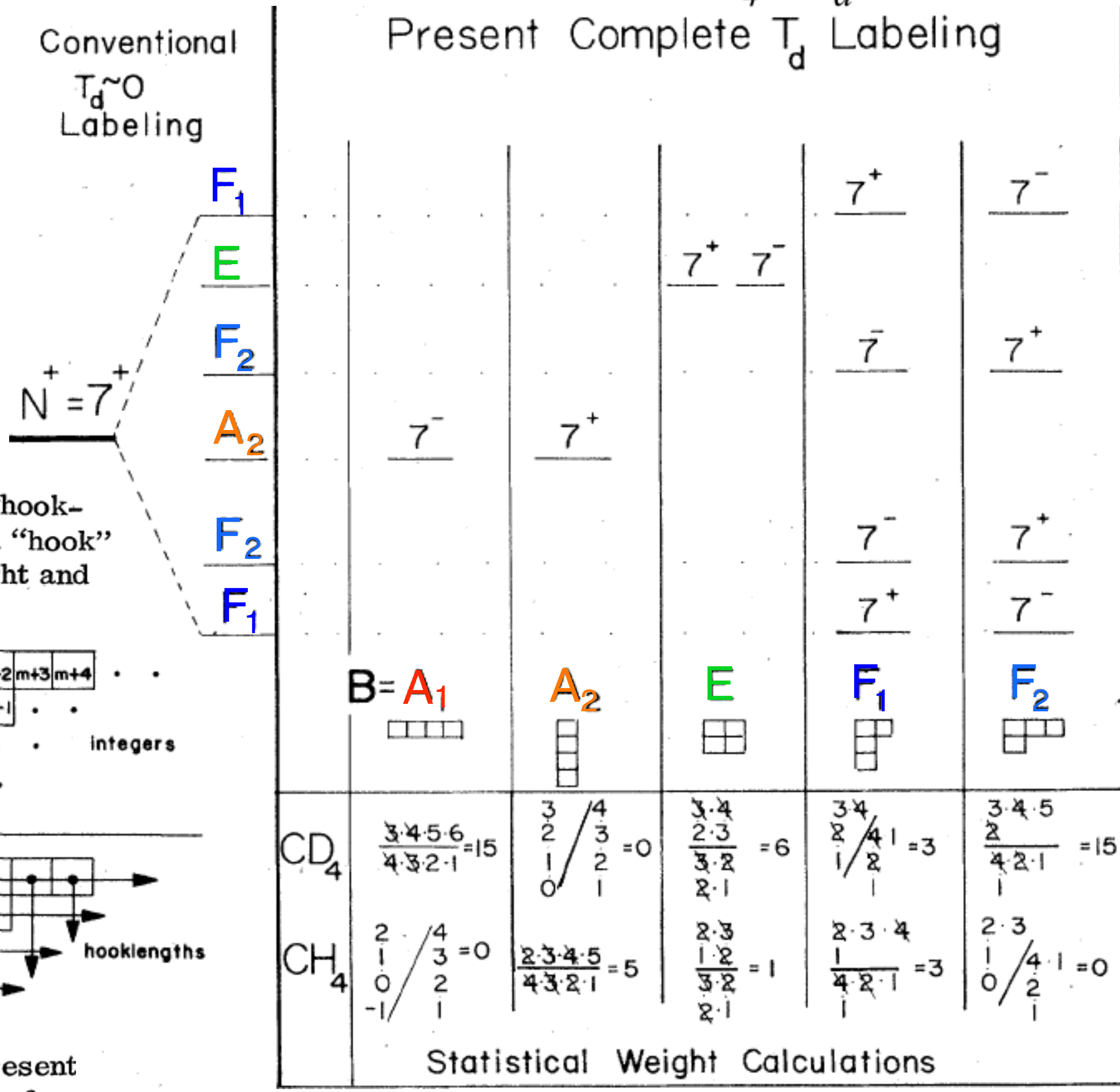


FIG. 36. Comparison of conventional CH_4 labeling with present labeling. The latter shows clearly the "hidden" structure of inversion doublets which has a structure very much like that of NH_3. For CH_4, however, only the E levels are actually double according to the statistical weight calculations.

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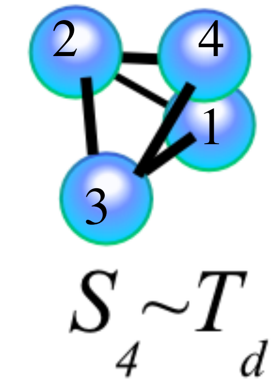
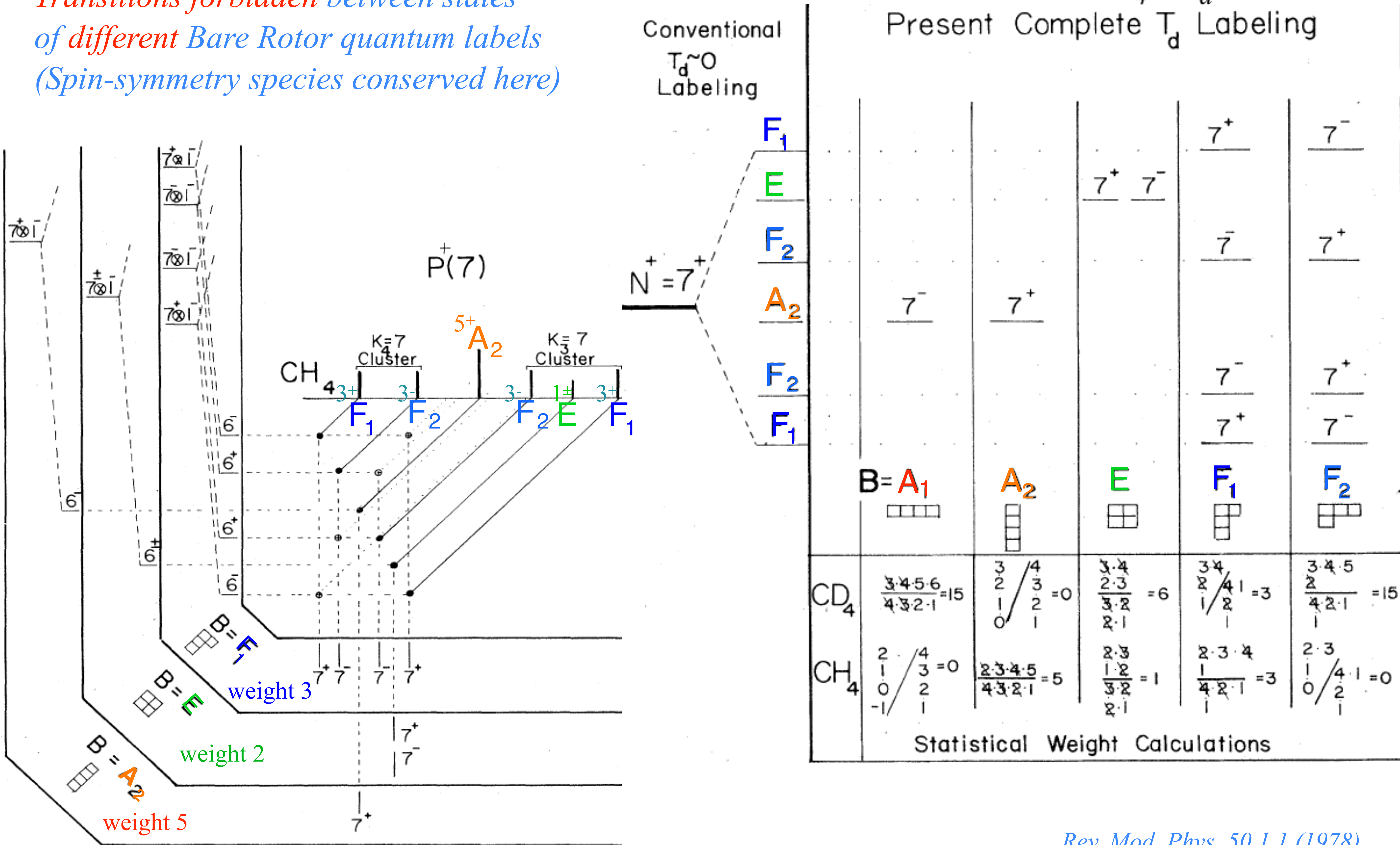


Introducing rovibrational spectral nomogram

Transitions forbidden between states of different Bare Rotor quantum labels (Spin-symmetry species conserved here)



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APPENDIX C. S_n CHARACTER FORMULA

We give a formula (Coleman, 1966) for S_n characters $x^{[\mu_1\cdots\mu_p]}_{1^\alpha 2^\beta 3^\gamma}$. Here the S_n IR is labeled by a tableau symbol $[\mu_1\cdots\mu_p]$ wherein μ_j means that row j has μ_j boxes. The S_n classes are labeled by the notation $1^\alpha 2^\beta 3^\gamma\cdots n$ wherein α, β, γ, ... are the number of permutation 1-cycles, 2-cycles, 3-cycles, ... respectively. For example, the permutation (1)(3)(2, 5)(4, 7, 6, 8) would be in the class $1^2 2^1 3^0 4^1 5^0 6^0 7^0 8^0$ of S_8. The character then is given by the following formula and definitions. Note that th formula starts with a column of numbers that are the hooklengths of the first column of the tableau. Then the definitions are used to whittle it down to a sum of sequentially numbered columns which each contribute unit according to Def. 2.

$$\chi^{[\mu_1\cdots\mu_p]}_{1^\alpha 2^\beta 3^\gamma\cdots} = \partial_1^\alpha \partial_2^\beta \partial_3^\gamma\cdots \begin{vmatrix} \mu_1+p-1 \\ \cdot \\ \cdot \\ \cdot \\ \mu_{p-2}+2 \\ \mu_{p-1}+1 \\ \mu_p \end{vmatrix};$$

For example, here is the character of the [56, 13] IR of class 2, 11, 56 of S_{69}:

$$\chi^{[56,13]}_{2,11,56} = \partial_2\partial_{11}\partial_{56}\begin{vmatrix} 57 \\ 13 \end{vmatrix} = \partial_2\partial_{11}\begin{vmatrix} 1 \\ 13 \end{vmatrix}$$

$$= \partial_2\begin{vmatrix} 1 \\ 2 \end{vmatrix} = \begin{vmatrix} 1 \\ 0 \end{vmatrix} = 1\,.$$

Def. 1:

$$\partial_m\begin{vmatrix} a \\ b \\ c \\ \cdot \\ \cdot \\ \cdot \end{vmatrix} = \begin{vmatrix} a-m \\ b \\ c \\ \cdot \\ \cdot \\ \cdot \end{vmatrix} + \begin{vmatrix} a \\ b-m \\ c \\ \cdot \\ \cdot \\ \cdot \end{vmatrix} + \begin{vmatrix} a \\ b \\ c-m \\ \cdot \\ \cdot \\ \cdot \end{vmatrix} + \cdots;$$

Def. 2:

$$\begin{vmatrix} p-1 \\ \cdot \\ \cdot \\ \cdot \\ 2 \\ 1 \\ 0 \end{vmatrix} = 1;$$

Def. 3:

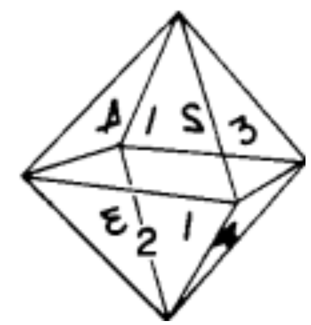
$$\begin{vmatrix} a \\ b \\ c \\ \cdot \\ \cdot \\ \cdot \end{vmatrix} = 0$$ if any two numbers in the column are equal, or if any number is less than zero;

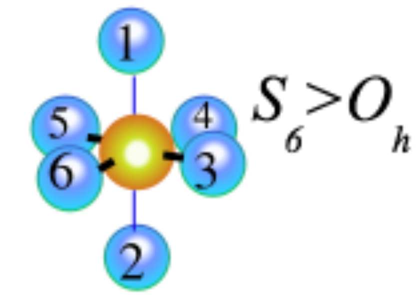
Def. 4:

$$\begin{vmatrix} a \\ b \\ c \\ \cdot \\ \cdot \\ \cdot \end{vmatrix} = -\begin{vmatrix} b \\ a \\ c \\ \cdot \\ \cdot \\ \cdot \end{vmatrix}$$ interchanging any two numbers gives a change of sign.

TABLE XV. Characters of permutation group (S_6) and octahedral (O_h) subgroup.

	1^6	3^2	2^2	4^1	2^3	2^3	6^1	2^1	$2^1 4^1$	$2^2 = S_6$ Class
$\{\mu\}=\{6\}$	1	1	1	1	1	1	1	1	1	1
$\{5,1\}$	5	−1	1	1	−1	−1	−1	3	−1	1
$\{4,2\}$	9	0	1	−1	3	3	0	3	1	1
$\{4,1,1\}$	10	1	−2	0	−2	−2	1	2	0	−2
$\{3,3\}$	5	2	1	−1	−3	−3	0	1	−1	1
$\{3,2,1\}$	16	−2	0	0	0	0	0	0	0	0
$\{2,2,2\}$	5	2	1	1	3	3	0	−1	−1	1
$\{3,1,1,1\}$	10	1	−2	0	2	2	−1	−2	0	−2
$\{2,2,1,1\}$	9	0	1	1	−3	−3	0	−3	1	1
$\{2,1,1,1,1\}$	5	−1	1	−1	1	1	1	−3	−1	1
$\{1,1,1,1,1,1\}$	1	1	1	−1	−1	−1	−1	−1	1	1
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1
E_g	2	−1	2	0	0	2	−1	2	0	0
T_{1g}	3	0	−1	1	−1	3	0	−1	1	−1
T_{2g}	3	0	−1	−1	1	3	0	−1	−1	1
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1
E_u	2	−1	2	0	0	−2	1	−2	0	0
T_{1u}	3	0	−1	1	−1	−3	0	1	−1	1
T_{2u}	3	0	−1	−1	1	−3	0	1	1	−1
	1	120° Class	180° Class	90° Class	180° Class	I				





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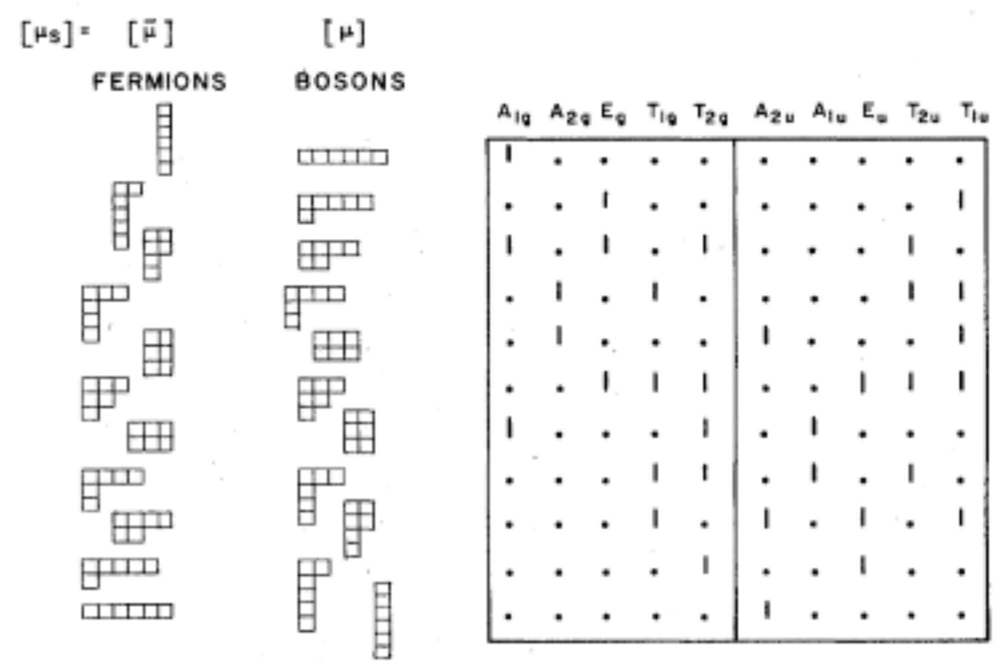

FIG. 27. Spin tableau-(B) correlation for octahedral XY_6 molecule (see Appendix D).

TABLE I. Permutational - octahedral correlation table $S_6 + O_h$. Only the last four rows are relevant for spin-$\frac{1}{2}$ nuclei.

Fermi nuclei	Bose nuclei	A_{1g}	A_{1u}	A_{2g}	A_{2u}	E_g	E_u	T_{1g}	T_{1u}	T_{2g}	T_{2u}	
[1,1,1,1,1,1]	[6]	1	·	·	·	·	·	·	·	·	·	
[2,1,1,1,1]	[5,1]	·	·	·	·	1	·	·	1	·	·	
[2,2,1,1]	[4,2]	1	·		·	1	·	·	·	1	1	
[3,1,1,1]	[4,1,1]	·	·	1	·	·	·	1	1	·	1	
[2,2,2]	[3,3]	·	·	1	1	·	·	·	1	·	·	
[3,2,1]	[3,2,1]	·	·	·	·	1	1	1	1	1	1	
[4,1,1]	[3,1,1,1]	·	1	·	·	·	·	1	·	1	1	
[3,3]	[2,2,2]	1	1	·	·	·	·	·	·	1	·	$I=0$
[4,2]	[2,2,1,1]	·	·	·	1	·	1	1	1	·	·	$I=1$ (Spin-$\frac{1}{2}$ nuclei)
[5,1]	[2,1,1,1,1]	·	·	·	·	·	1	·	·	1	·	$I=2$ (Spin-$\frac{1}{2}$ nuclei)
[6]	[1,1,1,1,1,1]	·	·	·	1	·	·	·	·	·	·	$I=3$ (Spin-$\frac{1}{2}$ nuclei)

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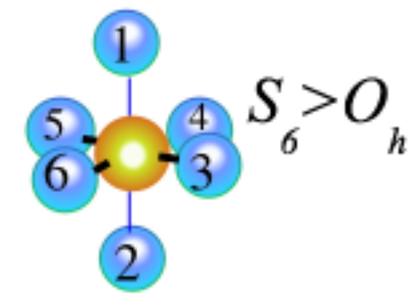


AMOP reference links on page 2

3.28.18 class 19.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

$S_1 \subset S_2 \subset S_3 \subset S_4 \subset S_5$ …permutation symmetry algebra and spinor-rotor correlations

Substitution Group products: S_n cycle notation

- Cyclic product algebra: bicycles tricycles quadricycles
  - Permutation unraveling
  - Product arrays shortcuts
- S_n class transformation algebra
- S_n class cycle labeling
- S_n class cycle counting

S_n tableaus spin-symmetry and characters: X_n and XY_n molecules

- Tableau dimension formulae
- Methane-like XY_4 Introducing rovibrational spectral nomogram
  - Large molecule character and correlation formulae
- Hexafluoride-like:XY_6.
  - How does level clustering affect nuclear hyperfine?

S_n Young Tableaus and spin-symmetry for X_n and XY_n molecules

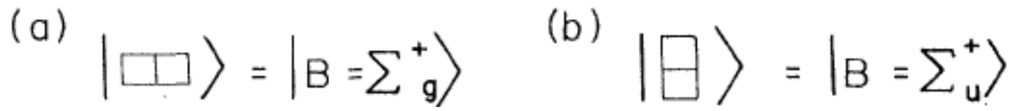
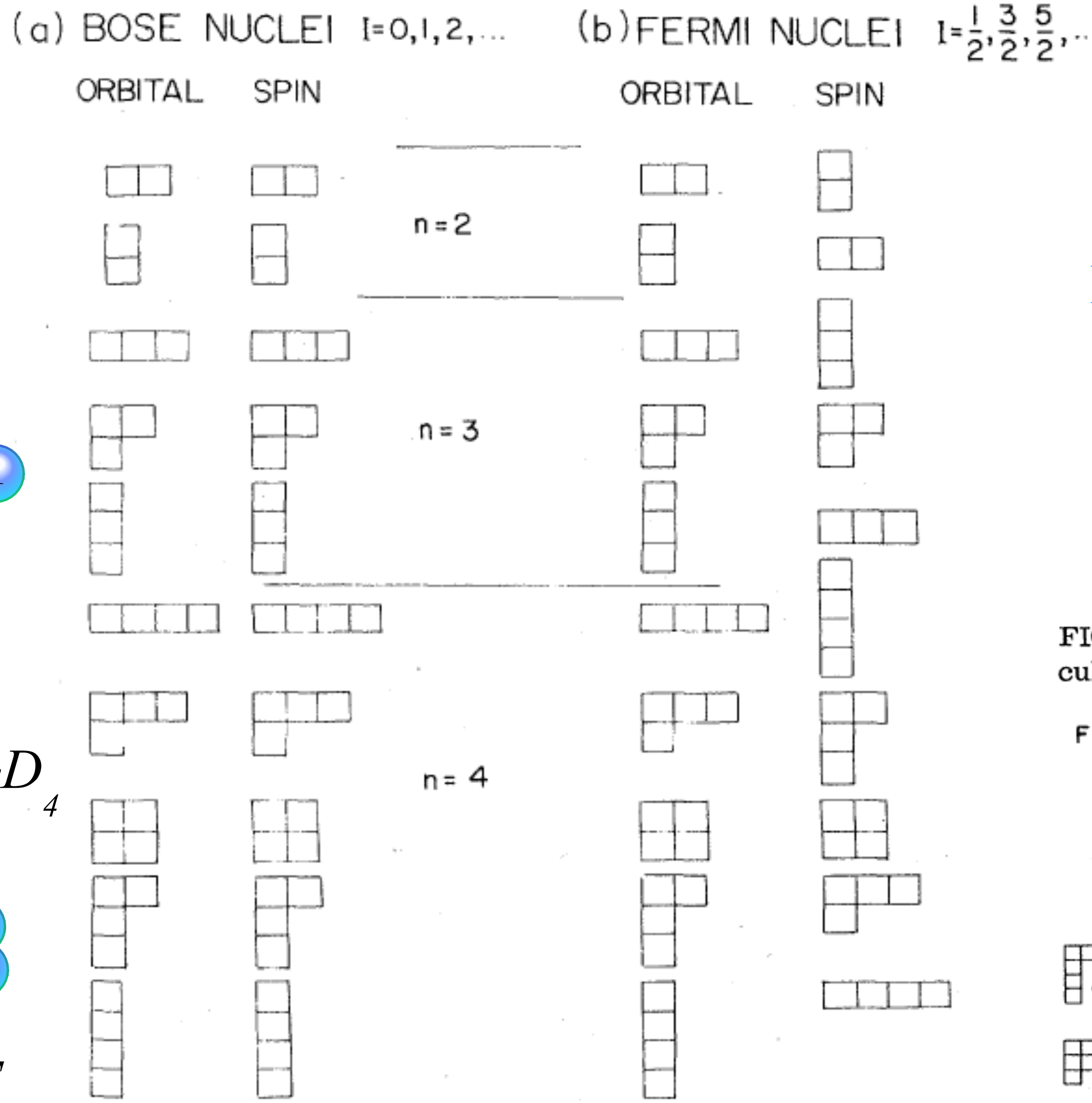
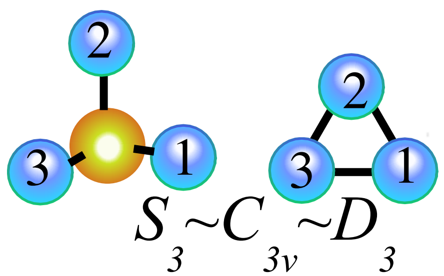
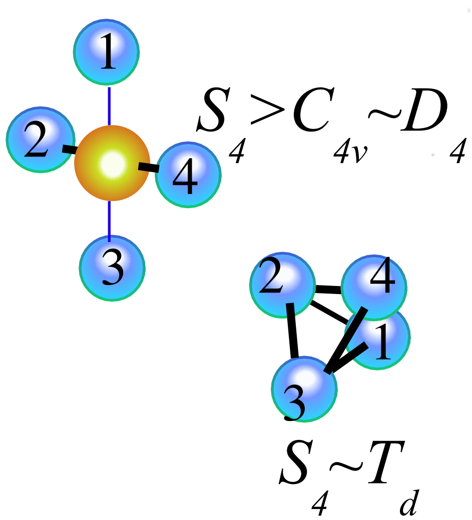


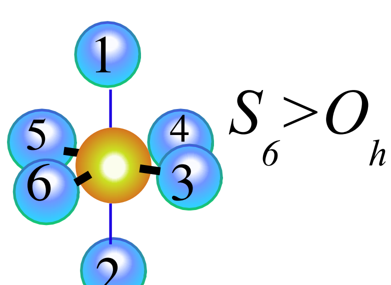
FIG. 25. Orbital tableau labeling of a homonuclear diatomic

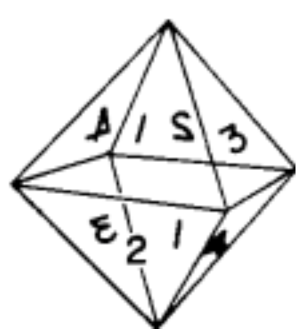
FIG. 26. Orbital and spin tableaus used to label homonuclear n-atomic molecules ($n=2,3,4,\ldots$).

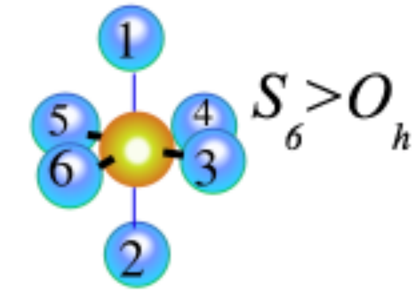












Hexa-flouride-like:XY_6

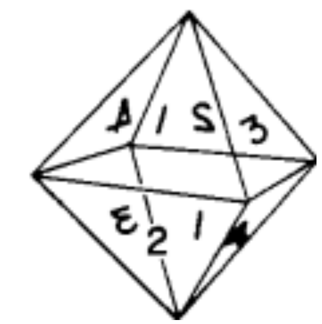
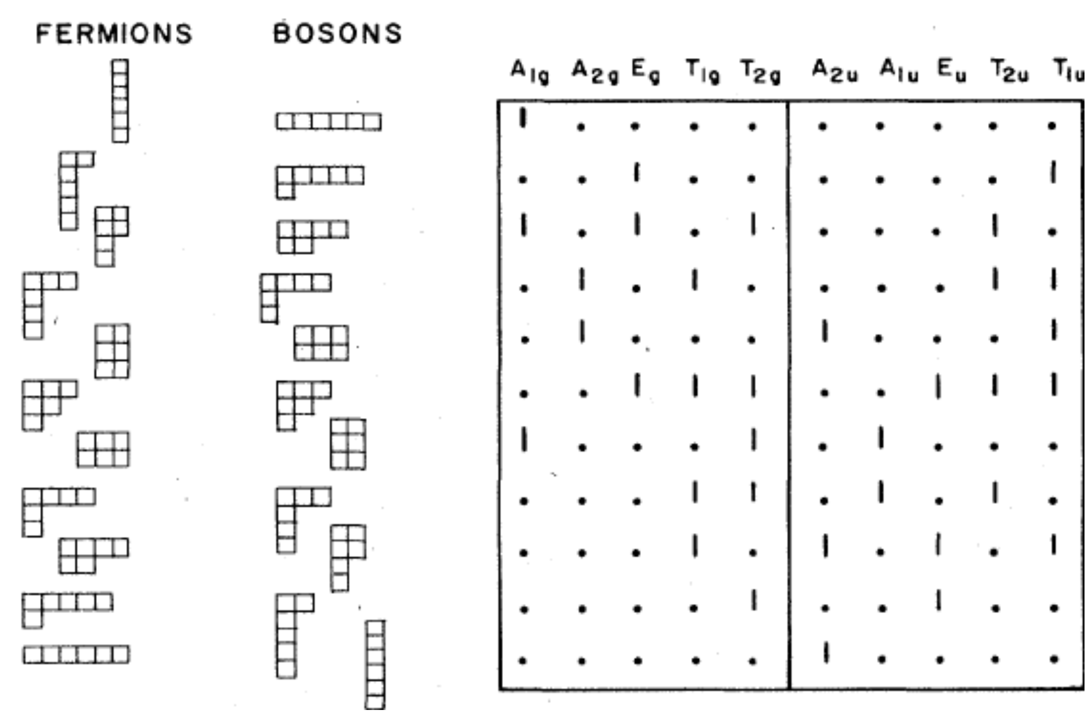


FIG. 27. Spin tableau-(B) correlation for octahedral XY_6 molecule (see Appendix D).



Rev. Mod. Phys. 50,1,1 (1978)

S_n Young Tableaus and spin-symmetry for X_n and XY_n molecules

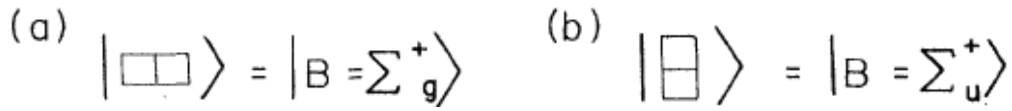
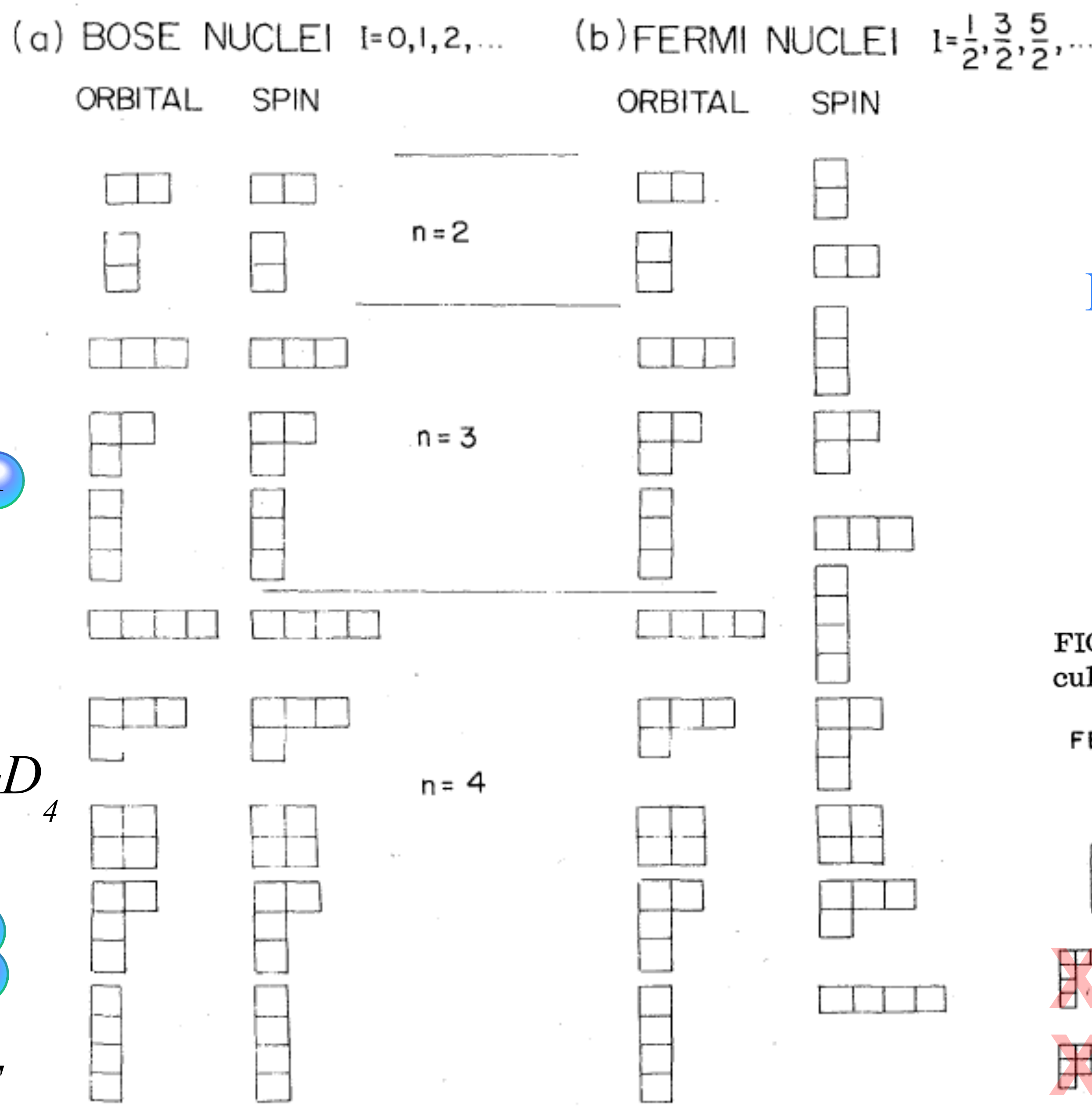
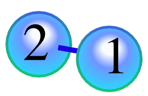


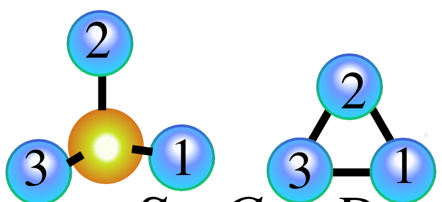
FIG. 25. Orbital tableau labeling of a homonuclear diatomic

FIG. 26. Orbital and spin tableaus used to label homonuclear n-atomic molecules ($n=2, 3, 4, \ldots$).

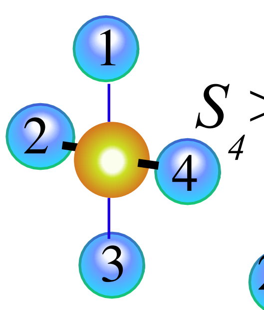




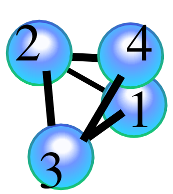
$S_2 \sim C_2$



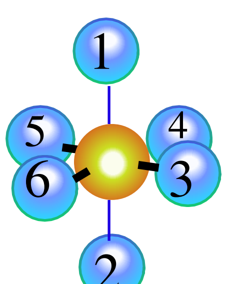
$S_3 \sim C_{3v} \sim D_3$



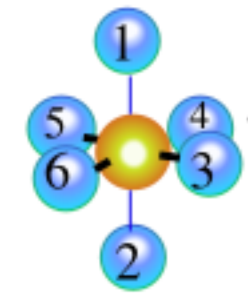
$S_4 > C_{4v} \sim D_4$



$S_4 \sim T_d$



$S_6 > O_h$



$S_6 > O_h$

Hexa-flouride-like:XY_6

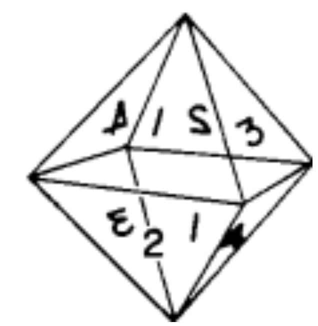
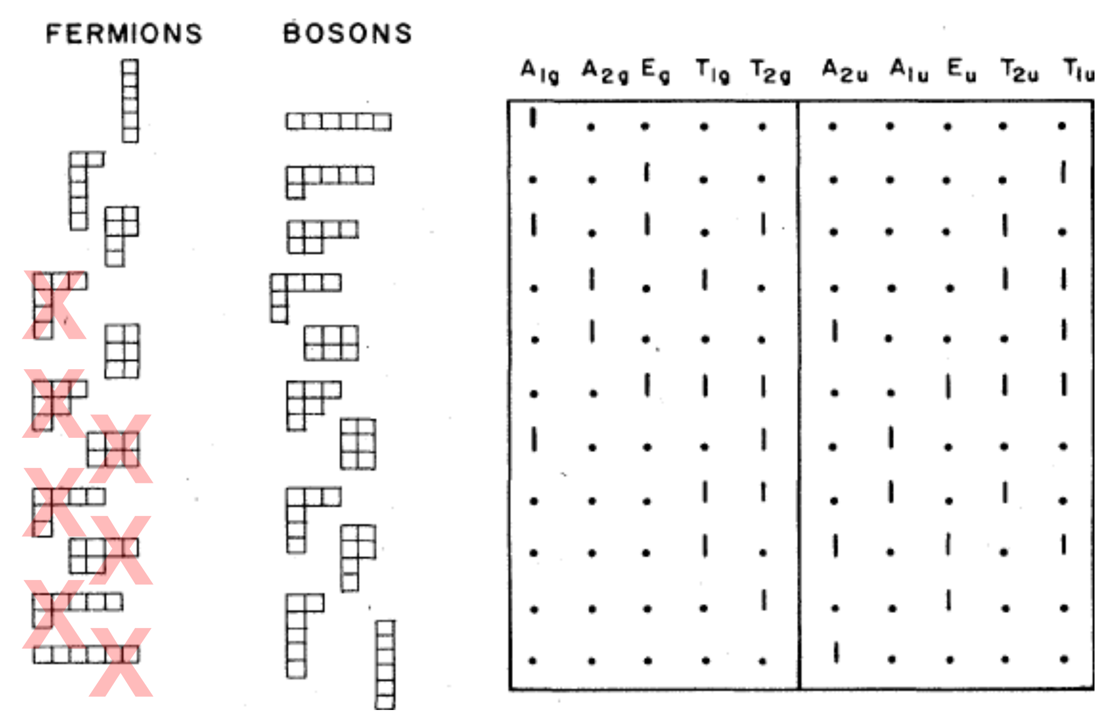


FIG. 27. Spin tableau-(B) correlation for octahedral XY_6 molecule (see Appendix D).



Compare to spin-½ case of $S_6 > O_h$ table that follows where orbit-tableau with more than 2 columns are *forbidden*

Rev. Mod. Phys. 50,1,1 (1978)

AMOP reference links on page 2

3.28.18 class 19.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

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$S_1 \subset S_2 \subset S_3 \subset S_4 \subset S_5$ …permutation symmetry algebra and spinor-rotor correlations

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S_n tableaus spin-symmetry and characters: X_n and XY_n molecules
- Tableau dimension formulae
- Methane-like XY_4 Introducing rovibrational spectral nomogram
  - Large molecule character and correlation formulae
- Hexafluoride-like:XY_6.
  - How does level clustering affect nuclear hyperfine?

Entanglement!

How F-nuclei become entangled

total-spin-I-symmetry O_h species

in SF_6.

C_4	0_4	1_4	2_4	3_4
A_1	1	.	.	.
A_2	.	.	1	.
E_1	1.	.	1	.
T_1	1	1	.	1
T_2	.	1	1	1

Spin-Permutation to Octahedral Correlations $S_6 \supset O_h$

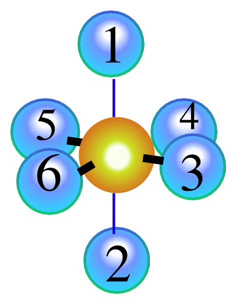
	E_u	T_{1g}	T_{1u}	T_{2g}	A_{1g}	A_{1u}	A_{2u}
I=0	.	.	.	1	1	1	.
I=1	1	1	1	.	.	.	1
I=2	1	.	.	1	.	.	.
I=3	.	.	.	.	.	.	1
Species Spin Weights	8	3	3	6	1	1	10

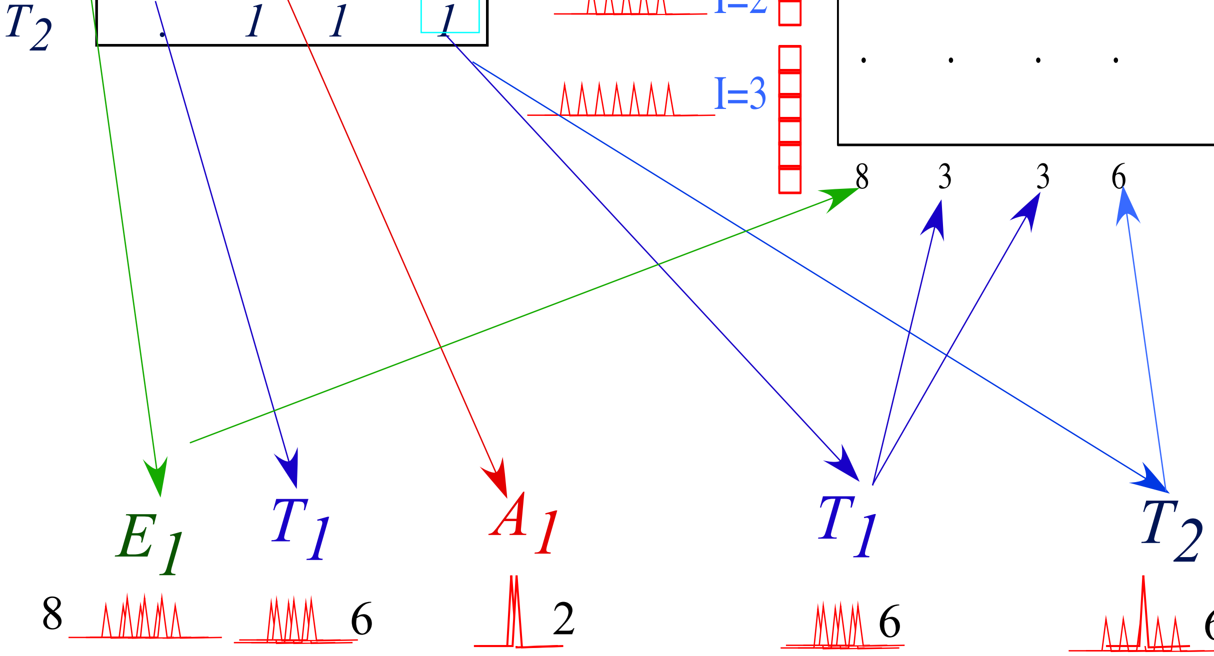
Forbidden SF_6 species: E_g, T_{2u}, A_{2g}

0 0 0

Compare to complete $S_6 > O_h$ table on p.86

With rotation all six nuclei are equivalent

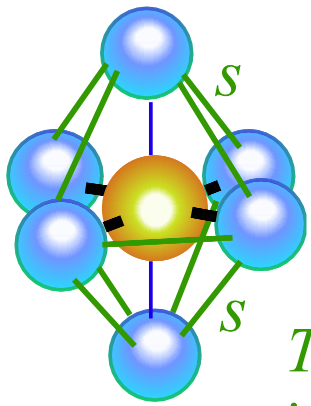




Greatly simplified sketches of ultra high resolution IR SF_6 spectroscopy of Christian Borde´, C. Saloman, and Oliver Pfister (Pfister did SiF_4, too.)

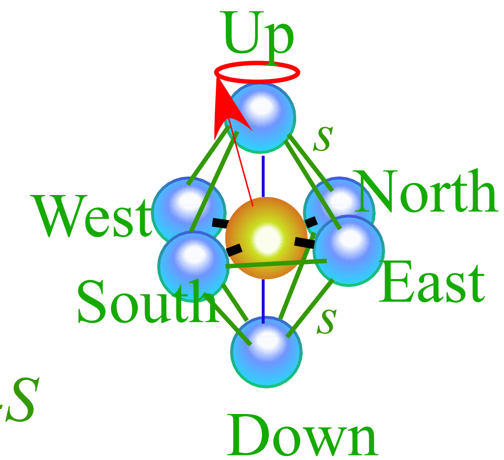
See SF_6 spectra with A_2 T_2 E level cluster that follows

S_6 and XY_6 molecules



Tunneling s=-S is negative here

*Internal **J** gets "stuck" on RES axes*
Must "tunnel" axis-to-axis at rate s



|U>|D>|E>|W>|N>|S>

$$\begin{pmatrix} H & 0 & s & s & s & s \\ 0 & H & s & s & s & s \\ s & s & H & 0 & s & s \\ s & s & 0 & H & s & s \\ s & s & s & s & H & 0 \\ s & s & s & s & 0 & H \end{pmatrix}$$

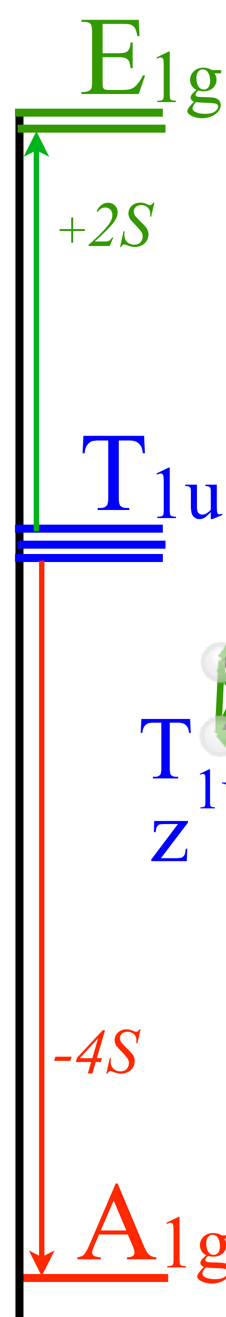
Review O(0_4)⊃C_4 cluster:

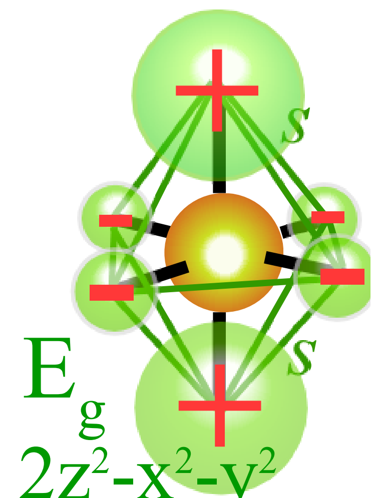
0_4 cluster splitting

$$\begin{pmatrix} H & 0 & s & s & s & s \\ 0 & H & s & s & s & s \\ s & s & H & 0 & s & s \\ s & s & 0 & H & s & s \\ s & s & s & s & H & 0 \\ s & s & s & s & 0 & H \end{pmatrix} \begin{pmatrix} +2 \\ +2 \\ -1 \\ -1 \\ -1 \\ -1 \end{pmatrix} \frac{1}{\sqrt{12}} = (H-2s) \begin{pmatrix} +2 \\ +2 \\ -1 \\ -1 \\ -1 \\ -1 \end{pmatrix} \frac{1}{\sqrt{12}}$$

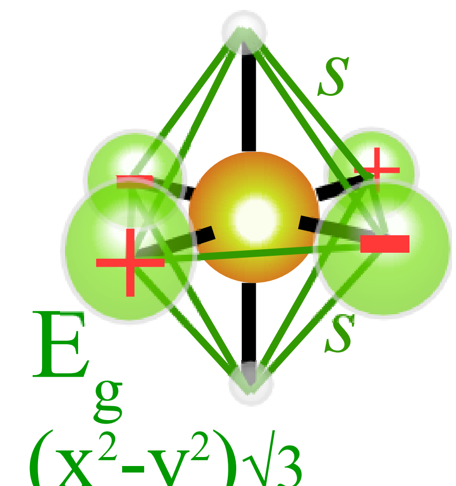
$$\begin{pmatrix} H & 0 & s & s & s & s \\ 0 & H & s & s & s & s \\ s & s & H & 0 & s & s \\ s & s & 0 & H & s & s \\ s & s & s & s & H & 0 \\ s & s & s & s & 0 & H \end{pmatrix} \begin{pmatrix} +1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \frac{1}{\sqrt{2}} = (H+0) \begin{pmatrix} +1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \frac{1}{\sqrt{2}}$$

$$\begin{pmatrix} H & 0 & s & s & s & s \\ 0 & H & s & s & s & s \\ s & s & H & 0 & s & s \\ s & s & 0 & H & s & s \\ s & s & s & s & H & 0 \\ s & s & s & s & 0 & H \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{6}} = (H+4s) \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{6}}$$

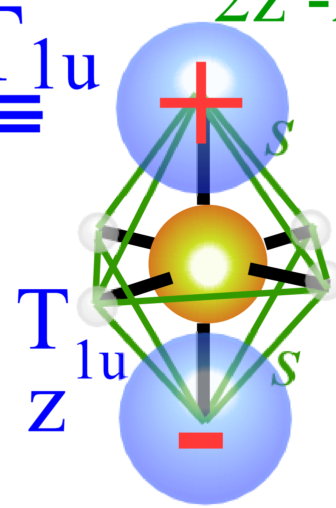




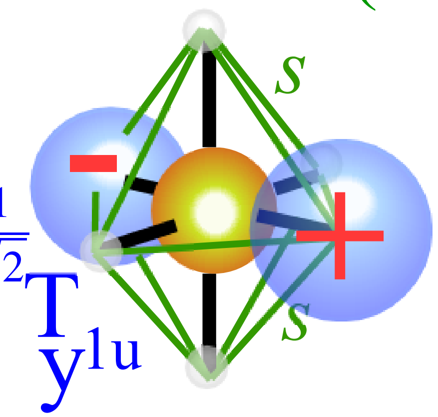
$\begin{pmatrix} +2 \\ +2 \\ -1 \\ -1 \\ -1 \\ -1 \end{pmatrix} \frac{1}{\sqrt{12}}$

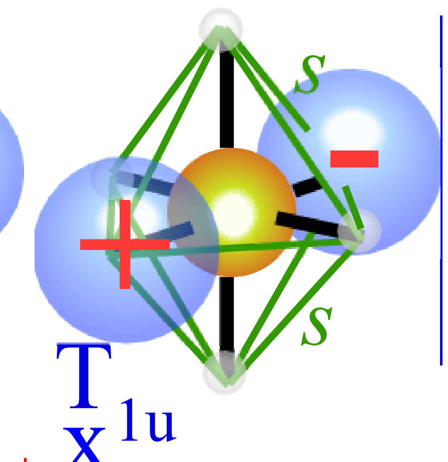


$\begin{pmatrix} 0 \\ 0 \\ -1 \\ -1 \\ +1 \\ +1 \end{pmatrix} \frac{1}{2}$

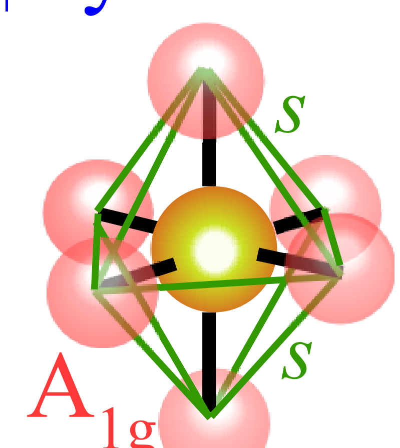


$\begin{pmatrix} 0 \\ 0 \\ +1 \\ -1 \\ 0 \\ 0 \end{pmatrix} \frac{1}{\sqrt{2}}$





$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -1 \\ +1 \end{pmatrix} \frac{1}{\sqrt{2}}$



$\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{6}}$

DISentanglement!

How F-nuclei become distinguished (but not distinguishable) in SF_6.

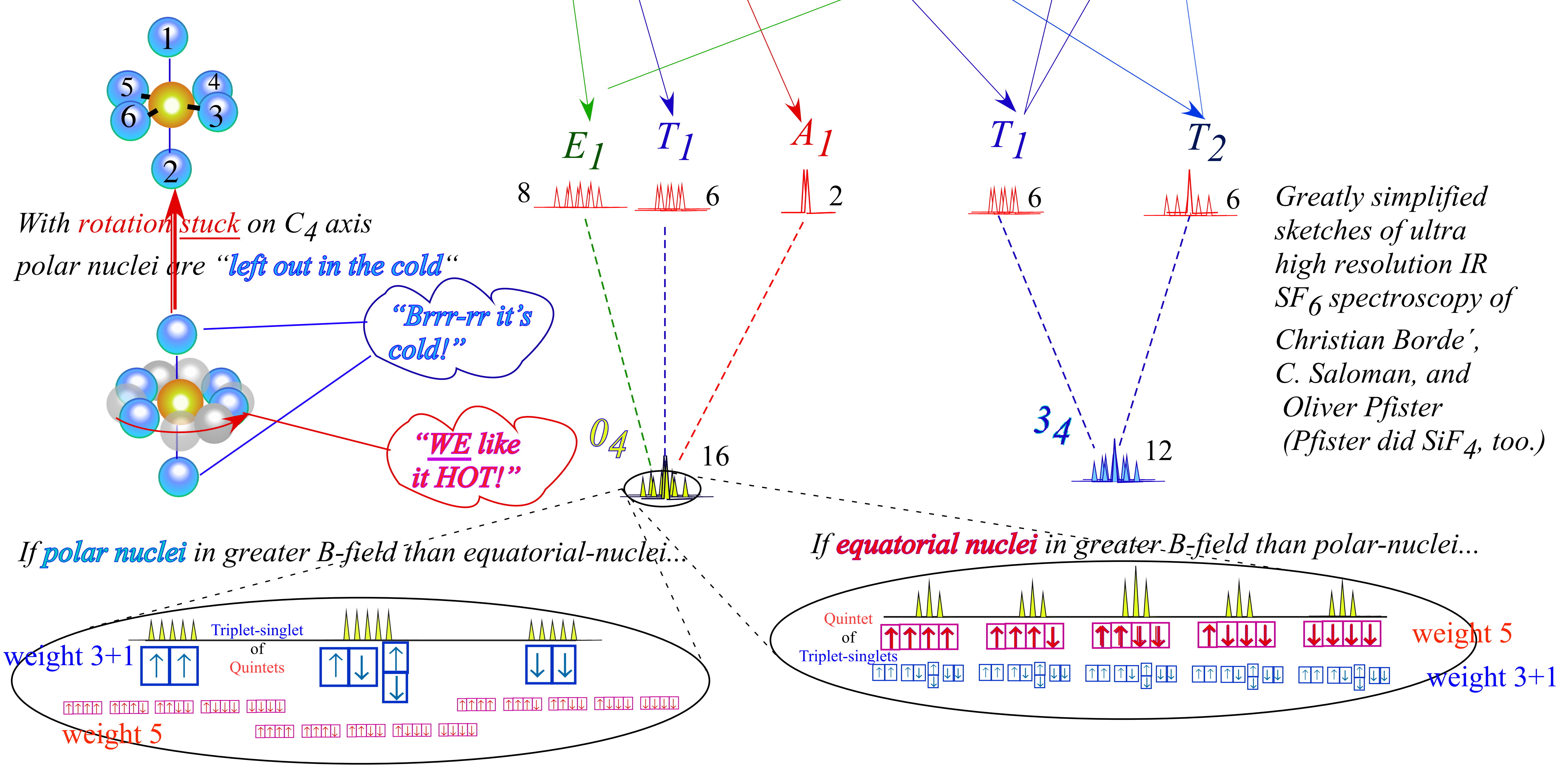
C_4	0_4	1_4	2_4	3_4
A_1	1	.	.	.
A_2	.	.	1	.
E_1	1.	.	1	.
T_1	1	1	.	1
T_2	.	1	1	1

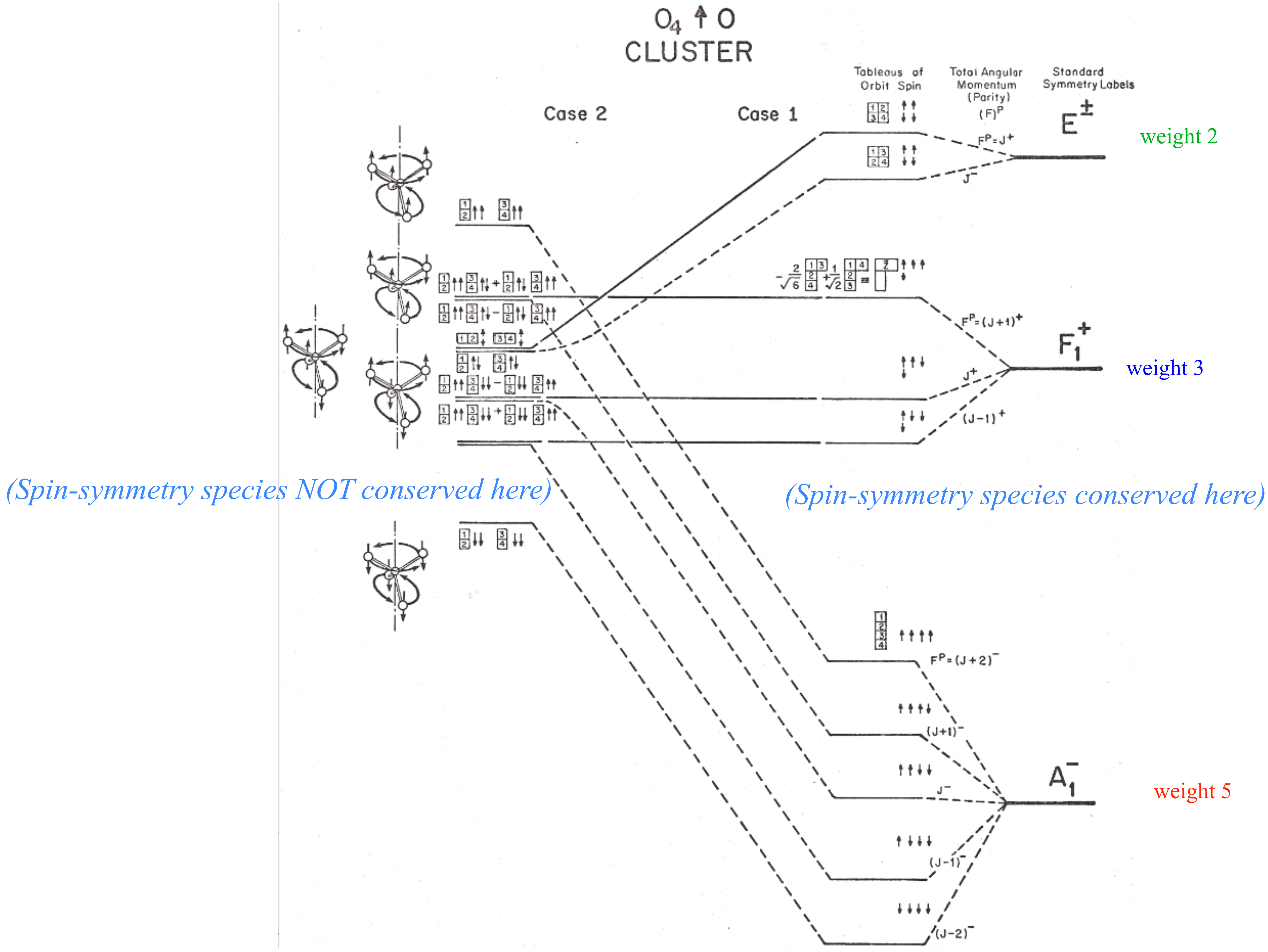
Spin-Permutation to Octahedral Correlations $S_6 \supset O_h$

Spin	E_u	T_{1g}	T_{1u}	T_{2g}	A_{1g}	A_{1u}	A_{2u}
weight 1, I=0	.	.	.	1	1	1	.
weight 3, I=1	1	1	1	.	.	.	1
weight 5, I=2	1	.	.	1	.	.	.
weight 7, I=3	.	.	.	.	.	.	1
Species Spin Weights	8	3	3	6	1	1	10

Forbidden SF_6 species: E_g, T_{2u}, A_{2g}

Without rotation being stuck on C_4 axis all six nuclei are equivalent

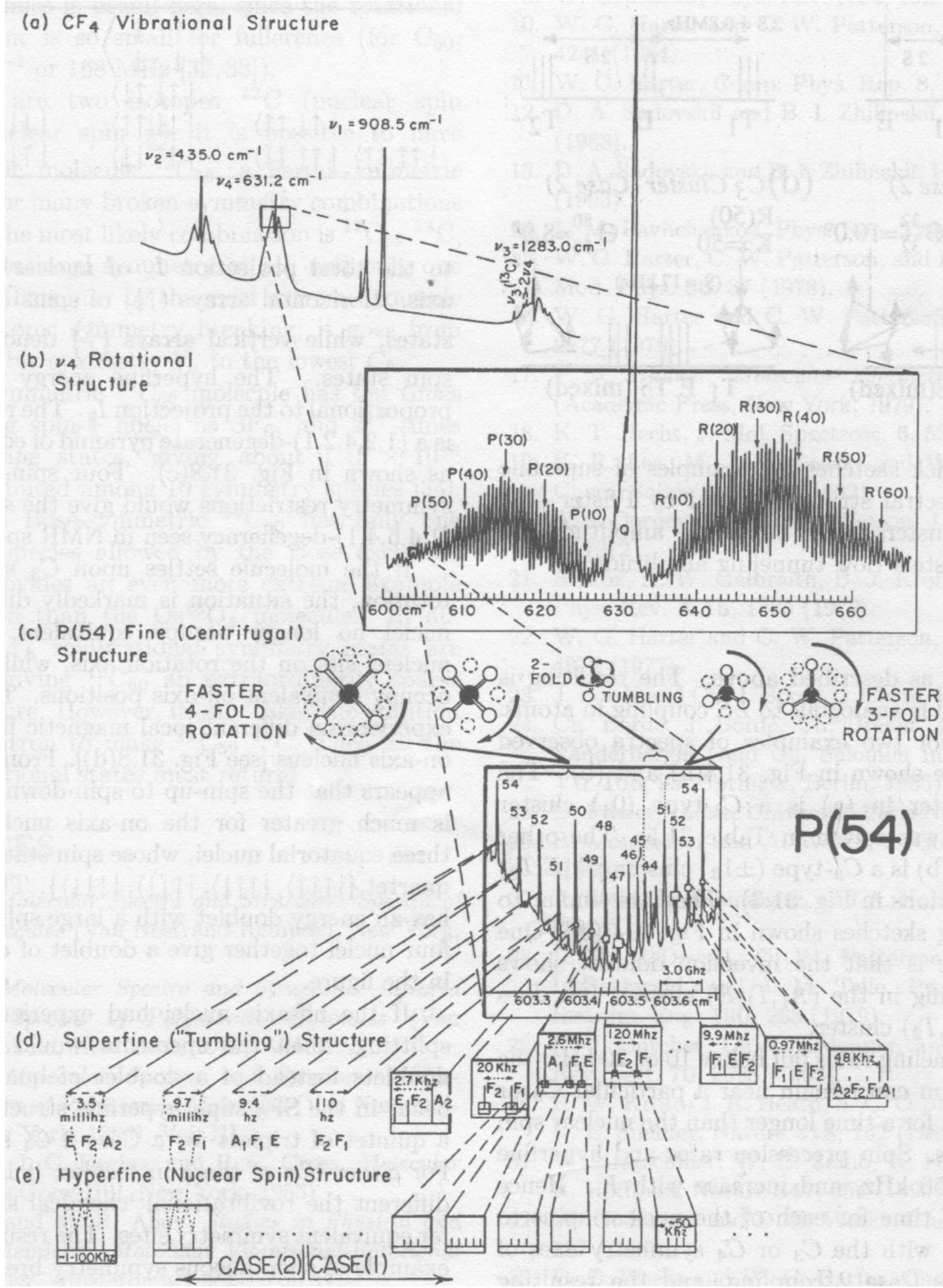


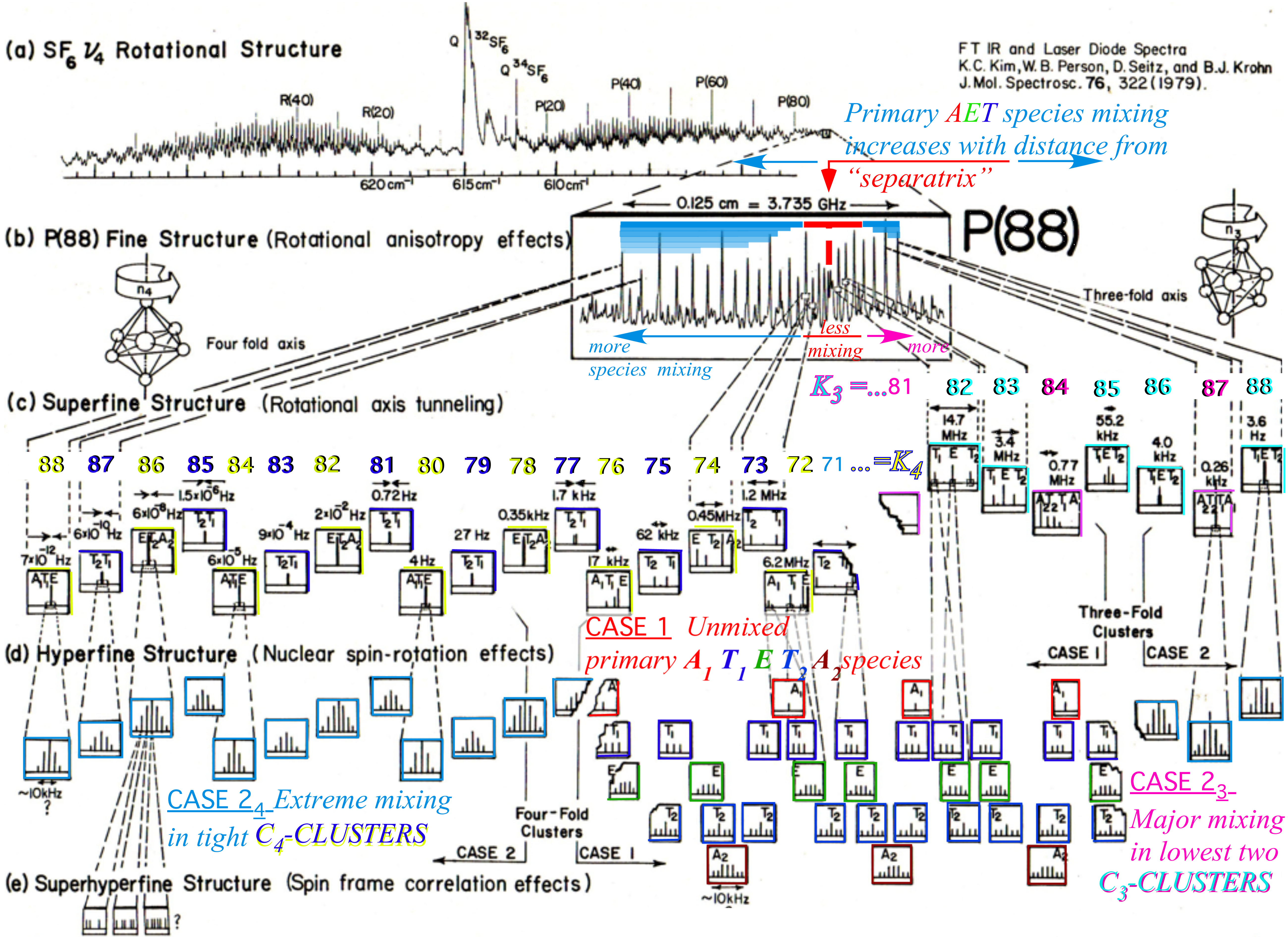


$O_4 \uparrow O$
CLUSTER
Case 2
Case 1
Tableaus of Orbit Spin
Total Angular Momentum (Parity) $(F)^P$
Standard Symmetry Labels
$E^{\pm}$
weight 2
$F^P = J^+$
J^-
$F^P = (J+1)^+$
J^+
$(J-1)^+$
F_1^+
weight 3
(Spin-symmetry species NOT conserved here)
(Spin-symmetry species conserved here)
$F^P = (J+2)^-$
$(J+1)^-$
J^-
$(J-1)^-$
$(J-2)^-$
A_1^-
weight 5

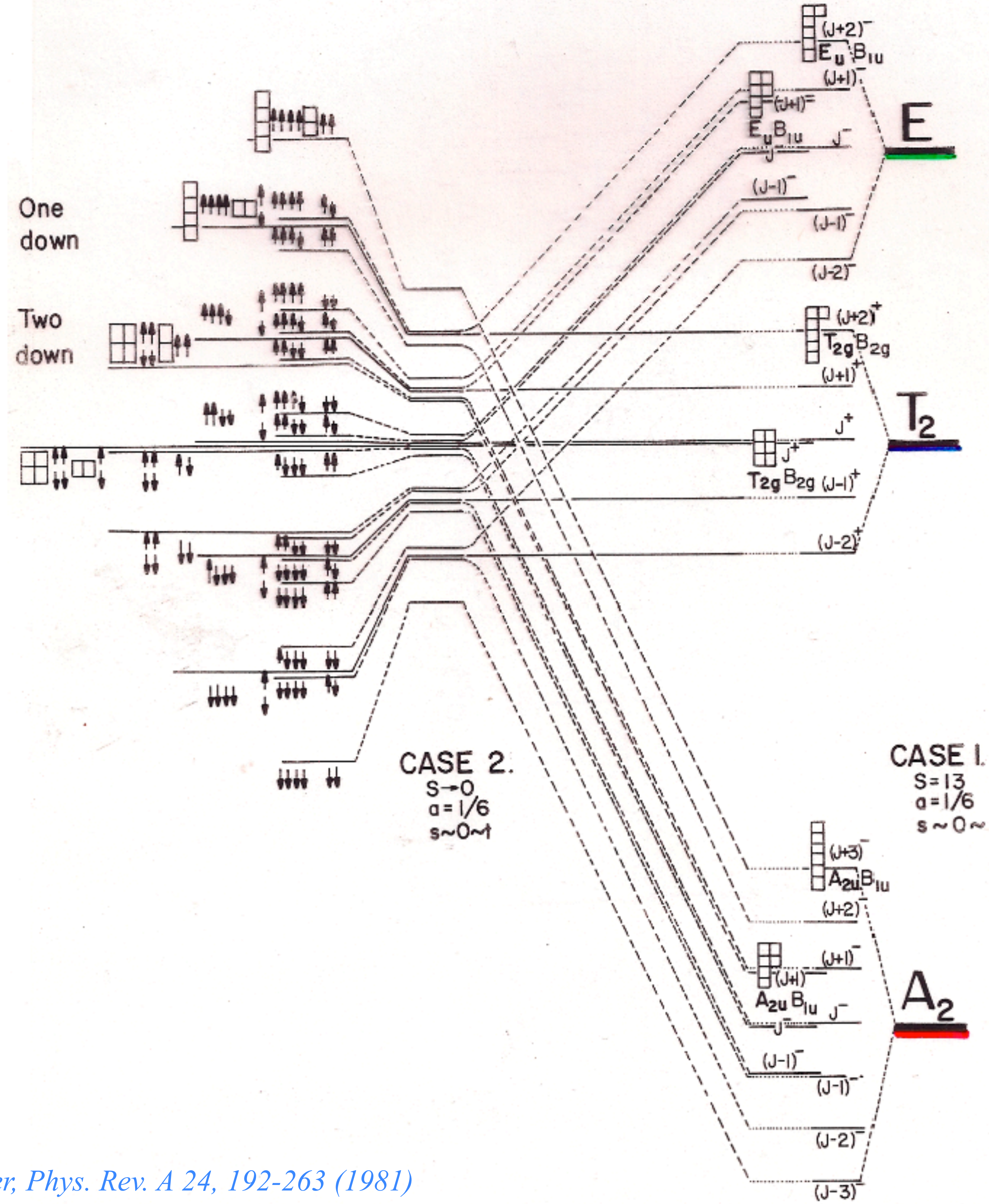
Example of frequency hierarchy for 16μm spectra of CF_4 (Freon-14)

W.G.Harter
Ch. 31
Atomic, Molecular, & Optical Physics Handbook
Am. Int. of Physics
Gordon Drake Editor
(1996)





Harter, Phys. Rev. A 24, 192-263 (1981)

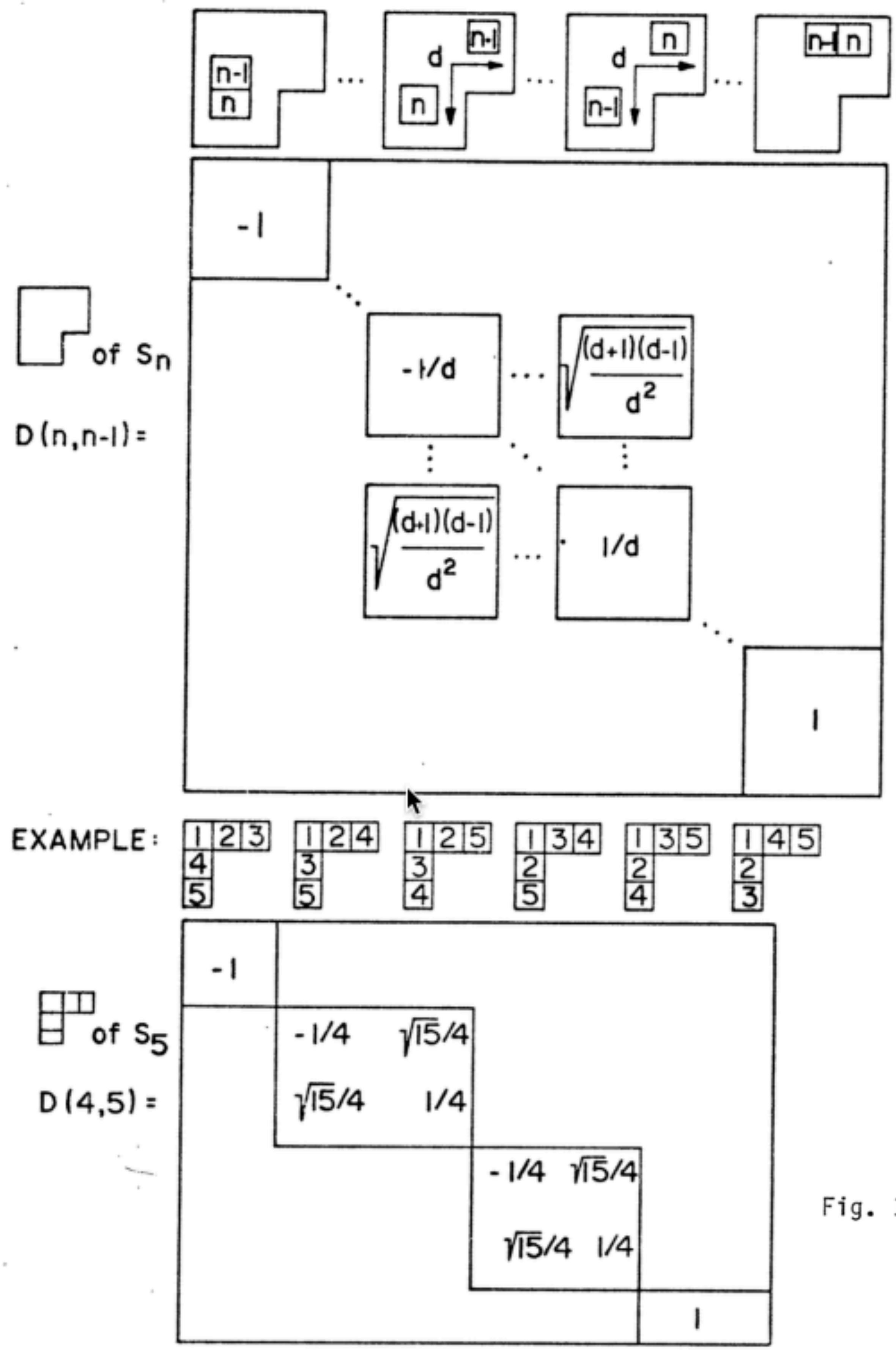


weight 8=5+3

weight 6=5+1

weight 10=7+3

Harter, Phys. Rev. A 24, 192-263 (1981)



$$D^{E}_{(\sigma_2)} = D^{[2,1]}(bc) = \begin{matrix} \begin{smallmatrix} ab \\ c \end{smallmatrix} \\ \\ \begin{smallmatrix} ac \\ b \end{smallmatrix} \end{matrix} \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ \\ \sqrt{3}/2 & 1/2 \end{pmatrix}$$

$$D^{[2,1]}(ab) = \begin{matrix} \begin{smallmatrix} ab \\ c \end{smallmatrix} \\ \\ \begin{smallmatrix} ac \\ b \end{smallmatrix} \end{matrix} \begin{pmatrix} 1 & 0 \\ \\ 0 & -1 \end{pmatrix}$$

From unpublished Ch.10 for
Principles of Symmetry, Dynamics & Spectroscopy

Fig. 10.1.2 Yamanouchi formulas for permutation operators. Integer d is the "city block" distance between (n) and (n-1) blocks, i.e., the minimum number of streets to be crossed when traveling from one to the other. Note that when numbers (n) and (n-1) are ordered smaller above larger, the permutation is negative (anti-symmetric if d=1), and positive (symmetric if d=1) when the smaller number is left of the larger number. [The (n-1) will never be above and left of (n) since that arrangement would be "non-standard."]