4.02.18 class 20: Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics

William G. Harter - University of Arkansas

Interwining  $(S_1 \subset S_2 \subset S_3 \subset S_4 \subset S_5 \dots)^* (U(1) \subset U(2) \subset U(3) \subset U(4) \subset U(5) \dots)$  algebras and tensor operator applications to spinor-rotor or orbital correlations

U(2) tensor product states and  $S_n$  permutation symmetry Rank-1 tensor (or spinor)

Rank-2 tensor (2 particles each with U(2) state space)2-particle U(2) transform and permutation operationS<sub>2</sub> symmetry of U(2): Trust but verify

Applying S<sub>2</sub> projection to build DTran Applying DTran for S<sub>2</sub> Applying DTran for U(2)

 $S_3$  permutations related to  $C_{3v}\!\!\sim\!\!D_3$  geometry

S<sub>3</sub> permutation matrices

Hooklength formula for  $S_n$  reps

S<sub>3</sub> symmetry of U(2): Applying S<sub>3</sub> projection (Note Pauli-exclusion principle basis) Building S<sub>3</sub> DTran T from projectors

Effect of S<sub>3</sub> DTran T: Introducing intertwining S<sub>3</sub> - U(2) irep matrices Multi-spin  $(1/2)^N$  product state (Comparison to previous cases)

#### 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

2014 AMOP 2017 Group Theory for QM 2018 AMOP

Classical Mechanics with a Bang!

#### Modern Physics and its Classical Foundations

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 Representaions Of Multidimensional Symmetries In Networks - harter-jmp-1973 Intro spin ½ coupling <u>Unit 8 Ch. 24 p3</u>.

*H atom hyperfine-B-level crossing* <u>Unit 8 Ch. 24 p15</u>.

Hyperf. theory Ch. 24 p48.

*Hyperf. theory Ch. 24 p48.* <u>Deeper theory ends p53</u>

> Intro 2p3p coupling <u>Unit 8 Ch. 24 p17</u>.

Intro LS-jj coupling <u>Unit 8 Ch. 24 p22</u>.

CG coupling derived (start) <u>Unit 8 Ch. 24 p39</u>. CG coupling derived (formula) <u>Unit 8 Ch. 24 p44</u>.

> Lande'g-factor <u>Unit 8 Ch. 24 p26</u>.

Irrep Tensor building <u>Unit 8 Ch. 25 p5</u>.

Irrep Tensor Tables <u>Unit 8 Ch. 25 p12</u>.

*Wigner-Eckart tensor Theorem.* <u>Unit 8 Ch. 25 p17</u>.

*Tensors Applied to d,f-levels.* <u>Unit 8 Ch. 25 p21</u>.

*Tensors Applied to high J levels.* <u>Unit 8 Ch. 25 p63</u>. *Intro 3-particle coupling.* <u>Unit 8 Ch. 25 p28</u>.

Intro 3,4-particle Young Tableaus <u>GrpThLect29 p42</u>.

Young Tableau Magic Formulae <u>GrpThLect29 p46-48</u>.

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

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U(2) tensor product states and S<sub>n</sub> permutation symmetry Rank-1 tensor (or spinor)

Rank-2 tensor (2 particles each with U(2) state space)
2-particle U(2) transform and permutation operation
S<sub>2</sub> symmetry of U(2): Trust but verify

Applying S<sub>2</sub> projection to build DTran Applying DTran for S<sub>2</sub> Applying DTran for U(2)

*U(2) tensor product states and*  $S_n$  *permutation symmetry* Typical U(2) transformations (Just like spin- $\frac{1}{2}$  irep in basis {1=+ $\frac{1}{2}$ ,1=- $\frac{1}{2}$ }) Rank-1 tensor

$$\phi_{1}' = \mathbf{u}\phi_{1} = \phi_{1}D_{11} + \phi_{2}D_{21}$$
  
where:  $D_{jk} = (\phi_{j}^{*}, \phi_{k}') = (\phi_{j}^{*}, \mathbf{u}\phi_{k})$ 

Dirac notation:

$$\begin{vmatrix} \mathbf{1'} \rangle = \mathbf{u} & |\mathbf{1}\rangle = |\mathbf{1}\rangle D_{11} + |\mathbf{2}\rangle D_{21} \\ |\mathbf{2'}\rangle = \mathbf{u} & |\mathbf{2}\rangle = |\mathbf{1}\rangle D_{12} + |\mathbf{2}\rangle D_{22} \end{aligned}$$
 where:  $D_{jk}(\mathbf{u}) = \langle j | \mathbf{k'} \rangle = \langle j | \mathbf{u} | \mathbf{k} \rangle$ 

U(2) tensor product states and  $S_n$  permutation symmetry Typical U(2) transformations (Just like spin- $\frac{1}{2}$  irep in basis {1=+ $\frac{1}{2}$ ,1=- $\frac{1}{2}$ }) Rank-1 tensor matrix representations

$$\phi_1' = \mathbf{u}\phi_1 = \phi_1 D_{11} + \phi_2 D_{21}$$
  

$$\phi_2' = \mathbf{u}\psi_2 = \phi_1 D_{12} + \phi_2 D_{22}$$
  
where:  $D_{jk} = (\phi_j^*, \phi_k') = (\phi_j^*, \mathbf{u}\phi_k)$   

$$\begin{vmatrix} 1 \rangle = \phi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
  

$$\begin{vmatrix} 2 \rangle = \phi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Dirac notation:

$$|1'\rangle = \mathbf{u} |1\rangle = |1\rangle D_{11} + |2\rangle D_{21}$$

$$|2'\rangle = \mathbf{u} |2\rangle = |1\rangle D_{12} + |2\rangle D_{22}$$
where:  $D_{jk}(\mathbf{u}) = \langle j|k'\rangle = \langle j|\mathbf{u}|k\rangle$ 

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 $\begin{array}{l} S_3 \mbox{ permutations related to $C_{3v}\sim D_3$ geometry} \\ S_3 \mbox{ permutation matrices} \\ \mbox{ Hooklength formula for $S_n$ reps} \\ S_3 \mbox{ symmetry of U(2): Applying $S_3$ projection (Note Pauli-exclusion principle basis)} \\ \mbox{ Building $S_3$ DTran $T$ from projectors} \\ \mbox{ Effect of $S_3$ DTran $T$: Introducing intertwining $S_3 - U(2)$ irep matrices} \\ \mbox{ Multi-spin (1/2)^N$ product state (Comparison to previous cases)} \end{array}$ 

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where:  $D_{jk}(\mathbf{u}) = \langle j|k'\rangle = \langle j|\mathbf{u}|k\rangle$ 

$$D_{jk}(\mathbf{u}) = \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix}$$

Rank-2 tensor (2 particles each with U(2) state space)

$$|1\rangle|1\rangle = \phi_1 \otimes \phi_1 = \begin{pmatrix} 1\\0\\0\\0 \end{pmatrix}, \ |1\rangle|2\rangle = \phi_1 \otimes \phi_2 = \begin{pmatrix} 0\\1\\0\\0 \end{pmatrix}, \ |2\rangle|1\rangle = \phi_2 \otimes \phi_1 = \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix}, \ |2\rangle|2\rangle = \phi_2 \otimes \phi_2 = \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix}$$

2-particle U(2) transform

$$|j'\rangle|k'\rangle = \mathbf{u}|j\rangle\mathbf{u}|k\rangle$$
$$= \sum_{j,k}|j\rangle|k\rangle D_{jj'}D_{kk'}$$
$$= \sum_{j,k}|j\rangle|k\rangle D\otimes D_{jk:j'k'}$$

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 where:  $D_{jk}(\mathbf{u}) = \langle j | \mathbf{k'} \rangle = \langle j | \mathbf{u} | \mathbf{k} \rangle$   $D_{jk}(\mathbf{u}) = \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix}$ 

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2-particle U(2) transform and outer-product U(2) transform matrix 
$$D_{jj'}D_{kk'} = D \otimes D_{jk;j'k'} = \\ |j'\rangle|k'\rangle = \mathbf{u}|j\rangle\mathbf{u}|k\rangle = \sum_{j,k}|j\rangle|k\rangle D_{jj'}D_{kk'} = \\ = \begin{pmatrix} D_{11}D_{11} & D_{11}D_{12} & D_{12}D_{11} & D_{12}D_{12} \\ D_{11}D_{21} & D_{11}D_{22} & D_{12}D_{21} & D_{12}D_{22} \\ D_{21}D_{11} & D_{21}D_{12} & D_{22}D_{11} & D_{22}D_{12} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{21} & D_{22}D_{22} \\ \end{pmatrix} = \begin{pmatrix} D_{11}\begin{pmatrix} D_{11} & D_{11}D_{12} & D_{12}D_{12} \\ D_{21}\begin{pmatrix} D_{11} & D_{12} & D_{12}D_{22} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{12} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{22} \\ \end{pmatrix} = \begin{pmatrix} D_{11}\begin{pmatrix} D_{11} & D_{12} & D_{12} \\ D_{11}\begin{pmatrix} D_{11} & D_{12} & D_{12} \\ D_{21}\begin{pmatrix} D_{11} & D_{12} & D_{22} \\ D_{21}\begin{pmatrix} D_{11} & D_{12} & D_{22} \\ D_{21}D_{21} & D_{22}D_{22} & D_{22}D_{22} \\ \end{pmatrix} = \begin{pmatrix} D_{11}\begin{pmatrix} D_{11} & D_{12} & D_{12} \\ D_{11}\begin{pmatrix} D_{11} & D_{12} & D_{12} \\ D_{21}\begin{pmatrix} D_{11} & D_{12} & D_{22} \\ D_{21} & D_{22} & D_{22} \\ \end{pmatrix} \end{pmatrix}$$

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 $\begin{array}{l} U(2) \ tensor \ product \ states \ and \ S_n \ permutation \ symmetry\\ \textbf{2-particle U(2) transform \ and \ outer-product U(2) \ transform \ matrix} \quad D_{jj'}D_{kk'} = D \otimes D_{jk;j'k'} = \\ |j'\rangle|k'\rangle = \mathbf{u}|j\rangle|k\rangle\\ = \sum_{j,k}|j\rangle|k\rangle D_{jj'}D_{kk'}\\ = \sum_{j,k}|j\rangle|k\rangle D \otimes D_{jk;j'k'} \end{array} \qquad = \begin{pmatrix} D_{11}D_{11} & D_{11}D_{12} & D_{12}D_{11} & D_{12}D_{12} \\ D_{11}D_{21} & D_{11}D_{22} & D_{12}D_{21} & D_{12}D_{22} \\ D_{21}D_{11} & D_{21}D_{12} & D_{22}D_{11} & D_{22}D_{12} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{21} & D_{22}D_{22} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{21} & D_{22}D_{22} \\ \end{array} \right) = \begin{pmatrix} D_{11}\begin{pmatrix}D_{11}D_{12} & D_{12}\\ D_{21}\begin{pmatrix}D_{11}D_{12} & D_{12}\\ D_{21}\begin{pmatrix}D_{11}D_{12} & D_{22}\\ D_{21}D_{22} & D_{22}\end{pmatrix} & D_{22}\begin{pmatrix}D_{11}D_{12} & D_{22}\\ D_{21}D_{21} & D_{22}\end{pmatrix} \\ \end{array} \right)$ 

 $\begin{array}{l} U(2) \ tensor \ product \ states \ and \ S_n \ permutation \ symmetry\\ \textbf{2-particle U(2) transform \ and \ outer-product U(2) \ transform \ matrix} \quad D_{jj'}D_{kk'} = D \otimes D_{jk;j'k'} = \\ |j'\rangle|k'\rangle = \textbf{u}|j\rangle \textbf{u}|k\rangle\\ = \sum_{j,k} |j\rangle|k\rangle D_{jj'}D_{kk'}\\ = \sum_{j,k} |j\rangle|k\rangle D \otimes D_{jk;j'k'} \end{array} = \begin{pmatrix} D_{11}D_{11} & D_{11}D_{12} & D_{12}D_{11} & D_{12}D_{12} \\ D_{11}D_{21} & D_{11}D_{22} & D_{12}D_{21} & D_{12}D_{22} \\ D_{21}D_{11} & D_{21}D_{12} & D_{22}D_{11} & D_{22}D_{12} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{21} & D_{22}D_{12} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{21} & D_{22}D_{22} \\ \end{array} = \begin{pmatrix} D_{11}\begin{pmatrix}D_{11} & D_{12} \\ D_{11}\begin{pmatrix}D_{11} & D_{12} \\ D_{21}\begin{pmatrix}D_{11} & D_{12} \\ D_{21}\begin{pmatrix}D_{11} & D_{12} \\ D_{21}\begin{pmatrix}D_{11} & D_{12} \\ D_{21}& D_{22}\end{pmatrix} & D_{22}\begin{pmatrix}D_{11} & D_{12} \\ D_{21}& D_{22}\end{pmatrix} \\ \end{array} \end{pmatrix}$ 

2-particle permutation operation:  $\mathbf{s}(ab)|j\rangle_{a}|k\rangle_{b} = |k\rangle_{a}|j\rangle_{b}$   $\mathbf{s}(ab)|1\rangle_{a}|1\rangle_{b} = |1\rangle_{a}|1\rangle_{b}, \mathbf{s}(ab)|1\rangle_{a}|2\rangle_{b} = |2\rangle_{a}|1\rangle_{b}, \mathbf{s}(ab)|2\rangle_{a}|1\rangle_{b} = |1\rangle_{a}|2\rangle_{b}, \mathbf{s}(ab)|2\rangle_{a}|2\rangle_{b} = |2\rangle_{a}|2\rangle_{b}$   $\mathbf{S}_{2} = \{(a)(b), (ab)\}$  represented by matrices: S((a)(b)) = S((ab)) =in basis:  $|1\rangle|1\rangle = |1\rangle|2\rangle = |2\rangle|1\rangle = |2\rangle|2\rangle = (1 \cdot \cdots )$  $\begin{pmatrix}1\\0\\0\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$ 

2-particle permutation  $\mathbf{s}(ab)$  commutes with U(2) transform matrix  $D \otimes D$ :  $\mathbf{s}(ab)D \otimes D\phi_{j}\phi_{k} = \sum_{m,n} \mathbf{s}(ab)\phi_{m}\phi_{n}D_{jm}D_{kn} = \sum_{m,n}\phi_{n}\phi_{m}D_{jm}D_{kn} = \sum_{m,n}\phi_{n}\phi_{m}D_{kn}D_{jm} = D \otimes D\phi_{k}\phi_{j} = D \otimes D\mathbf{s}(ab)\phi_{j}\phi_{k}$   $\begin{array}{l} U(2) \ tensor \ product \ states \ and \ S_n \ permutation \ symmetry \\ \textbf{2-particle U(2) transform \ and \ outer-product U(2) \ transform \ matrix \ D_{jj'}D_{kk'} = D \otimes D_{jk;j'k'} = \\ |j'\rangle|k'\rangle = \textbf{u}|j\rangle \textbf{u}|k\rangle \\ = \sum_{j,k} |j\rangle|k\rangle D_{jj'}D_{kk'} \\ = \sum_{j,k} |j\rangle|k\rangle D \otimes D_{jk;j'k'} \end{array} = \begin{pmatrix} D_{11}D_{11} \ D_{11}D_{12} \ D_{12}D_{12} \ D_{12}D_{21} \ D_{12}D_{21} \ D_{12}D_{22} \ D_{22}D_{11} \ D_{22}D_{22} \ D_{22}D_{11} \ D_{22}D_{22} \ D_{22}D_{21} \ D_{22}D_{22} \ D_{21}D_{22} \ D_{22}D_{22} \ D_{21}D_{22} \ D_{22}D_{22} \ D_{22}D_{22}D_{22} \ D_{22}D_{22} \ D_{22}D_{22} \ D_{22}D_{22} \ D_{2$ 

2-particle permutation operation:  $\mathbf{s}(ab)|j\rangle_{a}|k\rangle_{b} = |k\rangle_{a}|j\rangle_{b}$   $\mathbf{s}(ab)|1\rangle_{a}|1\rangle_{b} = |1\rangle_{a}|1\rangle_{b}, \mathbf{s}(ab)|1\rangle_{a}|2\rangle_{b} = |2\rangle_{a}|1\rangle_{b}, \mathbf{s}(ab)|2\rangle_{a}|1\rangle_{b} = |1\rangle_{a}|2\rangle_{b}, \mathbf{s}(ab)|2\rangle_{a}|2\rangle_{b} = |2\rangle_{a}|2\rangle_{b}$   $\mathbf{S}_{2}=\{(a)(b), (ab)\}$  represented by matrices:  $\mathbf{s}((a)(b)) = \mathbf{s}((ab)) =$ in basis:  $|1\rangle|1\rangle = |1\rangle|2\rangle = |2\rangle|1\rangle = |2\rangle|2\rangle = (1 \cdot \cdots + 1) \cdot (1 \cdot \cdots + 1)$ 

2-particle permutation  $\mathbf{s}(ab)$  commutes with U(2) transform matrix  $D \otimes D$ :  $\mathbf{s}(ab)D \otimes D\phi_{j}\phi_{k} = \sum_{m,n} \mathbf{s}(ab)\phi_{m}\phi_{n}D_{jm}D_{kn} = \sum_{m,n}\phi_{n}\phi_{m}D_{jm}D_{kn} = \sum_{m,n}\phi_{n}\phi_{m}D_{kn}D_{jm} = D \otimes D\phi_{k}\phi_{j} = D \otimes D\mathbf{s}(ab)\phi_{j}\phi_{k}$   $\mathbf{s}(ab)D \otimes D = D \otimes D\mathbf{s}(ab)$   $\begin{array}{l} U(2) \ tensor \ product \ states \ and \ S_n \ permutation \ symmetry \\ \textbf{2-particle U(2) transform \ and \ outer-product U(2) \ transform \ matrix \ D_{jj'}D_{kk'} = D \otimes D_{jk;j'k'} = \\ |j'\rangle|k'\rangle = \textbf{u}|j\rangle|\textbf{u}|k\rangle \\ = \sum_{j,k}|j\rangle|k\rangle D_{jj'}D_{kk'} \\ = \sum_{j,k}|j\rangle|k\rangle D \otimes D_{jk;j'k'} \end{array} = \begin{pmatrix} D_{11}D_{11} \ D_{11}D_{12} \ D_{12}D_{12} \ D_{12}D_{11} \ D_{12}D_{12} \ D_{12}D_{12} \ D_{12}D_{12} \ D_{12}D_{12} \ D_{12}(D_{11}D_{12}) \$ 

2-particle permutation operation:  $\mathbf{s}(ab)|j\rangle_{a}|k\rangle_{b} = |k\rangle_{a}|j\rangle_{b}$   $\mathbf{s}(ab)|1\rangle_{a}|1\rangle_{b} = |1\rangle_{a}|1\rangle_{b}, \mathbf{s}(ab)|1\rangle_{a}|2\rangle_{b} = |2\rangle_{a}|1\rangle_{b}, \mathbf{s}(ab)|2\rangle_{a}|1\rangle_{b} = |1\rangle_{a}|2\rangle_{b}, \mathbf{s}(ab)|2\rangle_{a}|2\rangle_{b} = |2\rangle_{a}|2\rangle_{b}$   $\mathbf{S}_{2} = \{(a)(b), (ab)\}$  represented by matrices:  $\mathbf{s}((a)(b)) = \mathbf{s}((ab)) =$ in basis:  $|1\rangle|1\rangle = |1\rangle|2\rangle = |2\rangle|1\rangle = |2\rangle|2\rangle =$  $\begin{pmatrix}1 & \cdots & 1 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix}0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix}0 & 0 & 0 \\$ 

2-particle permutation  $\mathbf{s}(ab)$  commutes with U(2) transform matrix  $D \otimes D$ :  $\mathbf{s}(ab)D \otimes D\phi_{j}\phi_{k} = \sum_{m,n} \mathbf{s}(ab)\phi_{m}\phi_{n}D_{jm}D_{kn} = \sum_{m,n}\phi_{n}\phi_{m}D_{jm}D_{kn} = \sum_{m,n}\phi_{n}\phi_{m}D_{kn}D_{jm} = D \otimes D\phi_{k}\phi_{j} = D \otimes D\mathbf{s}(ab)\phi_{j}\phi_{k}$ So  $\mathbf{S}_{2} = \{\mathbf{s}(ab)\}$  is symmetry of U(2)...  $\mathbf{s}(ab)D \otimes D = D \otimes D\mathbf{s}(ab)$  ...and vice-versa!

4.02.18 class 20: Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics

William G. Harter - University of Arkansas

Interwining  $(S_1 \subset S_2 \subset S_3 \subset S_4 \subset S_5 \dots)^* (U(1) \subset U(2) \subset U(3) \subset U(4) \subset U(5) \dots)$  algebras and tensor operator applications to spinor-rotor or orbital correlations

U(2) tensor product states and S<sub>n</sub> permutation symmetry Rank-1 tensor (or spinor)

Rank-2 tensor (2 particles each with U(2) state space)
2-particle U(2) transform and permutation operation
S<sub>2</sub> symmetry of U(2): Trust but verify

Applying S<sub>2</sub> projection to build DTran Applying DTran for S<sub>2</sub> Applying DTran for U(2)

S<sub>3</sub> permutations related to C<sub>3v</sub>~D<sub>3</sub> geometry
S<sub>3</sub> permutation matrices
Hooklength formula for S<sub>n</sub> reps
S<sub>3</sub> symmetry of U(2): Applying S<sub>3</sub> projection (Note Pauli-exclusion principle basis)
Building S<sub>3</sub> DTran T from projectors
Effect of S<sub>3</sub> DTran T: Introducing intertwining S<sub>3</sub> - U(2) irep matrices
Multi-spin (1/2)<sup>N</sup> product state (Comparison to previous cases)

It might help to matrix-verify the S<sub>2</sub> symmetry of 2-particle U(2) transformations

$S((ab)) \cdot D \otimes D$	?=?	$D \otimes D \cdot S((ab))$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{c} {}_{2}D_{12} \\ {}_{2}D_{22} \\ {}_{2}D_{12} \\ {}_{2}D_{22} \end{array} \end{array} \begin{array}{c} ? \\ = \\ ? \\ {}_{2}D_{12} \\ {}_{2}D_{22} \end{array} \end{array} \begin{array}{c} ? \\ = \\ ? \\ D_{21}D_{11} \\ D_{21}D_{21} \\ D_{21}D_{12} \\ D_{21}D_{21} \\ D_{21}D_{22} \end{array}$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$

It might help to matrix-verify the  $S_2$  symmetry of 2-particle U(2) transformations

S((ab))	$\cdot D \otimes D$				?=?				$D \otimes D$	$\cdot S((ab))$	
$ \left(\begin{array}{ccccccccc} 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \end{array}\right) $ (mid-rows)	$ \begin{pmatrix} D_{11}D_{11} \\ -D_{11}D_{21} \\ -D_{21}D_{11} \\ D_{21}D_{21} \end{pmatrix} $	$egin{array}{llllllllllllllllllllllllllllllllllll$	$D_{12}D_{11}$ $D_{12}D_{21}$ $D_{22}D_{11}$ $D_{22}D_{21}$	$ \begin{array}{c} D_{12}D_{12} \\ D_{12}D_{22} \\ D_{22}D_{12} \\ D_{22}D_{22} \end{array} $	? = ?	$\begin{pmatrix} D_{11}D_{11} & D_{11} \\ D_{11}D_{21} & D_{11} \\ D_{21}D_{11} & D_{21} \\ D_{21}D_{11} & D_{21} \\ D_{21}D_{21} & D_{21} \end{pmatrix}$	$D_{12}$	$D_{12}D_{11} \\ D_{12}D_{21} \\ D_{22}D_{11} \\ D_{22}D_{21} \\ \dots \\ $	$ \begin{array}{c} D_{12}D_{12} \\ D_{12}D_{22} \\ D_{22}D_{12} \\ D_{22}D_{22} \end{array} $	$ \left(\begin{array}{ccc} 1 & \cdot \\ \cdot & \cdot \\ \cdot & 1 \\ \cdot & \cdot \\ \cdot $	$\left.\begin{array}{c} \cdot & \cdot \\ 1 & \cdot \\ \cdot & \cdot \\ \cdot & 1 \end{array}\right)$
switched)	$\begin{array}{c} D_{11}D_{11} \\ D_{21}D_{11} \\ D_{11}D_{21} \\ D_{21}D_{21} \\ D_{21}D_{21} \end{array}$	$egin{array}{llllllllllllllllllllllllllllllllllll$	$egin{array}{llllllllllllllllllllllllllllllllllll$	$D_{12}D_{12} \\ D_{22}D_{12} \\ D_{12}D_{22} \\ D_{22}D_{22} \\ D_{22}D_{2} \\ D_{22}D_{2} \\ D_{2}D_{2} \\ D_{2}D_{2} \\ D_{2}D_{2}$	) =	$\begin{pmatrix} D_{11}D_{11} & D_{1} \\ D_{11}D_{21} & D_{1} \\ D_{21}D_{11} & D_{2} \\ D_{21}D_{11} & D_{2} \end{pmatrix}$	$D_{12}D_{11}$ $D_{12}D_{21}$ $D_{22}D_{11}$ $D_{22}D_{21}$	$D_{11}D_{12}$ $D_{11}D_{22}$ $D_{21}D_{12}$ $D_{21}D_{22}$	$D_{12}D_{12} \\ D_{12}D_{22} \\ D_{22}D_{12} \\ D_{22}D_{22} $		.ciica)

It might help to matrix-verify the S<sub>2</sub> symmetry of 2-particle U(2) transformations

 $S((ab)) \cdot D \otimes D$  $D \otimes D \cdot S((ab))$ ... but the matrices are numerically equal.

So  $S_2$ -symmetry of 2-particle U(2) tensor representation is verified.

It might help to matrix-verify the S<sub>2</sub> symmetry of 2-particle U(2) transformations

 $S((ab)) \cdot D \otimes D \qquad ?=? \qquad D \otimes D \cdot S((ab))$   $\begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & 1 & - & \cdot \\ \cdot & 2_1D_{11} & D_{21}D_{12} & D_{22}D_{11} & D_{22}D_{12} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{21} & D_{22}D_{22} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{21} & D_{22}D_{22} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{11} & D_{12}D_{12} \\ D_{21}D_{21} & D_{11}D_{22} & D_{12}D_{21} & D_{12}D_{22} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{11} & D_{22}D_{12} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{21} & D_{22}D_{22} \\ D_{21}D_{21} & D_{22}D_{22} & D_{22}D$ 

... but the matrices <u>are</u> numerically equal.

So  $S_2$ -symmetry of 2-particle U(2) tensor representation is verified.

So also is S<sub>2</sub>-symmetry of any 2-particle U(m) tensor. Showing S<sub>3</sub>-symmetry of any 3-particle U(m) tensor is treated later. S<sub>4</sub> 4

$S((ab)) \cdot D \otimes D \cdot S((ab))$ $\begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 \end{pmatrix} \begin{pmatrix} D_{11}D_{11} & D_{11}D_{12} & D_{12}D_{11} & D_{12}D_{12} \\ D_{11}D_{21} & D_{11}D_{22} & D_{12}D_{21} & D_{12}D_{22} \\ D_{21}D_{11} & D_{21}D_{12} & D_{22}D_{11} & D_{22}D_{12} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{21} & D_{22}D_{22} \end{pmatrix} \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \end{pmatrix}$	If <i>S(ab)</i> commuted with $D \otimes D$ you might assume it passes thru to give <i>S(ab) S(ab)</i> =1 leaving $D \otimes D$ unchanged. That is true numerically, but all components have flipped order.
$ \begin{pmatrix} D_{11}D_{11} & D_{11}D_{12} & D_{12}D_{11} & D_{12}D_{12} \\ D_{21}D_{11} & D_{21}D_{12} & D_{22}D_{11} & D_{22}D_{12} \\ D_{11}D_{21} & D_{11}D_{22} & D_{12}D_{21} & D_{12}D_{22} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{21} & D_{22}D_{22} \end{pmatrix} \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \end{pmatrix} = \begin{pmatrix} D_{11}D_{11} & D_{12}D_{11} \\ D_{21}D_{11} & D_{22}D_{11} \\ D_{11}D_{21} & D_{12}D_{21} \\ D_{21}D_{21} & D_{22}D_{21} \end{pmatrix} $	$ \begin{array}{ccc} D_{11}D_{12} & D_{12}D_{12} \\ D_{21}D_{12} & D_{22}D_{12} \\ D_{11}D_{22} & D_{12}D_{22} \\ D_{21}D_{22} & D_{22}D_{22} \end{array} \end{array} \begin{array}{c} \text{Each} \\ D_{ab}D_{cd} \\ \text{has become} \\ D_{cd}D_{ab} \end{array} $
$S((ab)) \cdot D \otimes D \cdot S((ab))$ $\begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \end{pmatrix} \begin{pmatrix} D_{11}D_{11} & D_{11}D_{12} & D_{12}D_{11} & D_{12}D_{12} \\ D_{11}D_{21} & D_{11}D_{22} & D_{12}D_{21} & D_{12}D_{22} \\ D_{21}D_{11} & D_{21}D_{12} & D_{22}D_{11} & D_{22}D_{12} \\ D_{21}D_{21} & D_{21}D_{22} & D_{22}D_{21} & D_{22}D_{22} \end{pmatrix} \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \end{pmatrix}$	
$= \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \end{pmatrix} \begin{pmatrix} D_{11}D_{11} & D_{12}D_{11} & D_{11}D_{12} & D_{12}D_{12} \\ D_{11}D_{21} & D_{12}D_{21} & D_{11}D_{22} & D_{12}D_{22} \\ D_{21}D_{11} & D_{22}D_{11} & D_{21}D_{12} & D_{22}D_{12} \\ D_{21}D_{21} & D_{22}D_{21} & D_{21}D_{22} & D_{22}D_{22} \end{pmatrix} = \begin{pmatrix} D_{11}D_{11} & D_{12}D_{12} & D_{12}D_{12} \\ D_{21}D_{11} & D_{22}D_{12} & D_{22}D_{12} \\ D_{21}D_{21} & D_{22}D_{21} & D_{21}D_{22} & D_{22}D_{22} \end{pmatrix}$	$ \begin{array}{cccc} D_{11} & D_{11}D_{12} & D_{12}D_{12} \\ D_{11} & D_{21}D_{12} & D_{22}D_{12} \\ D_{21} & D_{11}D_{22} & D_{12}D_{22} \\ D_{21} & D_{21}D_{22} & D_{22}D_{22} \end{array} $

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4.02.18 class 20: Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics

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Interwining  $(S_1 \subset S_2 \subset S_3 \subset S_4 \subset S_5 \dots)^* (U(1) \subset U(2) \subset U(3) \subset U(4) \subset U(5) \dots)$  algebras and tensor operator applications to spinor-rotor or orbital correlations

U(2) tensor product states and S<sub>n</sub> permutation symmetry Rank-1 tensor (or spinor)

Rank-2 tensor (2 particles each with U(2) state space) 2-particle U(2) transform and permutation operation S<sub>2</sub> symmetry of U(2): Trust but verify

Applying S<sub>2</sub> projection to build DTran Applying DTran for S<sub>2</sub> Applying DTran for U(2)

 $S_2$  matrix eigen-solution found by projectors: Minimal eq. (ab)<sup>2</sup>-1=0=((ab)+1)((ab)+1) yields:

Symmetric ( ):  $\mathbf{P}^{\square} = \frac{1}{2} [1 + (\mathbf{ab})]$  Anti-Symmetric ( ):  $\mathbf{P}^{\square} = \frac{1}{2} [1 - (\mathbf{ab})]$ 

 $S_2$  matrix eigen-solution found by projectors: Minimal eq. (ab)<sup>2</sup>-1=0=((ab)+1)((ab)+1) yields:

Symmetric ( 
$$\Box$$
 ):  $\mathbf{P}^{\Box\Box} = \frac{1}{2} [1 + (ab)]$ 

Matrix representations of projectors:

$$S(\mathbf{P}^{\Box\Box}) = \frac{1}{2} \Big[ S(\mathbf{1}) + S(\mathbf{ab}) \Big] = \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{2} & \frac{1}{2} & \cdot \\ \cdot & \frac{1}{2} & \frac{1}{2} & \cdot \\ \cdot & \frac{1}{2} & \frac{1}{2} & \cdot \\ \cdot & \cdot & 1 \end{pmatrix}$$

Anti-Symmetric ( $\square$ ):  $\mathbf{P}^{\square} = \frac{1}{2} [\mathbf{1} - (\mathbf{ab})]$ 

$$S(\mathbf{P}^{\square}) = \frac{1}{2} \left[ S(\mathbf{1}) - S(\mathbf{ab}) \right] = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{2} & \frac{-1}{2} & \cdot \\ \cdot & \frac{-1}{2} & \frac{1}{2} & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

 $S_2$  matrix eigen-solution found by projectors: Minimal eq. (ab)<sup>2</sup>-1=0=((ab)+1)((ab)+1) yields:

Symmetric ( ): 
$$\mathbf{P}^{\square} = \frac{1}{2} [1 + (\mathbf{ab})]$$
 Anti-Symmetric ( ):  $\mathbf{P}^{\square} = \frac{1}{2} [1 - (\mathbf{ab})]$ 

Matrix representation of *Diagonalizing Transform* (DTran T) is made by excerpting P-columns

$$S(\mathbf{P}^{\Box\Box}) = \frac{1}{2} \Big[ S(\mathbf{1}) + S(\mathbf{ab}) \Big] = \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{2} & \frac{1}{2} & \cdot \\ \cdot & \frac{1}{2} & \frac{1}{2} & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \qquad S(\mathbf{P}^{\Box}) = \frac{1}{2} \Big[ S(\mathbf{1}) - S(\mathbf{ab}) \Big] = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{2} & \frac{-1}{2} & \cdot \\ \cdot & \frac{-1}{2} & \frac{1}{2} & \cdot \\ \cdot & \frac{-1}{2} & \frac{1}{2} & \cdot \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{-1}{\sqrt{2}} \\ \cdot & \cdot & 1 & \cdot \end{pmatrix} = T$$

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Applying S<sub>2</sub> projection to build DTran Applying DTran for S<sub>2</sub> Applying DTran for U(2)

 $\begin{array}{l} S_3 \ \text{permutations related to } C_{3v} \sim D_3 \ \text{geometry} \\ S_3 \ \text{permutation matrices} \\ \text{Hooklength formula for } S_n \ \text{reps} \\ S_3 \ \text{symmetry of } U(2) : \ \text{Applying } S_3 \ \text{projection (Note Pauli-exclusion principle basis)} \\ \text{Building } S_3 \ \text{DTran } T \ \text{from projectors} \\ \text{Effect of } S_3 \ \text{DTran } T : \ \text{Introducing intertwining } S_3 - U(2) \ \text{irep matrices} \\ \text{Multi-spin } (1/2)^N \ \text{product state (Comparison to previous cases)} \end{array}$ 

S<sub>2</sub> symmetry of U(2): Applying S<sub>2</sub> projection  $S_2$  matrix eigen-solution found by projectors: Minimal eq. (ab)<sup>2</sup>-1=0=((ab)+1)((ab)+1) yields: Anti-Symmetric ( $\square$ ):  $\mathbf{P}^{\square} = \frac{1}{2} [\mathbf{1} - (\mathbf{ab})]$ Symmetric (  $\square$  ):  $\mathbf{P}^{\square\square} = \frac{1}{2} [\mathbf{1} + (\mathbf{ab})]$ Matrix representation of *Diagonalizing Transform* (DTran T) is made by excerpting **P**-columns  $S(\mathbf{P}^{\Box\Box}) = \frac{1}{2} \left[ S(\mathbf{1}) + S(\mathbf{ab}) \right] = \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \cdot \\ \cdot & \frac{1}{2} & \frac{1}{2}$  $\begin{pmatrix} \cdot & \cdot & \cdot & 1 \end{pmatrix} \begin{pmatrix} \cdot & \cdot & \cdot & 1 \end{pmatrix} \\ T^{\dagger} & S(ab) & T \\ 1 & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{\sqrt{2}} & \cdot \frac{1}{\sqrt{2}} & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & 1 & \cdot & 1 \end{pmatrix} \begin{pmatrix} 1 & \cdot & \cdot & 1 \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{-1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{-1}{\sqrt{2}} \\ \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & 1 & \cdot \end{pmatrix} = T^{\dagger}S(ab)T$ Next apply DTran T and its transpose  $T^{\dagger}$ to the *S*(*ab*) matrix to find  $T^{\dagger}S(ab)T$ .

S<sub>2</sub> symmetry of U(2): Applying S<sub>2</sub> projection  $S_2$  matrix eigen-solution found by projectors: Minimal eq. (ab)<sup>2</sup>-1=0=((ab)+1)((ab)+1) yields: Anti-Symmetric ( $\square$ ):  $\mathbf{P}^{\square} = \frac{1}{2} [\mathbf{1} - (\mathbf{ab})]$ Symmetric (  $\square$  ):  $\mathbf{P}^{\square\square} = \frac{1}{2} [\mathbf{1} + (\mathbf{ab})]$ Matrix representation of *Diagonalizing Transform* (DTran T) is made by excerpting **P**-columns  $S(\mathbf{P}^{\Box\Box}) = \frac{1}{2} \Big[ S(\mathbf{1}) + S(\mathbf{ab}) \Big] = \begin{bmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \cdot \\ \cdot & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \cdot \\ \cdot & \frac{1}{2} & \frac{1}$  $\begin{pmatrix} \cdot & \cdot & \cdot & 1 \\ T^{\dagger} & S(ab) \\ \cdot & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ \cdot &$ Next apply DTran T and its transpose  $T^{\dagger}$ to the *S*(*ab*) matrix to find  $T^{\dagger}S(ab)T$ .  $\begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \cdot \\ \cdot & \cdot & \cdot & 1 \\ \cdot & \frac{-1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & \cdot \end{pmatrix} \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{-1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{-1}{\sqrt{2}} \\ \cdot & \cdot & 1 & \cdot \end{pmatrix} = T^{\dagger}S(ab)T$ 

S<sub>2</sub> symmetry of U(2): Applying S<sub>2</sub> projection  $S_2$  matrix eigen-solution found by projectors: Minimal eq. (ab)<sup>2</sup>-1=0=((ab)+1)((ab)+1) yields: Anti-Symmetric ( $\square$ ):  $\mathbf{P}^{\square} = \frac{1}{2} [\mathbf{1} - (\mathbf{ab})]$ Symmetric ( $\Box$ ):  $\mathbf{P}^{\Box\Box} = \frac{1}{2} [\mathbf{1} + (\mathbf{ab})]$ Matrix representation of *Diagonalizing Transform* (DTran T) is made by excerpting **P**-columns  $S(\mathbf{P}^{\square\square}) = \frac{1}{2} \left[ S(\mathbf{1}) + S(\mathbf{ab}) \right] = \begin{bmatrix} \mathbf{1} & \cdots & \mathbf{1} \\ \vdots & \frac{1}{2} & \frac{1}{2} & \cdots \\ \vdots & \frac{1}{2} & \frac{1}{2} & \cdots \\ \vdots & \frac{1}{2} & \frac{1}{2} & \cdots \\ \vdots & \vdots & \ddots & 1 \end{bmatrix} \qquad S(\mathbf{P}^{\square}) = \frac{1}{2} \left[ S(\mathbf{1}) - S(\mathbf{ab}) \right] = \begin{bmatrix} \cdots & \cdots & \cdots & \cdots \\ \vdots & \frac{1}{2} & \frac{1}{2} & \cdots \\ \vdots & \frac{-1}{2} & \frac{1}{2} & \cdots \\ \vdots & \vdots & \cdots & \cdots \end{bmatrix}$  $\begin{pmatrix} T^{\dagger} & S(ab) \\ \cdot & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \cdot & \cdot & 1 \\ \cdot & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{-1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{-1}{\sqrt{2}} \\ \cdot & \cdot & 1 & \cdot \end{pmatrix} = T^{\dagger}S(ab)T$ Next apply DTran T and its transpose  $T^{\dagger}$ to the *S*(*ab*) matrix to find  $T^{\dagger}S(ab)T$ .  $T^{\dagger}S(ab)T = \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \cdot \\ \cdot & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \cdot \\ \cdot & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \cdot \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{-1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ \cdot & \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ \cdot & \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \cdot & \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \cdot & \frac{-1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\$ Three (3) symmetric ireps.  $D^{+}$ and one (1) anti-sym

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Interwining  $(S_1 \subset S_2 \subset S_3 \subset S_4 \subset S_5 \dots)^* (U(1) \subset U(2) \subset U(3) \subset U(4) \subset U(5) \dots)$  algebras and tensor operator applications to spinor-rotor or orbital correlations

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$$\begin{pmatrix} T^{\dagger} & D \otimes D & T & \text{Finally, apply DTran}T \\ 1 & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \\ \cdot & \cdot & \cdot & 1 \\ \cdot & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \cdot \end{pmatrix} \begin{pmatrix} D_{11\,11} & D_{11\,12} & D_{12\,11} & D_{12\,12} \\ D_{11\,21} & D_{11\,22} & D_{12\,21} & D_{12\,22} \\ D_{11\,21} & D_{12\,21} & D_{11\,22} & D_{12\,22} \\ D_{21\,21} & D_{21\,22} & D_{21\,22} & D_{22\,22} \end{pmatrix} \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{1}{\sqrt{2}} \\ \cdot & \frac{1}{\sqrt{2}} & \cdot & -\frac{1}{\sqrt{2}} \\ \cdot & \cdot & 1 & \cdot \end{pmatrix} = T^{\dagger}D \otimes DT$$



$$\begin{aligned}
 T^{\dagger} & D \otimes D & T & \text{Finally, apply DTran } T \\
 1 & \cdot & \cdot & \cdot \\
 \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
 \cdot & \cdot & \cdot & 1 \\
 \cdot & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
 \cdot & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}$$

$$\begin{bmatrix} T^{*} & D \otimes D & T & \text{Finally, apply DTran} T \\ 1 & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \cdot & \cdot & \cdot & 1 \\ \cdot & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \cdot \\ \end{bmatrix} \begin{bmatrix} D_{1121} & D_{1221} & D_{1222} & D_{1222} \\ D_{2121} & D_{2122} & D_{2122} & D_{2222} \\ D_{2122} & D_{2122} & D_{2222} \\ D_{2121} & D_{2122} & D_{2122} & 0 \\ D_{2121} & D_{2122} & D_{2122} & 0 \\ 0 & 0 & 0 & D_{1122} + D_{122} \\ 0 & 0 & 0 & D_{1122} + D_{122} \end{bmatrix} = \begin{bmatrix} T^{*}D \otimes DT \\ T^{*}D \otimes DT \end{bmatrix} = \begin{bmatrix} P_{1101} & \frac{f_{1}}{2} P_{112} & P_{122} & 0 \\ \frac{g_{2}}{2} P_{112} & D_{1122} + D_{122} & \frac{g_{2}}{2} P_{222} & 0 \\ 0 & 0 & 0 & D_{1122} + D_{122} \end{bmatrix} = \begin{bmatrix} D^{+}(0) & 0 \\ 0 & 0 & D^{-}(0) & D^{-}(0) \end{bmatrix} = D^{-p^{-p}} \end{bmatrix}$$

$$\begin{bmatrix} T^{*}D \otimes DT \\ \frac{g_{2}}{2} P_{122} & D_{1122} + D_{122} & \frac{g_{2}}{2} P_{222} & 0 \\ 0 & 0 & 0 & D_{1122} + D_{122} \end{bmatrix} = \begin{bmatrix} D^{+}(0) & 0 \\ 0 & 0 & D^{-}(0) & D^{-}(0) \end{bmatrix} = D^{-p^{-p}} \end{bmatrix}$$

$$\begin{bmatrix} T^{*}D \otimes DT \\ \frac{g_{2}}{2} P_{122} & D_{1122} + D_{122} & \frac{g_{2}}{2} P_{222} & 0 \\ 0 & 0 & 0 & D_{1122} + D_{122} \end{bmatrix} = \begin{bmatrix} D^{+}(0) & 0 \\ 0 & 0 & D^{-}(0) & D^{-}(0) \end{bmatrix} = D^{-p^{-p}} \end{bmatrix}$$

$$\begin{bmatrix} T^{*}D \otimes DT \\ \frac{g_{2}}{2} P_{12} & \frac{g_{2}}{2} P_{22} & \frac{g_{2}}{2} P_{222} & 0 \\ 0 & 0 & 0 & D_{1122} + D_{122} \end{bmatrix} = \begin{bmatrix} D^{+}(0) & 0 \\ 0 & 0 & D^{-}(0) & D^{-}(0) \end{bmatrix} = D^{-p^{-p}} \end{bmatrix}$$

$$\begin{bmatrix} T^{*}D \otimes DT \\ \frac{g_{2}}{2} P_{12} & \frac{g_{2}}{2} P_{22} & \frac{g_{2}}{2} P_{222} & 0 \\ 0 & 0 & 0 & D_{1122} + D_{122} \end{bmatrix} = \begin{bmatrix} D^{+}(0) & 0 & D^{-}(0) \\ 0 & 0 & D^{-}(0) & D^{-}(0) \end{bmatrix} = D^{-p^{-p}} \end{bmatrix}$$

$$\begin{bmatrix} T^{*}D \otimes DT \\ \frac{g_{2}}{2} P_{22} & \frac{g_{2}}{2} & \frac{g_{2}}{2} P_{22} & \frac{g_{2}}{2} & \frac$$

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 $S_3$  permutations related to  $C_{3v} \sim D_3$  geometry

D3<C3v nomogram</th>D3<D6 nomogram</th>AMOP Class 12 pdf p30AMOP Class 14 pdf p28



### **S**<sub>3</sub> permutations related to $C_{3v} \sim D_3$ geometry

D3<C3v nomogram</th>D3<D6 nomogram</th>AMOP Class 12 pdf p30AMOP Class 14 pdf p28

Fig. 25.3.0 QTforCA Unit 8 Ch.25 pdf p28







 $[123] |1_a, 2_b, 3_c\rangle = |3_a, 1_b, 2_c\rangle$ 

<u>5 pdf p29</u> <b>O</b>	2			Ŏ	1		
plan	e la	_		pla	ne		
				$\wedge$			
			$\mathbb{N}$				
σ	3		/0	3		C	<b>5</b> 3
plan	e Tp2	2/	1			pla	ine
		/0	2				
				$\checkmark$			
σ	1		2		$\mathbf{J}_2$		
plan	e			p	lane		
	1	$r^2$	r	$\dot{i}_1$	$i_2$	i <sub>3</sub>	
	r	1	$r^2$	$\dot{l}_2$	i <sub>3</sub>	<i>i</i> <sub>1</sub>	
	$r^2$	r	1	i <sub>3</sub>	$\dot{i}_1$	$\dot{l}_2$	
	<i>i</i> <sub>1</sub>	$i_2$	i <sub>3</sub>	1	$r^2$	r	
	$\dot{l}_2$	$\dot{l}_3$	$\dot{l}_1$	r	1	$r^2$	
	i <sub>3</sub>	$\dot{l}_1$	$i_2$	$r^2$	r	1	
$C_{3_{V}} \mathbf{g} \mathbf{g}^{\dagger}$ form	1	$\mathbf{r}^2$	$\mathbf{r}^1$	$\sigma_1$	$\sigma_2$	σ	3
(a)(b)(c) = 1	1	r <sup>2</sup>	$\mathbf{r}^1$	<b>σ</b> <sub>1</sub>	$\sigma_2$	σ	3
$(abc) = \mathbf{r}^1$	$\mathbf{r}^1$	1	r <sup>2</sup>	$\sigma_2$	σ <sub>3</sub>	<b>σ</b> <sub>1</sub>	
$(acb) = \mathbf{r}^2$	<b>r</b> <sup>2</sup>	$\mathbf{r}^{1}$	1	<b>σ</b> <sub>3</sub>	$\boldsymbol{\sigma}_1$	$\sigma_2$	2
$(bc) = \sigma_1$	<b>σ</b> <sub>1</sub>	$\sigma_2$	σ3	1	$\mathbf{r}^2$	r <sup>1</sup>	
$(ac) = \sigma_2$	$\sigma_2$	$\sigma_3$	$\mathbf{\sigma}_1$	$\mathbf{r}^1$	1	r <sup>2</sup>	
$(ab) = \sigma_3$	$\sigma_3$	$\boldsymbol{\sigma}_1$	$\sigma_2$	<b>r</b> <sup>2</sup>	$\mathbf{r}^1$	1	

(1)	(acb)	(abc)	( <i>bc</i> )	( <i>ac</i> )	<i>(ab)</i>
(abc)	(1)	(acb)	( <i>ac</i> )	<i>(ab)</i>	( <i>bc</i> )
(acb)	(abc)	(1)	<i>(ab)</i>	( <i>bc</i> )	( <i>ac</i> )
( <i>bc</i> )	( <i>ac</i> )	<i>(ab)</i>	(1)	(acb)	(abc)
( <i>ac</i> )	<i>(ab)</i>	( <i>bc</i> )	(abc)	(1)	(acb)
( <i>ab</i> )	(bc)	<i>(ac)</i>	(acb)	(abc)	(1)

[1]	[132]	[123]	[23]	[13]	[12]
[123]	[1]	[132]	[13]	[12]	[23]
[132]	[123]	[1]	[12]	[23]	[13]
[23]	[13]	[12]	[1]	[132]	[123]
[13]	[12]	[23]	[123]	[1]	[132]
[12]	[23]	[13]	[132]	[123]	[1]

S<sub>3</sub> permutations related to C<sub>3v</sub>~D<sub>3</sub> geometry Fig. 25.3.1 QTforCA Unit 8 Ch. 25 pdf p29



S<sub>3</sub> permutations related to C<sub>3v</sub>~D<sub>3</sub> geometry Fig. 25.3.1 QTforCA Unit 8 Ch. 25 pdf p29



 $S_3$  permutations related to  $C_{3\nu} \sim D_3$  geometry Fig. 25.3.1 QTforCA Unit 8 Ch.25 pdf p29



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Rank-3 tensor basis  $|ijk\rangle$  (3 particles each with U(2) state space)

[1][2][3]	111	112	121	122	211	212	221	$ 222\rangle$
(111	1	•	•	•	•	•	•	•
(112		1					•	
(121			1					
(122				1				
(211					1			
(212						1		
(221							1	
(222)		•					•	1

Representation of bicycle (ab) or [12]

[12]	111	112>	121	$ 122\rangle$	211	$ 212\rangle$	221	$ 222\rangle$
(111)	1	•	•	•	•	•	•	•
(112)	•	1	•	•	•	•	•	
(121	•	•	•	•	1	•	•	•
(122)	•	•	•	•	•	1	•	•
<b>(211</b>	•	•	1	•	•	•	•	•
<b>(212</b>	•	•	•	1	•	•	•	
<b>(221</b>	•	•	•	•	•	•	1	
<b>(222</b>	•	•	•	•	•	•	•	1

Rank-3 tensor basis  $|ijk\rangle$  (3 particles each with U(2) state space)

[1][2][3]	111	112	121	$ 122\rangle$	211	$ 212\rangle$	221	$ 222\rangle$
(111	1	•	•	•	•	•	•	•
(112	•	1	•					
(121			1					
(122				1				
(211					1			
(212						1		
(221	•						1	
(222	•							1

# Representation of bicycle (ab) or [12]

[12]	111	112	121	122	211	212	221	$ 222\rangle$
(111	1	•	•	•	•	•	•	•
(112	•	1	•	•			•	
(121			•		1			
(122	•					1		
(211	•		1					
(212				1				
(221							1	
<b>(222</b>								1

# Representation of bicycle (ac) or [13]

[13]	111	112>	121	122>	211	$ 212\rangle$	221	$ 222\rangle$
(111)	1	•	•	•	•	•	•	•
(112)	•	•	•	•	1	•	•	•
(121	•	•	1	•	•	•	•	•
(122)	•	•	•	•	•	•	1	
(211)	•	1					•	
<b>(212</b>	•					1	•	
<b>221</b>	•	•	•	1	•	•	•	
<b>\langle 222</b>	•	•	•	•	•	•	•	1

Rank-3 tensor basis  $|ijk\rangle$  (3 particles each with U(2) state space)

[1][2][3]	111	112>	121	$ 122\rangle$	211	212	221	$ 222\rangle$
(111	1	•	•	•	•	·	•	
(112	•	1						
(121			1					
(122				1				
(211					1			
(212						1		
(221							1	
(222	•							1

# Representation of bicycle (ab) or [12]

[12]	111	112	121	122	211	212	221	$ 222\rangle$
(111	1	•	•	•	•	•	•	•
(112	•	1	•					
(121	•		•		1			
(122)	•					1		
(211	•		1					
(212	•			1				
(221	•						1	
<b>(222</b>	•	•				•		1

# Representation of bicycle (ac) or [13]

[13]	111>	112>	121	$ 122\rangle$	211	$ 212\rangle$	221	$ 222\rangle$
(111)	1	•	•	·	·	•	·	·
(112	•	•	•		1	•		
(121	•	•	1			•		
(122)	•	•	•				1	
(211	•	1						
(212	•	•				1		
(221	•	•		1				
222								1

# Representation of bicycle (bc) or [23]

[23]	111	112>	121	122	211	212	221	$ 222\rangle$
(111)	1	•	•	•	•	•	•	•
(112			1					
(121		1						
(122				1				
(211					1			•
(212							1	
(221						1		•
(222								1

Rank-3 tensor basis  $|ijk\rangle$  (3 particles each with U(2) state space)

[1][2][3]	111	112	121	122	211	$ 212\rangle$	221	$ 222\rangle$
(111	1	•	•	•	•	•	•	•
(112	•	1	•	•	•	•		
(121			1					
(122)	•			1				
(211	•				1			
(212						1		
(221	•						1	
(222	•							1

	111	112	121	122	211	212	221	222
111								
112								
121								
122								
211								
212								
221								
222								

# Representation of tricycle (abc) or [123]

[123]	111	112	121	122>	211	$ 212\rangle$	221	$ 222\rangle$
(111)	1	•	•	•	•	•	•	•
(112	•	•	1	•	•	•	•	
(121	•				1			
(122	•						1	
(211)		1						
<b>(212</b>				1				
<b>221</b>						1		
<b>\(222)</b>	•	•	•		•	•		1

## Representation of tricycle (acb) or [132]

### [132] is transpose or inverse of [123]

[132]	111	$ 112\rangle$	<b> 121</b>	$ 122\rangle$	$ 211\rangle$	$ 212\rangle$	$ 221\rangle$	$ 222\rangle$
(111)	1	•	•	•	•	•	•	•
(112	•				1			•
(121	•	1						•
(122)	•			•		1	•	•
(211	•		1					•
(212)	•						1	•
(221				1				
(222	•		•			•		1

Rank-3 tensor basis  $|ijk\rangle$  (3 particles each with U(2) state space)

[1][2][3]	111	112	121	$ 122\rangle$	211	$ 212\rangle$	221	$ 222\rangle$
(111	1	•	•	•	•	•	•	•
(112	•	1	•	•				•
(121			1					
(122				1				
(211					1			
(212						1		
(221							1	
<b>(222</b> )								1

	111	112	121	122	211	212	221	222
111								
112								
121								
122								
211								
212								
221								
222								

#### Need smaller boxes!

[12]	111>	112	121	122	211	212	221	$ 222\rangle$	
(111	1	•	•	•	•	•	•	•	
(112		1							
(121					1				
(122						1			
(211			1						
(212				1					
(221							1		
(222								1	

[13]	111>	112>	121	122	211	212	221	$ 222\rangle$	[23]	[23]	111
(111	1	·	•	·	•	·	·	•	(111	(111)	1
(112					1				(112	(112	•
(121			1						(121	(121	
(122							1		(122	(122	
(211		1							(211	(211)	
(212						1			(212	(212	
(221				1					(221	(221	
(222								1	(222	(222	
	1								1		

[23]	111>	112>	121	122	211	212	221	$ 222\rangle$
(111)	1	•	•	•	•	•	•	•
(112	•		1					
(121		1						
(122				1				
(211					1			
(212							1	
(221						1		
<b>(222</b>	•		•		•			1

[123]	111	112	121	122	211	212	221	$ 222\rangle$
(111	1	•	•	•	•	•	•	•
(112	•		1				•	
(121					1			
(122							1	
(211	•	1					•	
(212	•			1			•	
(221						1		
<b>(222</b> )	•							1

11	112	121	$ 122\rangle$	211	$ 212\rangle$	$ 221\rangle$	$ 222\rangle$
1	•	•	•	•	•	•	
		1					
				1			
						1	
•	1						
			1				
•					1		
							1

4.02.18 class 20: Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics

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Interwining  $(S_1 \subset S_2 \subset S_3 \subset S_4 \subset S_5 \dots)^* (U(1) \subset U(2) \subset U(3) \subset U(4) \subset U(5) \dots)$  algebras and tensor operator applications to spinor-rotor or orbital correlations

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

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

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."]

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$$\frac{\mathbf{g} = |\mathbf{1} = (1)(2)(3) \mathbf{r} = (123) \mathbf{r}^{2} = (132) \mathbf{i}_{1} = (23) \mathbf{i}_{2} = (13) \mathbf{i}_{3} = (12)}{D^{\square\square}(\mathbf{g}) = |\mathbf{f}|_{1} \mathbf{g}|_{1} \mathbf$$

 $\mathbf{P}^{\square\square} = \frac{1}{6} ((1)(1) + (1)(123) + (1)(132) + (1)(13) + (1)(13) + (1)(12))$ 

111 112 121 122	211 212 221 222	111 112 121 122 211	212 221 222   111 1	112 121 122 211 212 221 222	111 112 121 122 211 2	212 221 222   111 112 121 12	2 211 212 221 222	111 112 121 122 211 212 221 222
111 1		111 1	111 1		111 1	111 1	11	1 1
112 1		112 1	112	1	112 1	112	1 11	2 1
121 1		121 1	121	1	121 1	121 1	12	1 1
122 1		122	1 122	1	122 1	122	1 12	2 1
211	1	211 1	211	1	211 1	211 1	21	1 1
212	1	212 1	212	1	212	1 212	1 21	2 1
221	1	221	1 221	1	221	1 221 1	22	1
222	1	222	1 222	1	222	1 222	1 22	2 1
[1][2][3]		[123]	[13]	2]	[23]	[13]	t	[12]



$$\frac{\mathbf{g} = \mathbf{1} = (1)(2)(3) \quad \mathbf{r} = (123) \quad \mathbf{r}^{2} = (132) \quad \mathbf{i}_{1} = (23) \quad \mathbf{i}_{2} = (13) \quad \mathbf{i}_{3} = (12)}{\mathbf{D}^{\square\square}(\mathbf{g}) = \mathbf{D}^{\square\square}(\mathbf{g}) = \mathbf{$$

 $\mathbf{P}^{\text{I}} = \frac{1}{6} \left( (1)(1) + (1)(123) + (1)(132) + (1)(13) + (1)(12) \right)$ 





Difficult and tedious to sum? Try MathType overlays (next page)

	g =	<b>1</b> = (1)(2)	(3)	<b>r</b> = (123)		$r^2 = (132)$	2)	$i_1 = (23)$	3)		$i_2 = (13)$		$i_3 = (12)$					
	$D^{\Box\Box\Box}(\mathbf{g}) = D^{\Box}_{\mathbf{g}}(\mathbf{g}) = D^{\Box\Box}_{x_2y_2}(\mathbf{g}) = D^{\Box\Box}_{x_2y_2}(\mathbf{g}) = D^{\Box\Box}_{x_2y_2}(\mathbf{g}) = D^{\Box\Box}_{x_2y_2}(\mathbf{g}) = D^{\Box\Box\Box}_{x_2y_2}(\mathbf{g}) = D^{\Box\Box\Box}_{x_2y_2}(\mathbf{g}) = D^{\Box\Box\Box}_{x_2y_2}(\mathbf{g}) = D^{\Box\Box\Box}_{x_2y_2}(\mathbf{g}) = D^{\Box\Box\Box}_{x_2y_2}(\mathbf{g}) = D^{\Box\Box}_{x_2y_2}(\mathbf{g}) = D^{\Box\Box}_{x_$	$ \begin{array}{c} 1\\ 1\\ \begin{pmatrix} 1 & 0\\ 0 & 1 \end{array} $	$\left(\begin{array}{c} -1\\ \sqrt{2}\end{array}\right)$	$ \begin{array}{c} 1 \\ 1 \\ 1/2 \\ -\sqrt{3}/2 \\ -1/2 \end{array} $	$\begin{pmatrix} 2\\ 2 \end{pmatrix}$	$ \begin{array}{c} 1 \\ 1 \\ -1/2 \\ \sqrt{3}/2 \\ -\sqrt{3}/2 \end{array} $	$\left(\frac{\overline{3}}{2}\right)$	$ \begin{array}{c} 1 \\ -1 \\ \left( \begin{array}{c} -1/2 \\ \sqrt{3}/2 \end{array} \right) $	√3/2 1/2		$ \begin{array}{r} 1 \\ -1 \\ -\sqrt{3} \\ -\sqrt{3} \\ 2 \\ 1 \\ \end{array} $	$\left(\begin{array}{c} \overline{3}/2\\2\end{array}\right)$	$ \begin{array}{c} 1 \\ -1 \\ \left(\begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array}\right) \end{array} $	)				
111       112       122       211       212       222         111       1       1       111       112         112       1       1       121       121         121       1       1       122       121         122       1       1       122       122         211       1       1       211       212         212       1       1       212       212         212       1       1       212       212         221       1       1       212       212         212       1       1       212       212         212       1       1       212       212         212       1       1       212       212         212       1       1       212       212         221       1       1       221       221         222       1       1       222       223         1       1       223       224       224         1       1       224       1       225         1       1       225       1       225         1 <td< td=""><td>111       112       121       1         1       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         1       1       1       1         2       1       1       1         1       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         1       1       1       1         1       1       1       1         2       1       1       1         1       1       1       1       1         1       1       1       1       1</td><td>22 211 212 1 1 1 1 1</td><td>221     222       1     1       1     1       1     1       1     1       1     1       1     1       1     2       1     2</td><td>111     112       11     1       12     1       21     2       22     2       211     1       212     2       221     2       221     1       212     1       213     1</td><td></td><td></td><td>222     111       112     121       122     211       212     221       1     222</td><td>111 112 121 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1</td><td>122 2</td><td>11 212 2 1 1 1 1</td><td>21     222       111       112       121       122       1       21       1       21       1       22       1       22       1       22       1</td><td>1111 112 1 1 2 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 1 2 1 1 1 2 1 1 1 2 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1</td><td>1 122 21 1 1 1 1 1 1 1 1 1 1 1 1</td><td></td><td>222     111       112     121       122     211       212     212       1     222</td><td>111 112 1 1 1 1 1 1 1 1 1 1 1 1 1 1</td><td>21 122 211 1 1 1 1 1</td><td>212 221 222 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1</td></td<>	111       112       121       1         1       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         1       1       1       1         2       1       1       1         1       1       1       1         2       1       1       1         2       1       1       1         2       1       1       1         1       1       1       1         1       1       1       1         2       1       1       1         1       1       1       1       1         1       1       1       1       1	22 211 212 1 1 1 1 1	221     222       1     1       1     1       1     1       1     1       1     1       1     1       1     2       1     2	111     112       11     1       12     1       21     2       22     2       211     1       212     2       221     2       221     1       212     1       213     1			222     111       112     121       122     211       212     221       1     222	111 112 121 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	122 2	11 212 2 1 1 1 1	21     222       111       112       121       122       1       21       1       21       1       22       1       22       1       22       1	1111 112 1 1 2 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 1 2 1 1 1 2 1 1 1 2 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1	1 122 21 1 1 1 1 1 1 1 1 1 1 1 1		222     111       112     121       122     211       212     212       1     222	111 112 1 1 1 1 1 1 1 1 1 1 1 1 1 1	21 122 211 1 1 1 1 1	212 221 222 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
	111	112	121	122	211	212	221	222										
11	1										6							
11	2	11	11		11							2	2		2			
12	21	11	11		11							2	2		2			
12	2			11		11	11							2		2	2	
21	1	11	11		11						-	2	2		2			
21	2			11	•	11	11	6	1					2		2	2	
$\overline{)}$	21			11	•	11	11							2		2	2	
2.2	2							111111										6

$$\frac{\mathbf{g} = \mathbf{1} = (1)(2)(3) \quad \mathbf{r} = (123) \quad \mathbf{r}^{2} = (132) \quad \mathbf{i}_{1} = (23) \quad \mathbf{i}_{2} = (13) \quad \mathbf{i}_{3} = (12)}{D^{\square\square}(\mathbf{g}) = \mathbf{1} \quad \mathbf{$$

$$\mathbf{P}_{11}^{\Box} = \frac{1}{6} \Big( (2)(1) + (-1)(123) + (-1)(132) + (-1)(23) + (-1)(13) + (+2)(12) \Big)$$

111 112 121	122 211 212 221 222	111 112 121 122 211 212 221 222	111 112 121 122 211 212 221 222	111 112 121 122 211 212 221 222	111 112 121 122 211 212 221 222	111 112 121 122 211 212 221 222
111 1		111 1	111 1	111 1	111 1	111 1
112 1		112 1	112 1	112 1	112 1	112 1
121 1		121 1	121 1	121 1	121 1	121 1
122	1	122 1	122 1	122 1	122 1	122 1
211	1	211 1	211 1	211 1	211 1	211 1
212	1	212 1	212 1	212 1	212 1	212 1
221	1	221 1	221 1	221 1	221 1	221 1
222	1	222 1	222 1	222 1	222 1	222 1
[1][2][3]		[123]	[132]	[23]	[13]	[12]



$$\frac{\mathbf{g}}{D^{\square\square}(\mathbf{g})} = \frac{1 = (1)(2)(3) \quad \mathbf{r} = (123) \quad \mathbf{r}^{2} = (132) \quad \mathbf{i}_{1} = (23) \quad \mathbf{i}_{2} = (13) \quad \mathbf{i}_{3} = (12)}{\mathbf{p}^{\square\square}(\mathbf{g})} = \frac{1}{D^{\square\square}(\mathbf{g})} = \frac{1}{1} \quad \frac{1}$$



1	1111	12 12	1 122	211 2	12 221	222		111 1	12 121	122 2	211 212	221 22	2	111 112	121 12	2 211 21	2 221 222	11	1 112 12	1 122 2	11 212	221 222	11	1 112 12	1 1 2 2	211 212	221 222		111 112	121 12	2 211	212 221	222
111	1						111	1					111	1				111 1					111 1					111	1				
112		1					112		1				112			1		112	1				112			1		112	1				
121		1					121				1		121	1				121	1				121	1		l		121		Ī	1		1
122			1				122					1	122			1		122		1			122				1	122				1	1
211				1			211	]	1				211		1			211			1		211	1				211		1			
212					1		212			1			212				1	212				1	212			1		212		1			
221					1		221				1		221		1			221			1		221		1			221				1	
222						1	222					1	222				1	222				1	222				1	222					1
[	1][2]	[3]						[123]						[132]				[]	23]				[1]	3]				]	12]				



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# Note all $\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ (totally antisymmetric) U(2) (spin-1/2) states $\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ $\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ $\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ are non-existent.

$$\begin{vmatrix} \widehat{1} \\ \widehat{1}$$

It takes at least 3 distinct (U(3)) states to make a 3<sup>rd</sup> rank "determinant" state  $\frac{a}{b}{c}$ .

This is the symmetry basis of the Pauli-exclusion principle.

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S<sub>3</sub> symmetry of U(2): Effect of S<sub>3</sub> DTran T on intertwining S<sub>3</sub> - U(2) irep matrices

#### S<sub>3</sub> matrices:

#### *U*(2) *matrices*:



#### $T^{\dagger}D \otimes D \otimes D(\mathbf{u})T =$

$D_{11}({f u})$	$D_{12}({f u})$	$D_{13}({f u})$	$D_{14}(\mathbf{u})$				
$D_{21}({f u})$	$D_{22}({f u})$	$D_{23}({f u})$	$D_{24}(\mathbf{u})$				
$D_{31}({\bf u})$	$D_{31}({\bf u})$	$D_{31}({\bf u})$	$D_{31}({\bf u})$				
$D_{41}({f u})$	$D_{42}(\mathbf{u})$	$D_{43}({f u})$	$D_{44}(\mathbf{u})$				
				$D_{11}({\bf u})$		$D_{12}({f u})$	
					$D_{12}({f u})$		$D_{12}(\mathbf{u})$
				$D_{21}({f u})$		$D_{22}(\mathbf{u})$	
					$D_{21}({f u})$		$D_{22}(\mathbf{u})$

S<sub>3</sub> symmetry of U(2): Effect of S<sub>3</sub> DTran T on intertwining S<sub>3</sub> - U(2) irep matrices

#### S<sub>3</sub> matrices:

#### *U*(2) *matrices*:



#### $T^{\dagger}D \otimes D \otimes D(\mathbf{u})T =$

$D_{11}({\bf u})$	$D_{12}({f u})$	$D_{13}({f u})$	$D_{14}({f u})$				
$D_{21}({f u})$	$D_{22}({f u})$	$D_{23}({f u})$	$D_{24}(\mathbf{u})$				
$D_{31}({\bf u})$	$D_{31}({\bf u})$	$D_{31}({\bf u})$	$D_{31}({\bf u})$				
$D_{41}({f u})$	$D_{42}(\mathbf{u})$	$D_{43}({f u})$	$D_{44}(\mathbf{u})$				
				$D_{11}({f u})$		$D_{12}({f u})$	
					$D_{12}({\bf u})$		$D_{12}({\bf u})$
				$D_{21}({\bf u})$		$D_{22}(\mathbf{u})$	
					$D_{21}({f u})$		$D_{22}(\mathbf{u})$

*After flipping rows and columns (6\Leftrightarrow7) of T matrix* 

$T_{\epsilon}$	$_{57}$ <sup>†</sup> S(	$(\mathbf{p}_{abc})$	$T_{67}$	, =				
f	lip	I	fli	р		1	1	1
	<i>D</i> ( <b>p</b> )							
		<i>D</i> ( <b>p</b> )						
			<i>D</i> ( <b>p</b> )					
				<i>D</i> ( <b>p</b> )				
					$D_{11}({\bf p})$		$D_{12}({\bf p})$	
						$D_{11}({\bf p})$		$D_{12}({\bf p})$
					$D_{21}({\bf p})$		$D_{22}({\bf p})$	
						$D_{21}({\bf p})$		$D_{22}({\bf p})$

$T_{67}^{\dagger} D \otimes L$	)(8	D(u	$T_{67}$	=					
flip			flip						
		$D_{11}({f u})$	$D_{12}({f u})$	$D_{13}({\bf u})$	$D_{14}({f u})$				
		$D_{21}({f u})$	$D_{22}(\mathbf{u})$	$D_{23}({f u})$	$D_{24}({f u})$				
		$D_{31}({\bf u})$	$D_{31}({\bf u})$	$D_{31}({\bf u})$	$D_{31}({\bf u})$				
		$D_{41}({f u})$	$D_{42}(\mathbf{u})$	$D_{43}(\mathbf{u})$	$D_{44}(\mathbf{u})$				
						$D_{11}({\bf u})$	$D_{12}(\mathbf{u})$		
						$D_{21}({\bf u})$	$D_{22}(\mathbf{u})$		
								$D_{11}({\bf u})$	$D_{12}({f u})$
								$D_{21}({\bf u})$	$D_{22}({f u})$

S<sub>3</sub> symmetry of U(2): Effect of S<sub>3</sub> DTran T on intertwining S<sub>3</sub> - U(2) irep matrices



*After flipping rows and columns (6\Leftrightarrow7) of T matrix* 



4.02.18 class 20: Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics

William G. Harter - University of Arkansas

Interwining  $(S_1 \subset S_2 \subset S_3 \subset S_4 \subset S_5 \dots)^* (U(1) \subset U(2) \subset U(3) \subset U(4) \subset U(5) \dots)$  algebras and tensor operator applications to spinor-rotor or orbital correlations

U(2) tensor product states and S<sub>n</sub> permutation symmetry Rank-1 tensor (or spinor)

Rank-2 tensor (2 particles each with U(2) state space)
2-particle U(2) transform and permutation operation
S<sub>2</sub> symmetry of U(2): Trust but verify

Applying S<sub>2</sub> projection to build DTran Applying DTran for S<sub>2</sub> Applying DTran for U(2)

S<sub>3</sub> permutations related to C<sub>3v</sub>~D<sub>3</sub> geometry
S<sub>3</sub> permutation matrices
Hooklength formula for S<sub>n</sub> reps
S<sub>3</sub> symmetry of U(2): Applying S<sub>3</sub> projection (Note Pauli-exclusion principle basis)
Building S<sub>3</sub> DTran T from projectors
Effect of S<sub>3</sub> DTran T: Introducing intertwining S<sub>3</sub> - U(2) irep matrices
Multi-spin (1/2)<sup>N</sup> product state (Comparison to previous cases)

*Multi-spin (1/2)*<sup>N</sup> *product states* 



*Multi-spin (1/2)*<sup>N</sup> *product states* 



	g =	1 = (1)(2)(3)	r = (123)	$r^2 = (132)$	$i_1 = (23)$	$i_2 = (13)$	$i_3 = (12)$		
	$D^{\Box\Box\Box}(\mathbf{g}) =$								
	E C	1	1	1	1	1	1		
	$D^{\square}(\mathbf{g}) =$	1	1	1	-1	-1	-1		
		$\begin{pmatrix} 1 & 0 \end{pmatrix}$	$-1/2 - \sqrt{3}/2$	$-1/2  \sqrt{3}/2$	$\left( -\frac{1}{2} \sqrt{3}/2 \right)$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \end{pmatrix}$		
	$D_{x_2y_2}^{[\bot]}\left(\mathbf{g}\right) =$		$\sqrt{3}/2$ $-1/2$	$-\sqrt{3}/2$ $-1/2$	$\sqrt{3/2}$ $1/2$	$\left( -\sqrt{3}/2 + 1/2 \right)$	( 0 -1 )		
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	2	1	122	1	122 1	122	1	122	1
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	2 1		212		212	1 212		212	1
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