

# 4.16.18 class 23: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

## (S<sub>n</sub>)\*(U(m)) shell model of electrostatic quadrupole-quadrupole-e interactions

Complete set of E<sub>jk</sub> matrix elements for the doublet (spin-1/2) p<sup>3</sup> orbits

Detailed sample applications of “Jawbone” formulae

Number operators

1-jump E<sub>i-1,i</sub> operators

2-jump E<sub>i-2,i</sub> operators

Angular momentum operators (for later application)

Multipole expansions and Coulomb (e-e)-electrostatic interaction

Linear multipoles; P<sub>1</sub>-dipole, P<sub>2</sub>-quadrupole, P<sub>3</sub>-octupole,...

Moving off-axis: On-z-axis linear multipole P<sub>ℓ</sub> (cosθ) wave expansion:

**Multipole Addition Theorem (should be called Group Multiplication Theorem)**

Coulomb (e-e)-electrostatic interaction and its Hamiltonian Matrix, Slater integrals

2-particle elementary e<sub>jk</sub> operator expressions for (e-e)-interaction matrix

Tensor tables are (2ℓ+1)-by-(2ℓ+1) arrays (p<sup>k</sup><sub>q</sub>) giving V<sub>q</sub><sup>k</sup> in terms of E<sub>p,q</sub>.

Relating V<sub>q</sub><sup>k</sup> to E<sub>m',m</sub> by (m'<sup>k</sup><sub>m</sub>) arrays

Atomic p-shell ee-interaction in elementary operator form

[2,1] tableau basis (from p.29) and matrices of v<sup>1</sup> dipole and v<sup>1</sup>•v<sup>1</sup>=L•L

[2,1] tableau basis (from p.29) and matrices of v<sup>2</sup> and v<sup>2</sup>•v<sup>2</sup> quadrupole

<sup>4</sup>S, <sup>2</sup>P, and <sup>2</sup>D energy calculation of quartet and doublet (spin-1/2) p<sup>3</sup> orbits

Corrected level diagrams Nitrogen p<sup>3</sup>

## *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](#)

[Gallop 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](#)

**[Representations Of Multidimensional Symmetries In Networks - harter-jmp-1973](#)**

*[\\*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.](#)*

*Intro spin  $\frac{1}{2}$  coupling*  
*Unit 8 Ch. 24 p3.*

*H atom hyperfine-B-level crossing*  
*Unit 8 Ch. 24 p15.*

*Hyperf. theory Ch. 24 p48.*

*Hyperf. theory Ch. 24 p48.*  
*Deeper theory ends p53*

*Intro 2p3p coupling*  
*Unit 8 Ch. 24 p17.*

*Intro LS-jj coupling*  
*Unit 8 Ch. 24 p22.*

*CG coupling derived (start)*  
*Unit 8 Ch. 24 p39.*

*CG coupling derived (formula)*  
*Unit 8 Ch. 24 p44.*

*Lande' g-factor*  
*Unit 8 Ch. 24 p26.*

*Irrep Tensor building*  
*Unit 8 Ch. 25 p5.*

*Irrep Tensor Tables*  
*Unit 8 Ch. 25 p12.*

*Wigner-Eckart tensor Theorem.*  
*Unit 8 Ch. 25 p17.*

*Tensors Applied to d,f-levels.*  
*Unit 8 Ch. 25 p21.*

*Tensors Applied to high J levels.*  
*Unit 8 Ch. 25 p63.*

*Intro 3-particle coupling.*  
*Unit 8 Ch. 25 p28.*

*Intro 3,4-particle Young Tableaus*  
*GrpThLect29 p42.*

*Young Tableau Magic Formulae*  
*GrpThLect29 p46-48.*

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

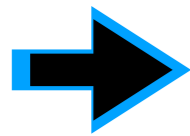
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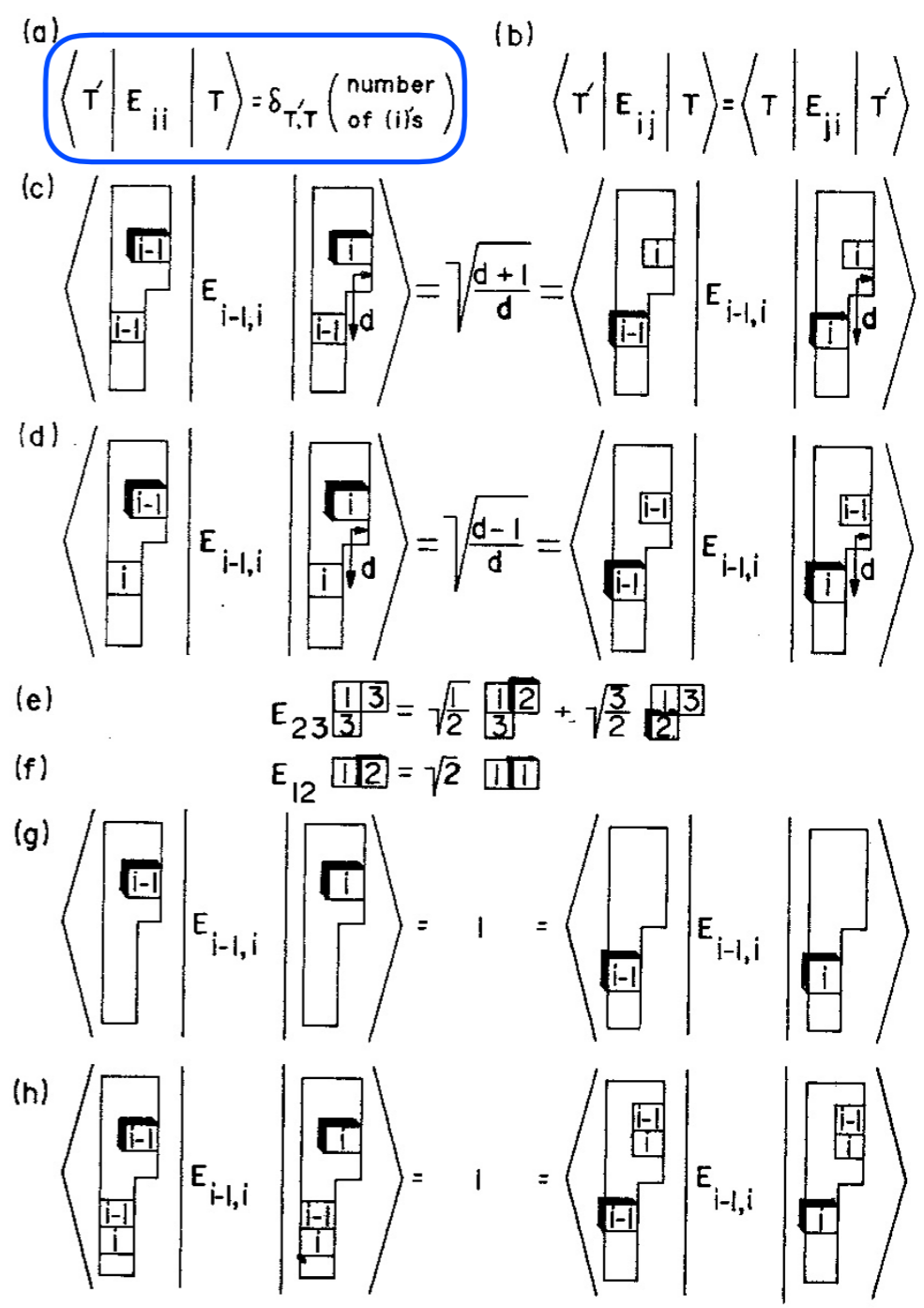
# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

		$M=2$	$M=1$		$M=0$	$M=-1$	$M=-2$		
		$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$E_{jk} =$	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{matrix} (11) & (22) \\ 2 & + & 1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{\frac{1}{2}} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{\frac{3}{2}} \end{matrix}$	.	.	.
	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$		$\begin{matrix} (11) & (22) \\ 1 & + & 2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{\frac{1}{2}} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{\frac{3}{2}} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$		.	$\begin{matrix} (11) & (33) \\ 2 & + & 1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$				$\begin{matrix} (11) & (22) & (33) \\ 1 & + & 1 & + & 1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{\frac{1}{2}} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{\frac{1}{2}} \end{matrix}$
	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$				.	$\begin{matrix} (11) & (22) & (33) \\ 1 & + & 1 & + & 1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{\frac{3}{2}} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{\frac{3}{2}} \end{matrix}$
	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$						$\begin{matrix} (11) & (33) \\ 1 & + & 2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$						.	$\begin{matrix} (22) & (33) \\ 2 & + & 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$								$\begin{matrix} (22) & (33) \\ 1 & + & 2 \end{matrix}$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $		.	$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $				.	$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $						.	$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



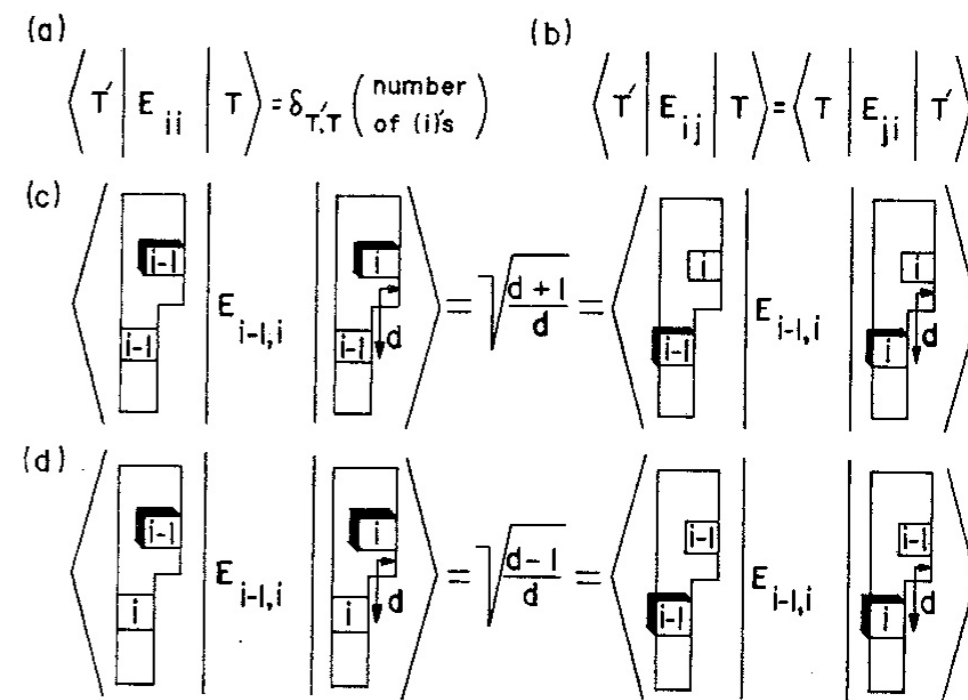
## Sample applications of "Jawbone" number operators

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$	$M=-2$	
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
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$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $		.	$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $				.	$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
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$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



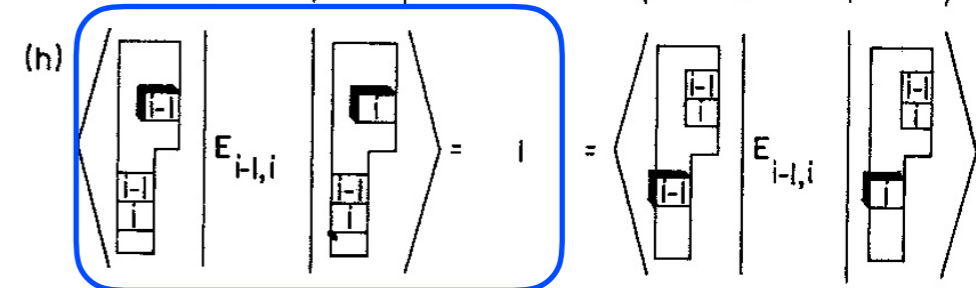
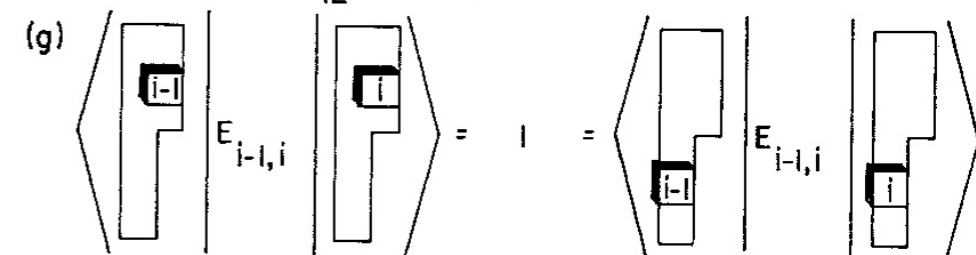
## Sample applications of "Jawbone" formulae

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{12} | \begin{vmatrix} 12 \\ 2 \end{vmatrix} \rangle = 1$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 11 \\ 3 \end{vmatrix} \rangle = 1 \quad \text{(1-jump } E_{i-1,i})$$

(e)  $E_{23} \begin{vmatrix} 13 \\ 3 \end{vmatrix} = \frac{1}{\sqrt{2}} \begin{vmatrix} 12 \\ 3 \end{vmatrix} + \frac{\sqrt{3}}{\sqrt{2}} \begin{vmatrix} 13 \\ 2 \end{vmatrix}$

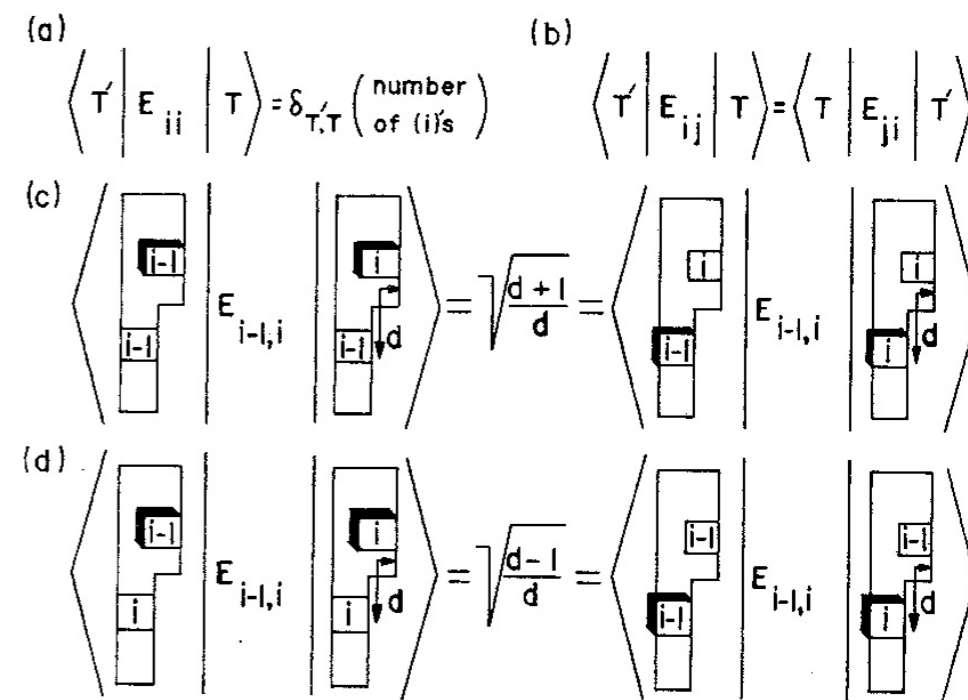
(f)  $E_{12} \begin{vmatrix} 11 \\ 2 \end{vmatrix} = \sqrt{2} \begin{vmatrix} 11 \\ 3 \end{vmatrix}$



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$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
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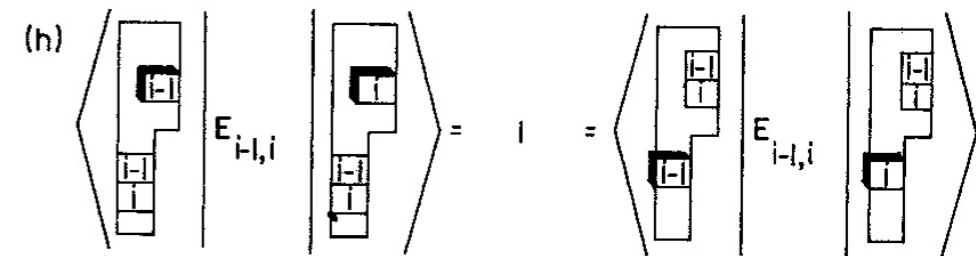
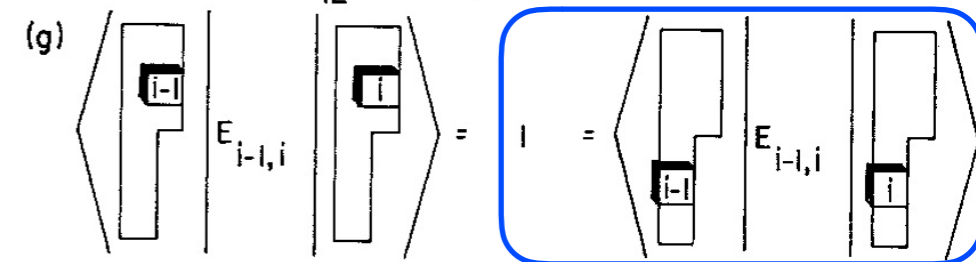
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(1-jump  $E_{i-1,i}$ )

(e)  $E_{23} \begin{vmatrix} 13 \\ 3 \end{vmatrix} = \frac{1}{\sqrt{2}} \begin{vmatrix} 12 \\ 3 \end{vmatrix} + \frac{\sqrt{3}}{\sqrt{2}} \begin{vmatrix} 13 \\ 2 \end{vmatrix}$

(f)  $E_{12} \begin{vmatrix} 11 \\ 2 \end{vmatrix} = \sqrt{2} \begin{vmatrix} 11 \\ 1 \end{vmatrix}$





# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

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	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$	
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $		.	$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $				.	$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $						.	$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$	

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$

(a)  $\langle T | E_{ii} | T \rangle = \delta_{T,T} \left( \begin{matrix} \text{number} \\ \text{of } (i)'s \end{matrix} \right)$       (b)  $\langle T | E_{ij} | T \rangle = \langle T | E_{ji} | T \rangle$

(c)  $\langle \begin{vmatrix} i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \end{vmatrix} \rangle = \sqrt{\frac{d+1}{d}} = \langle \begin{vmatrix} i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \end{vmatrix} \rangle$

(d)  $i=2, d=2$   
 $\langle \begin{vmatrix} i-1 \\ i \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \end{vmatrix} \rangle = \sqrt{\frac{d-1}{d}} = \langle \begin{vmatrix} i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i-1 \\ i \end{vmatrix} \rangle$

(e)  $E_{23} \begin{vmatrix} 13 \\ 3 \end{vmatrix} = \frac{1}{\sqrt{2}} \begin{vmatrix} 12 \\ 3 \end{vmatrix} + \frac{\sqrt{3}}{\sqrt{2}} \begin{vmatrix} 13 \\ 2 \end{vmatrix}$

(f)  $E_{12} \begin{vmatrix} 11 \\ 2 \end{vmatrix} = \sqrt{2} \begin{vmatrix} 11 \\ 3 \end{vmatrix}$

(g)  $\langle \begin{vmatrix} i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \end{vmatrix} \rangle = 1 = \langle \begin{vmatrix} i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \end{vmatrix} \rangle$

(h)  $\langle \begin{vmatrix} i-1 \\ i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \\ i \end{vmatrix} \rangle = 1 = \langle \begin{vmatrix} i-1 \\ i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \\ i \end{vmatrix} \rangle$

## Sample applications of "Jawbone" formulae

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{12} | \begin{vmatrix} 12 \\ 2 \end{vmatrix} \rangle = 1$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 11 \\ 3 \end{vmatrix} \rangle = 1$$

(1-jump  $E_{i-1,i}$ )

$$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = \sqrt{\frac{1}{2}}$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$	$M=-2$	
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$	
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $		.	$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $				.	$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $						.	$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$

(a)  $\langle T | E_{ii} | T \rangle = \delta_{T,T} \left( \begin{matrix} \text{number} \\ \text{of } (i)'s \end{matrix} \right)$       (b)  $\langle T | E_{ij} | T \rangle = \langle T | E_{ji} | T \rangle$

(c)  $i=2, d=2$   
 $\langle \begin{vmatrix} i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \end{vmatrix} \rangle = \sqrt{\frac{d+1}{d}} = \langle \begin{vmatrix} i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \end{vmatrix} \rangle$

(d)  $\langle \begin{vmatrix} i-1 \\ i \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \end{vmatrix} \rangle = \sqrt{\frac{d-1}{d}} = \langle \begin{vmatrix} i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \end{vmatrix} \rangle$

(e)  $E_{23} \begin{vmatrix} 13 \\ 3 \end{vmatrix} = \frac{1}{\sqrt{2}} \begin{vmatrix} 12 \\ 3 \end{vmatrix} + \frac{\sqrt{3}}{\sqrt{2}} \begin{vmatrix} 13 \\ 2 \end{vmatrix}$

(f)  $E_{12} \begin{vmatrix} 11 \\ 2 \end{vmatrix} = \sqrt{2} \begin{vmatrix} 11 \\ 3 \end{vmatrix}$

(g)  $\langle \begin{vmatrix} i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \end{vmatrix} \rangle = 1 = \langle \begin{vmatrix} i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \end{vmatrix} \rangle$

(h)  $\langle \begin{vmatrix} i-1 \\ i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \\ i \end{vmatrix} \rangle = 1 = \langle \begin{vmatrix} i-1 \\ i-1 \\ i-1 \end{vmatrix} | E_{i-1,i} | \begin{vmatrix} i \\ i \\ i \end{vmatrix} \rangle$

## Sample applications of "Jawbone" formulae

(1-jump  $E_{i-1,i}$ )

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{12} | \begin{vmatrix} 12 \\ 2 \end{vmatrix} \rangle = 1$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 11 \\ 3 \end{vmatrix} \rangle = 1$$

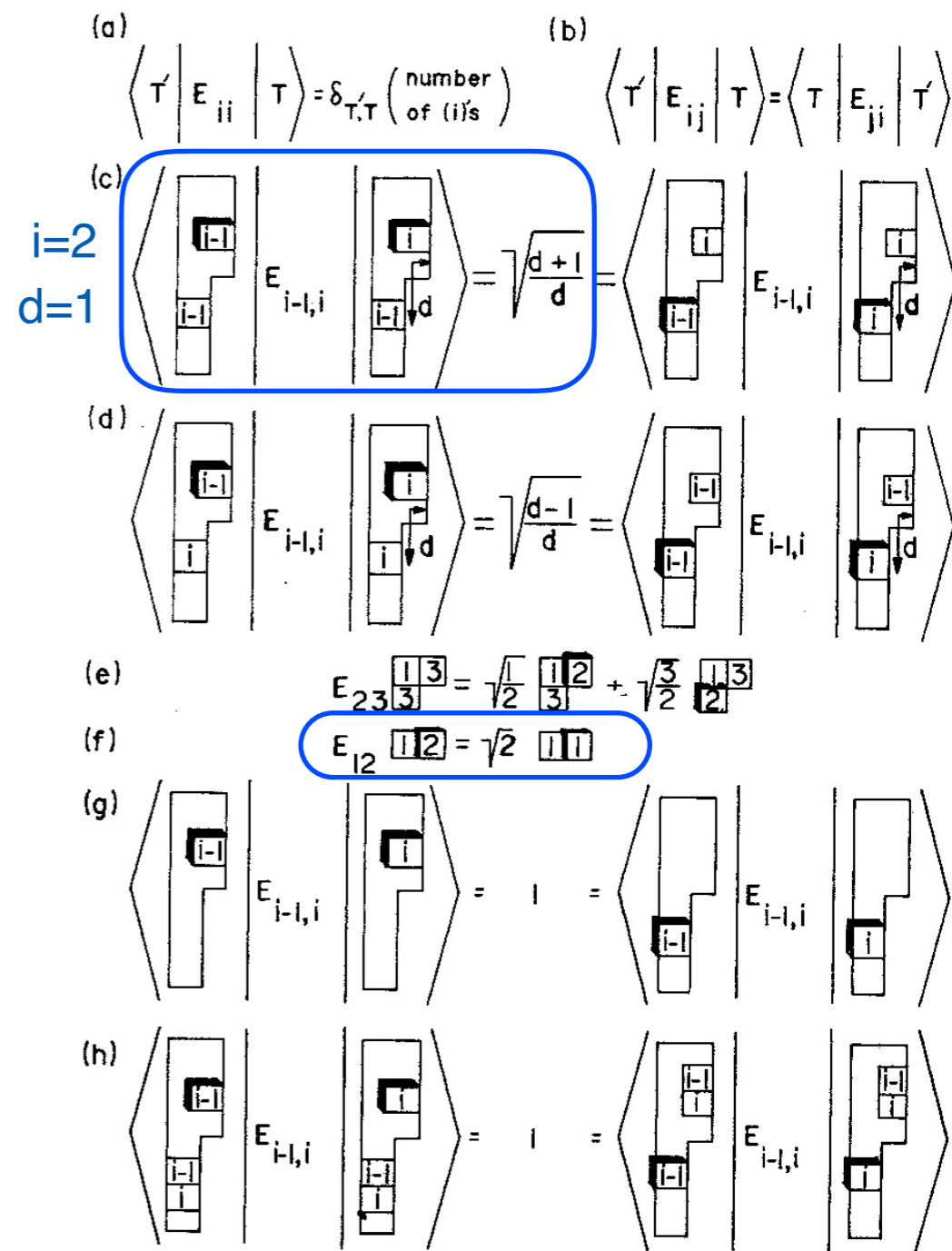
$$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 13 \\ 2 \end{vmatrix} \rangle = \sqrt{\frac{3}{2}}$$

$$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = \sqrt{\frac{1}{2}}$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$	$M=-2$	
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $		.	$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $				.	$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $						.	$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



## Sample applications of "Jawbone" formulae

(1-jump  $E_{i-1,i}$ )

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{12} | \begin{vmatrix} 12 \\ 2 \end{vmatrix} \rangle = 1 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 11 \\ 3 \end{vmatrix} \rangle = 1$$

$$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 13 \\ 2 \end{vmatrix} \rangle = \sqrt{\frac{3}{2}} \quad \langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = \sqrt{\frac{1}{2}}$$

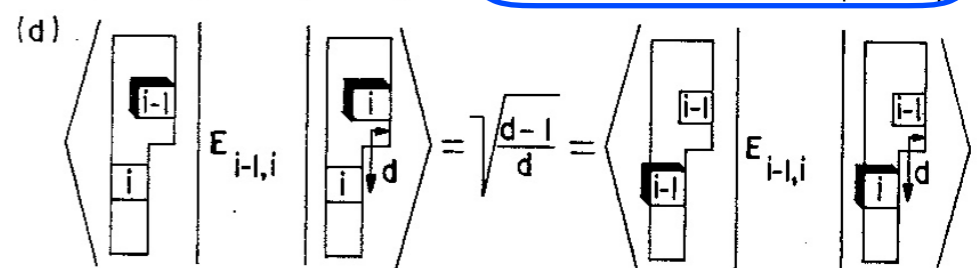
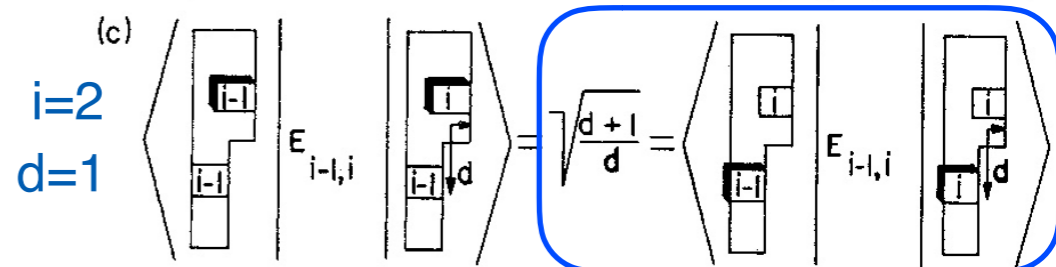
$$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix} | E_{12} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = \sqrt{2}$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

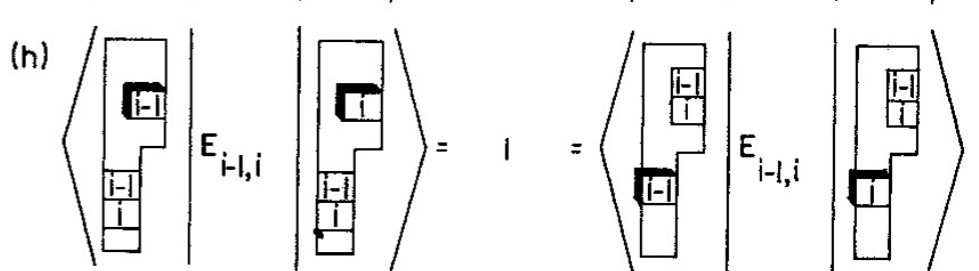
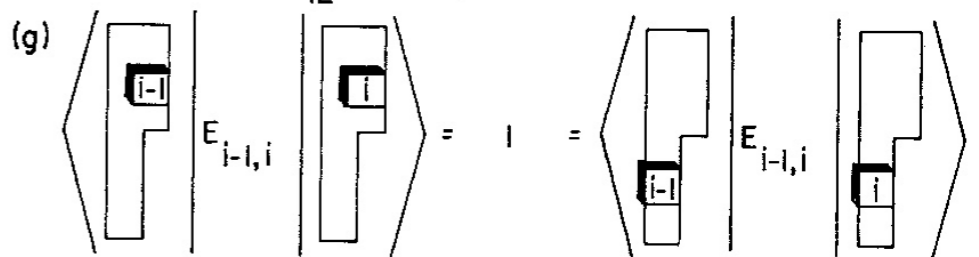
$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$

(a)  $\langle T | E_{ii} | T \rangle = \delta_{T,T} \left( \begin{matrix} \text{number} \\ \text{of } (i)'s \end{matrix} \right)$       (b)  $\langle T | E_{ij} | T \rangle = \langle T | E_{ji} | T \rangle$



(e)  $E_{23} \begin{vmatrix} 13 \\ 3 \end{vmatrix} = \frac{1}{\sqrt{2}} \begin{vmatrix} 12 \\ 3 \end{vmatrix} + \frac{\sqrt{3}}{\sqrt{2}} \begin{vmatrix} 13 \\ 2 \end{vmatrix}$

(f)  $E_{12} \begin{vmatrix} 11 \\ 2 \end{vmatrix} = \sqrt{2} \begin{vmatrix} 11 \\ 3 \end{vmatrix}$



## Sample applications of "Jawbone" formulae

(1-jump  $E_{i-1,i}$ )

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{12} | \begin{vmatrix} 12 \\ 2 \end{vmatrix} \rangle = 1 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 11 \\ 3 \end{vmatrix} \rangle = 1$$

$$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 13 \\ 2 \end{vmatrix} \rangle = \sqrt{\frac{3}{2}} \quad \langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = \sqrt{\frac{1}{2}}$$

$$\langle \begin{vmatrix} 12 \\ 3 \end{vmatrix} | E_{12} | \begin{vmatrix} 22 \\ 3 \end{vmatrix} \rangle = \sqrt{2} \quad \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix} | E_{12} | \begin{vmatrix} 22 \\ 3 \end{vmatrix} \rangle = \sqrt{2}$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$-\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\sqrt{2}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{2}$	$\sqrt{\frac{1}{2}}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\sqrt{\frac{3}{2}}$	.	$\sqrt{\frac{3}{2}}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$

(a)  $\langle T | E_{ii} | T \rangle = \delta_{T,T} \left( \begin{matrix} \text{number} \\ \text{of } (i\text{'s}) \end{matrix} \right)$       (b)  $\langle T | E_{ij} | T \rangle = \langle T | E_{ji} | T \rangle$

(c)  $\langle \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} | E_{i-1,i} | \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} \rangle = \sqrt{\frac{d+1}{d}} = \langle \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} | E_{i-1,i} | \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} \rangle$

(d)  $i=3$   
 $d=2$   
 $\langle \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} | E_{i-1,i} | \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} \rangle = \sqrt{\frac{d-1}{d}} = \langle \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} | E_{i-1,i} | \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} \rangle$

(e)  $E_{23} \begin{vmatrix} 13 \\ 3 \end{vmatrix} = \frac{1}{\sqrt{2}} \begin{vmatrix} 12 \\ 3 \end{vmatrix} + \frac{\sqrt{3}}{\sqrt{2}} \begin{vmatrix} 13 \\ 2 \end{vmatrix}$

(f)  $E_{12} \begin{vmatrix} 11 \\ 2 \end{vmatrix} = \sqrt{2} \begin{vmatrix} 11 \\ 3 \end{vmatrix}$

(g)  $\langle \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} | E_{i-1,i} | \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} \rangle = 1 = \langle \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} | E_{i-1,i} | \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} \rangle$

(h)  $\langle \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} | E_{i-1,i} | \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} \rangle = 1 = \langle \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} | E_{i-1,i} | \begin{matrix} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{matrix} \rangle$

## Sample applications of "Jawbone" formulae

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{12} | \begin{vmatrix} 12 \\ 2 \end{vmatrix} \rangle = 1$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 11 \\ 3 \end{vmatrix} \rangle = 1$$

(1-jump  $E_{i-1,i}$ )

$$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 13 \\ 2 \end{vmatrix} \rangle = \sqrt{\frac{3}{2}}$$

$$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = \sqrt{\frac{1}{2}}$$

$$\langle \begin{vmatrix} 12 \\ 3 \end{vmatrix} | E_{12} | \begin{vmatrix} 22 \\ 3 \end{vmatrix} \rangle = \sqrt{2}$$

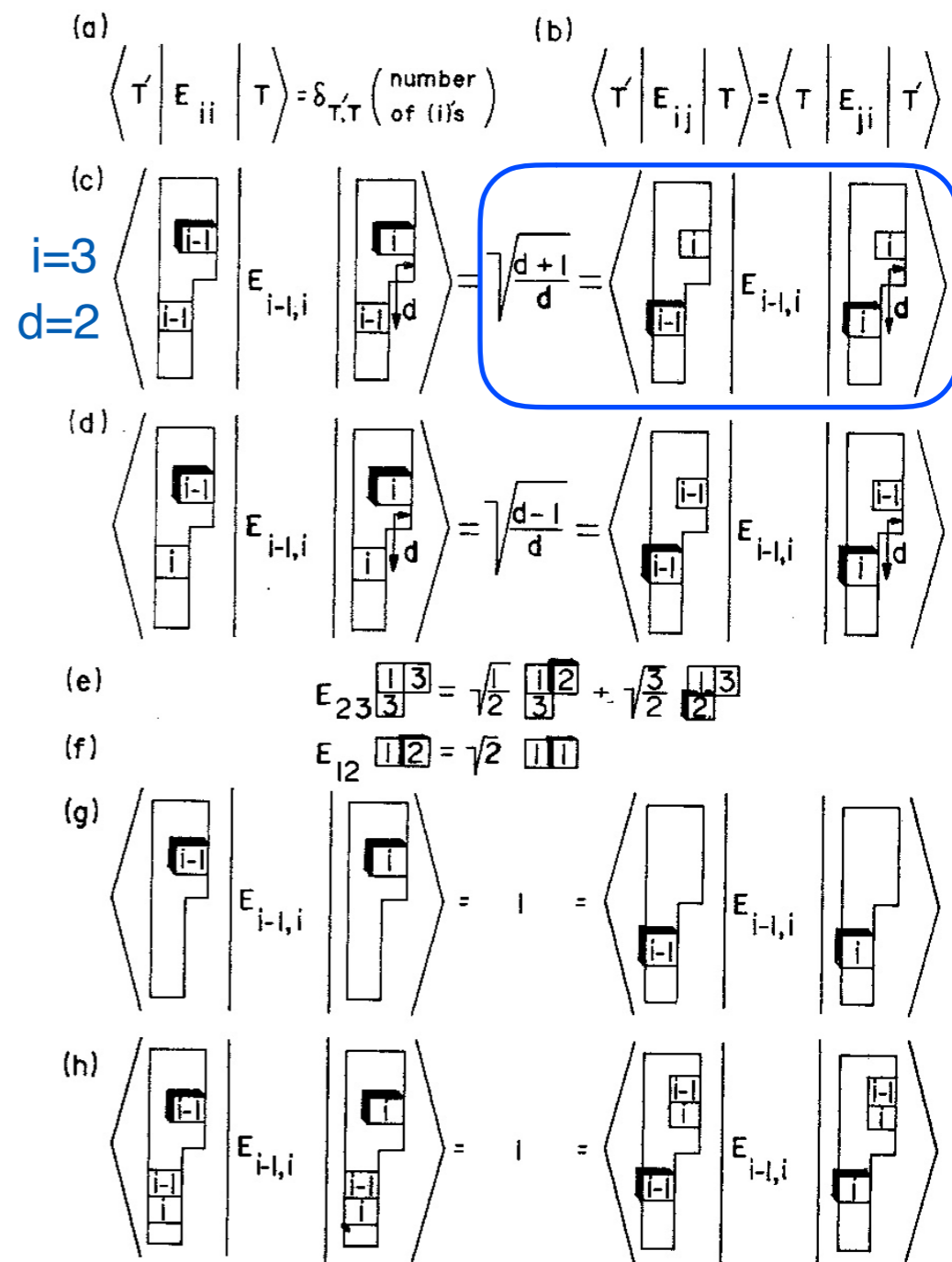
$$\langle \begin{vmatrix} 12 \\ 3 \end{vmatrix} | E_{12} | \begin{vmatrix} 22 \\ 3 \end{vmatrix} \rangle = \sqrt{2}$$

$$\langle \begin{vmatrix} 12 \\ 3 \end{vmatrix} | E_{23} | \begin{vmatrix} 13 \\ 3 \end{vmatrix} \rangle = \sqrt{\frac{1}{2}}$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



## Sample applications of "Jawbone" formulae

(1-jump  $E_{i-1,i}$ )

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{12} | \begin{vmatrix} 12 \\ 2 \end{vmatrix} \rangle = 1 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 11 \\ 3 \end{vmatrix} \rangle = 1$$

$$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 13 \\ 2 \end{vmatrix} \rangle = \sqrt{\frac{3}{2}} \quad \langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = \sqrt{\frac{1}{2}}$$

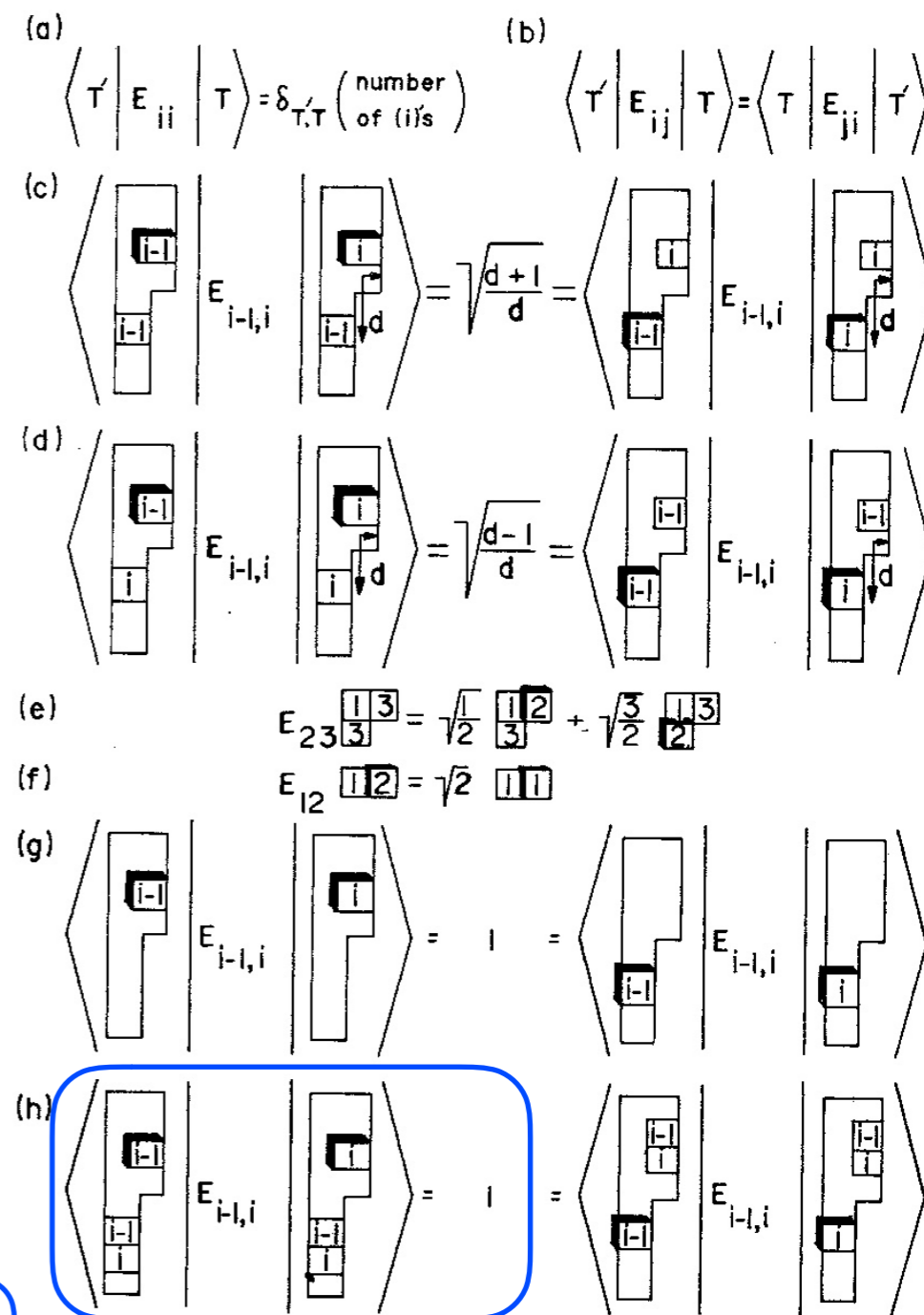
$$\langle \begin{vmatrix} 12 \\ 3 \end{vmatrix} | E_{12} | \begin{vmatrix} 22 \\ 3 \end{vmatrix} \rangle = \sqrt{2} \quad \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix} | E_{12} | \begin{vmatrix} 22 \\ 3 \end{vmatrix} \rangle = \sqrt{2}$$

$$\langle \begin{vmatrix} 12 \\ 3 \end{vmatrix} | E_{23} | \begin{vmatrix} 13 \\ 3 \end{vmatrix} \rangle = \sqrt{\frac{1}{2}} \quad \langle \begin{vmatrix} 13 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 13 \\ 3 \end{vmatrix} \rangle = \sqrt{\frac{3}{2}}$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$-\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	$(13)$ -1	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\sqrt{2}$	.	$(13)$ 1	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{2}$	$\sqrt{\frac{1}{2}}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\sqrt{\frac{3}{2}}$	.	$\sqrt{\frac{3}{2}}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$(12)$ 1
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



## Sample applications of "Jawbone" formulae

(1-jump  $E_{i-1,i}$ )

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{12} | \begin{vmatrix} 12 \\ 2 \end{vmatrix} \rangle = 1 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 11 \\ 3 \end{vmatrix} \rangle = 1$$

$$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 13 \\ 2 \end{vmatrix} \rangle = \sqrt{\frac{3}{2}} \quad \langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = \sqrt{\frac{1}{2}}$$

$$\langle \begin{vmatrix} 12 \\ 3 \end{vmatrix} | E_{12} | \begin{vmatrix} 22 \\ 3 \end{vmatrix} \rangle = \sqrt{2} \quad \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix} | E_{12} | \begin{vmatrix} 22 \\ 3 \end{vmatrix} \rangle = \sqrt{2}$$

$$\langle \begin{vmatrix} 12 \\ 3 \end{vmatrix} | E_{23} | \begin{vmatrix} 13 \\ 3 \end{vmatrix} \rangle = \sqrt{\frac{1}{2}} \quad \langle \begin{vmatrix} 13 \\ 2 \end{vmatrix} | E_{23} | \begin{vmatrix} 13 \\ 3 \end{vmatrix} \rangle = \sqrt{\frac{3}{2}}$$

$$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix} | E_{23} | \begin{vmatrix} 23 \\ 3 \end{vmatrix} \rangle = 1$$

# 4.16.18 class 23: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

## (S<sub>n</sub>)\*(U(m)) shell model of electrostatic quadrupole-quadrupole-e interactions

Complete set of E<sub>jk</sub> matrix elements for the doublet (spin-1/2) p<sup>3</sup> orbits

Detailed sample applications of “Jawbone” formulae

Number operators

1-jump E<sub>i-1,i</sub> operators

➔ 2-jump E<sub>i-2,i</sub> operators

Angular momentum operators (for later application)

Multipole expansions and Coulomb (e-e)-electrostatic interaction

Linear multipoles; P<sub>1</sub>-dipole, P<sub>2</sub>-quadrupole, P<sub>3</sub>-octupole,...

Moving off-axis: On-z-axis linear multipole P<sub>ℓ</sub> (cosθ) wave expansion:

**Multipole Addition Theorem (should be called Group Multiplication Theorem)**

Coulomb (e-e)-electrostatic interaction and its Hamiltonian Matrix, Slater integrals

2-particle elementary e<sub>jk</sub> operator expressions for (e-e)-interaction matrix

Tensor tables are (2ℓ+1)-by-(2ℓ+1) arrays (p<sup>k</sup><sub>q</sub>) giving V<sub>q</sub><sup>k</sup> in terms of E<sub>p,q</sub>.

Relating V<sub>q</sub><sup>k</sup> to E<sub>m',m</sub> by (m'<sup>k</sup><sub>m</sub>) arrays

Atomic p-shell ee-interaction in elementary operator form

[2,1] tableau basis (from p.29) and matrices of v<sup>1</sup> dipole and v<sup>1</sup>•v<sup>1</sup>=L•L

[2,1] tableau basis (from p.29) and matrices of v<sup>2</sup> and v<sup>2</sup>•v<sup>2</sup> quadrupole

<sup>4</sup>S, <sup>2</sup>P, and <sup>2</sup>D energy calculation of quartet and doublet (spin-1/2) p<sup>3</sup> orbits

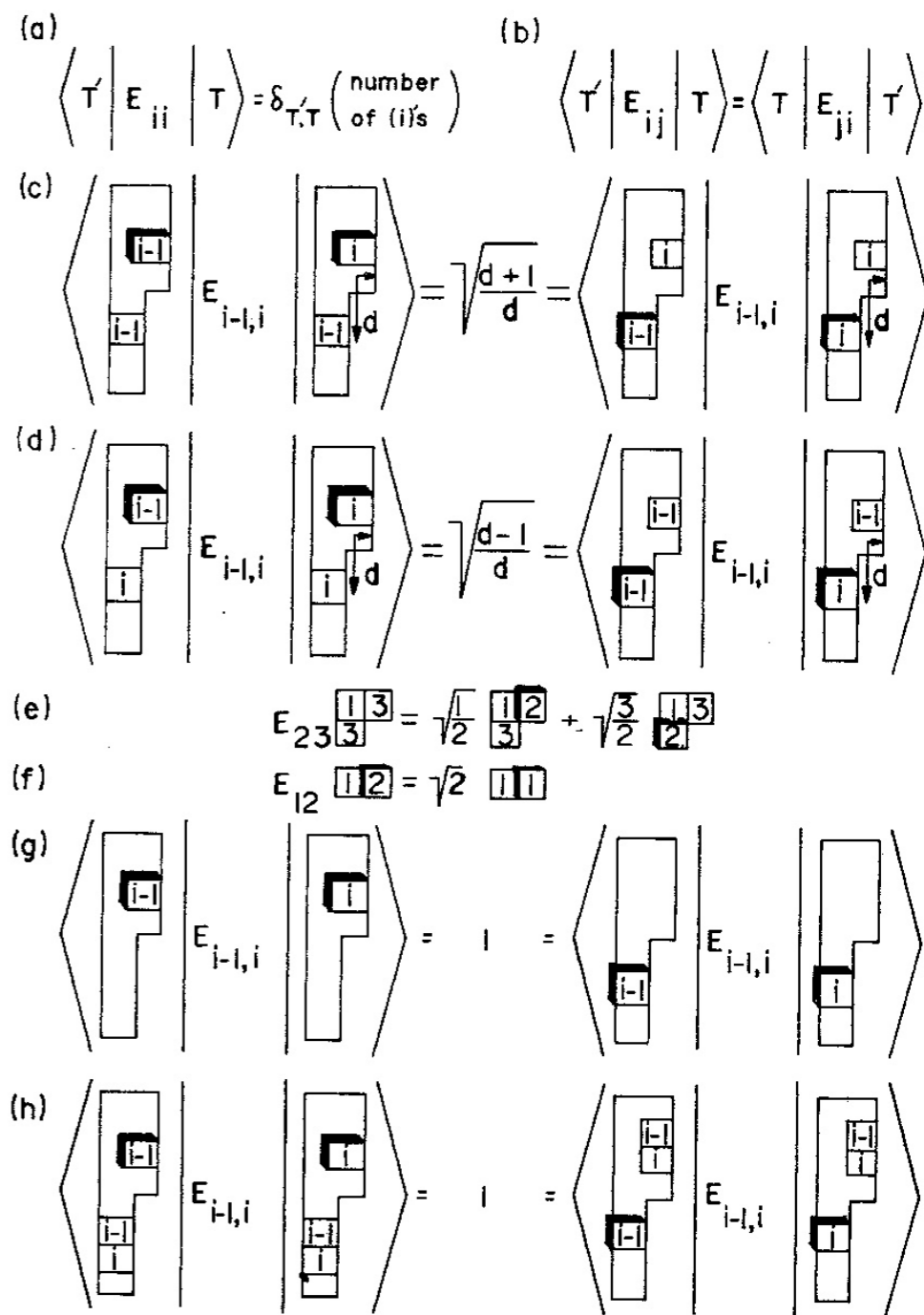
Corrected level diagrams Nitrogen p<sup>3</sup>



# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $		.	$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $				.	$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $						.	$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



## Sample applications of "Jawbone" formulae

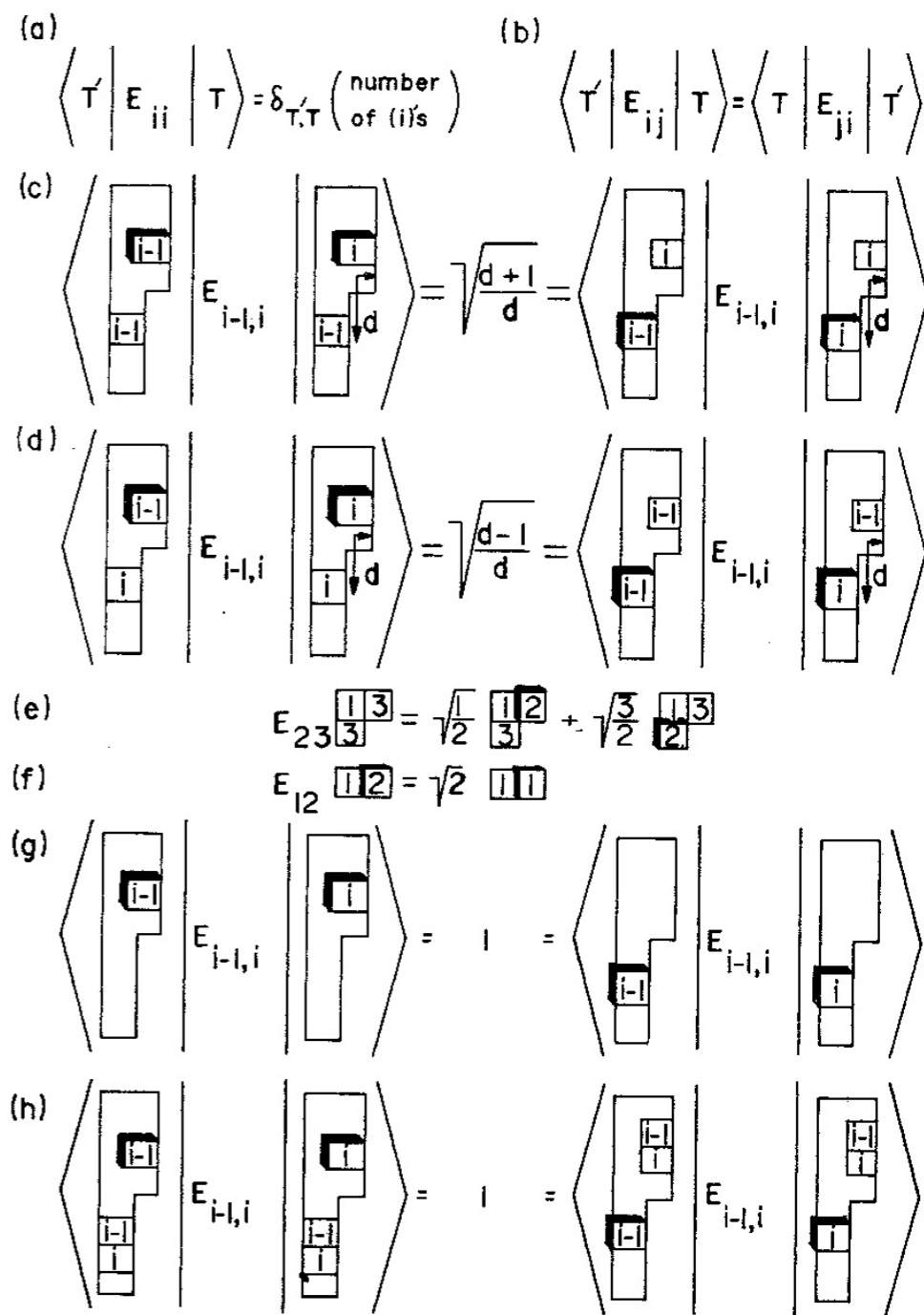
$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} - E_{23}E_{12} \quad (2\text{-jump } E_{i-2,i})$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = ??$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$	$M=-2$	
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



## Sample applications of "Jawbone" formulae

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} - E_{23}E_{12} \quad (2\text{-jump } E_{i-2,i})$$

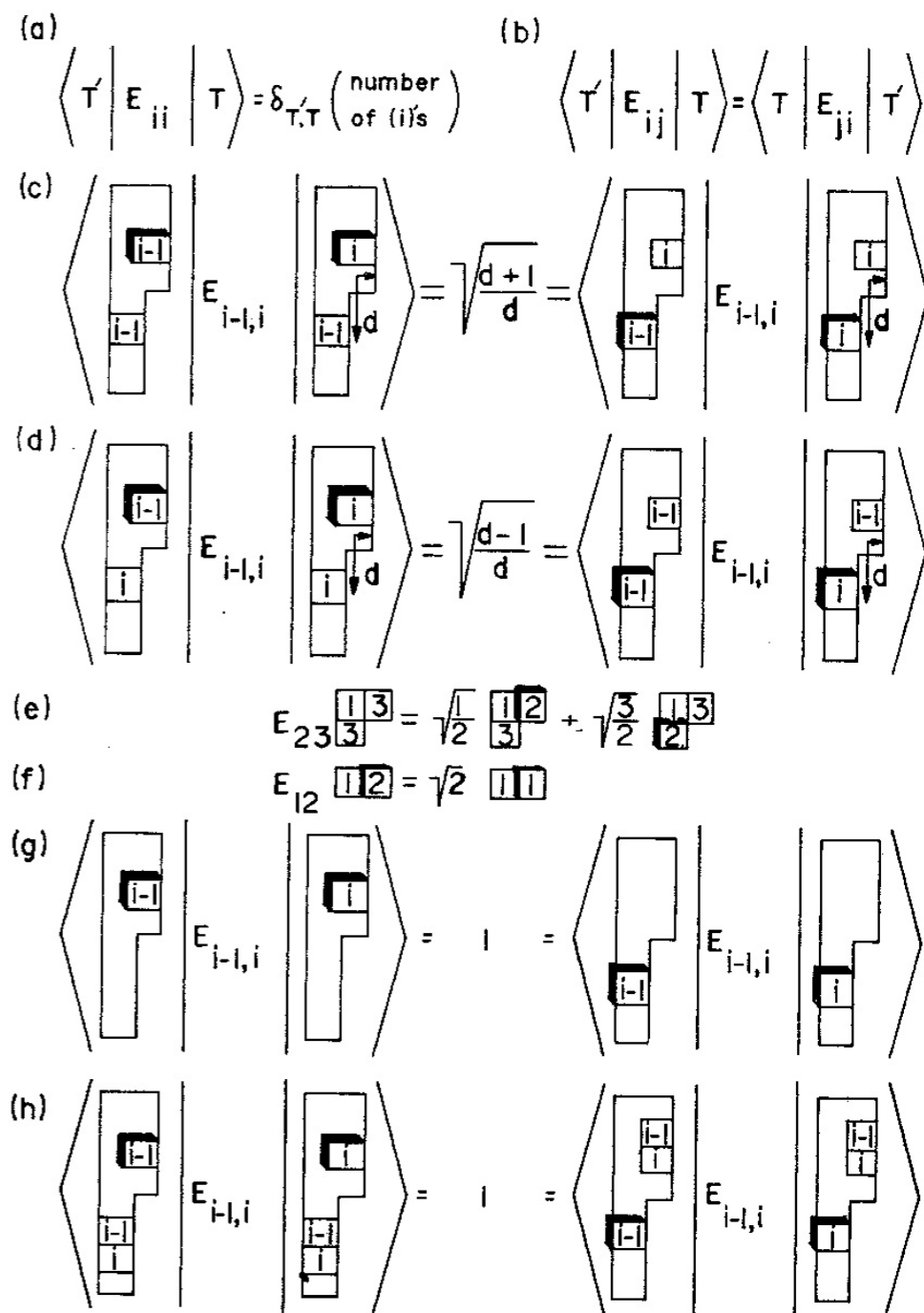
$$E_{13} \begin{vmatrix} 12 \\ 3 \end{vmatrix} = E_{12}E_{23} \begin{vmatrix} 12 \\ 3 \end{vmatrix} - E_{23}E_{12} \begin{vmatrix} 12 \\ 3 \end{vmatrix}$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = ??$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$	$M=-2$	
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



## Sample applications of "Jawbone" formulae

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} - E_{23}E_{12} \quad (2\text{-jump } E_{i-2,i})$$

$$E_{13} \begin{vmatrix} 12 \\ 3 \end{vmatrix} = E_{12} E_{23} \begin{vmatrix} 12 \\ 3 \end{vmatrix} - E_{23} E_{12} \begin{vmatrix} 12 \\ 3 \end{vmatrix}$$

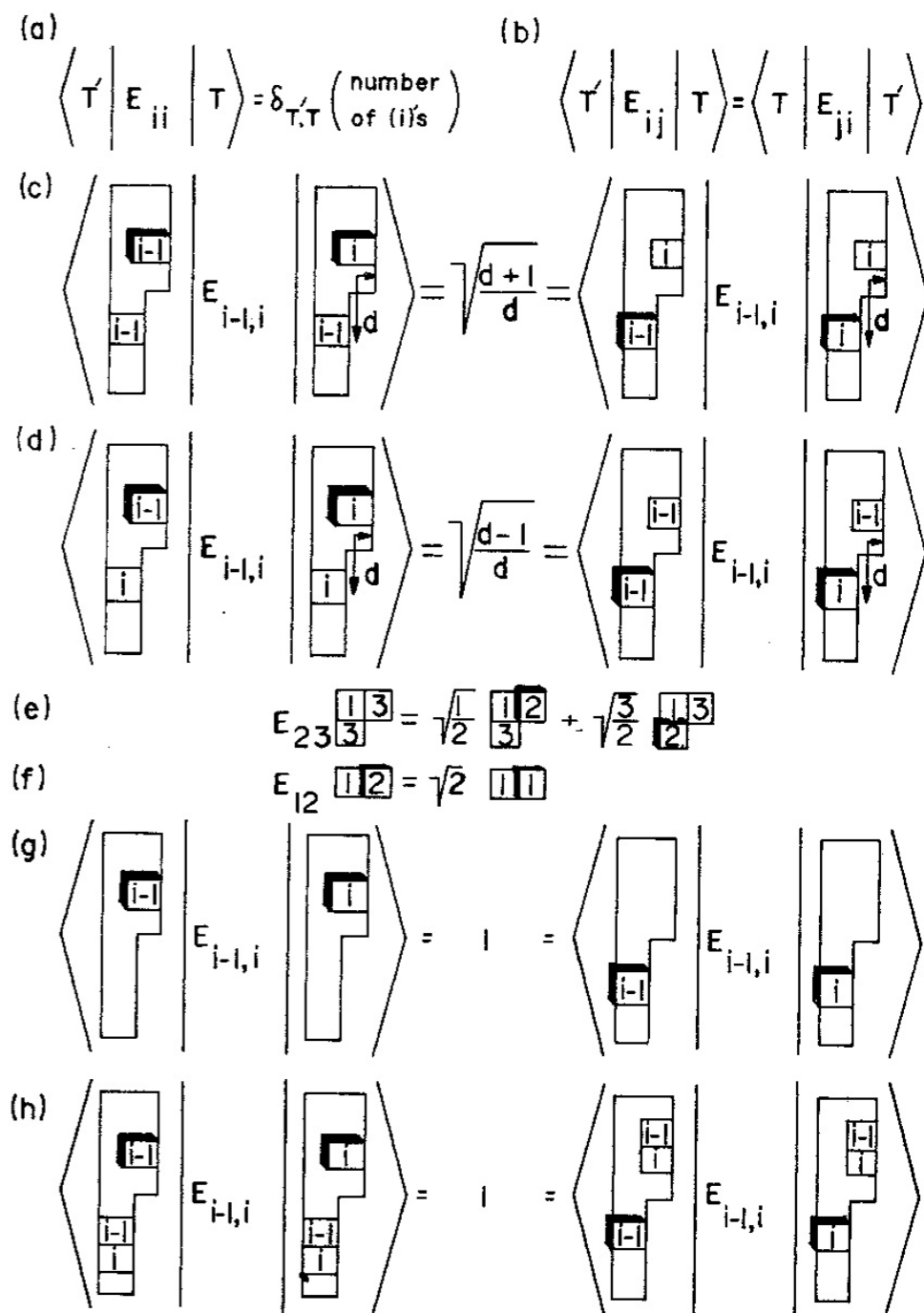
$$= E_{12} \sqrt{\frac{1}{2}} \begin{vmatrix} 12 \\ 2 \end{vmatrix} - E_{23} \sqrt{2} \begin{vmatrix} 11 \\ 3 \end{vmatrix}$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = ??$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$	$M=-2$	
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $		.	$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $				.	$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $						.	$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



## Sample applications of "Jawbone" formulae

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} - E_{23}E_{12} \quad (2\text{-jump } E_{i-2,i})$$

$$E_{13} \begin{vmatrix} 12 \\ 3 \end{vmatrix} = E_{12} E_{23} \begin{vmatrix} 12 \\ 3 \end{vmatrix} - E_{23} E_{12} \begin{vmatrix} 12 \\ 3 \end{vmatrix}$$

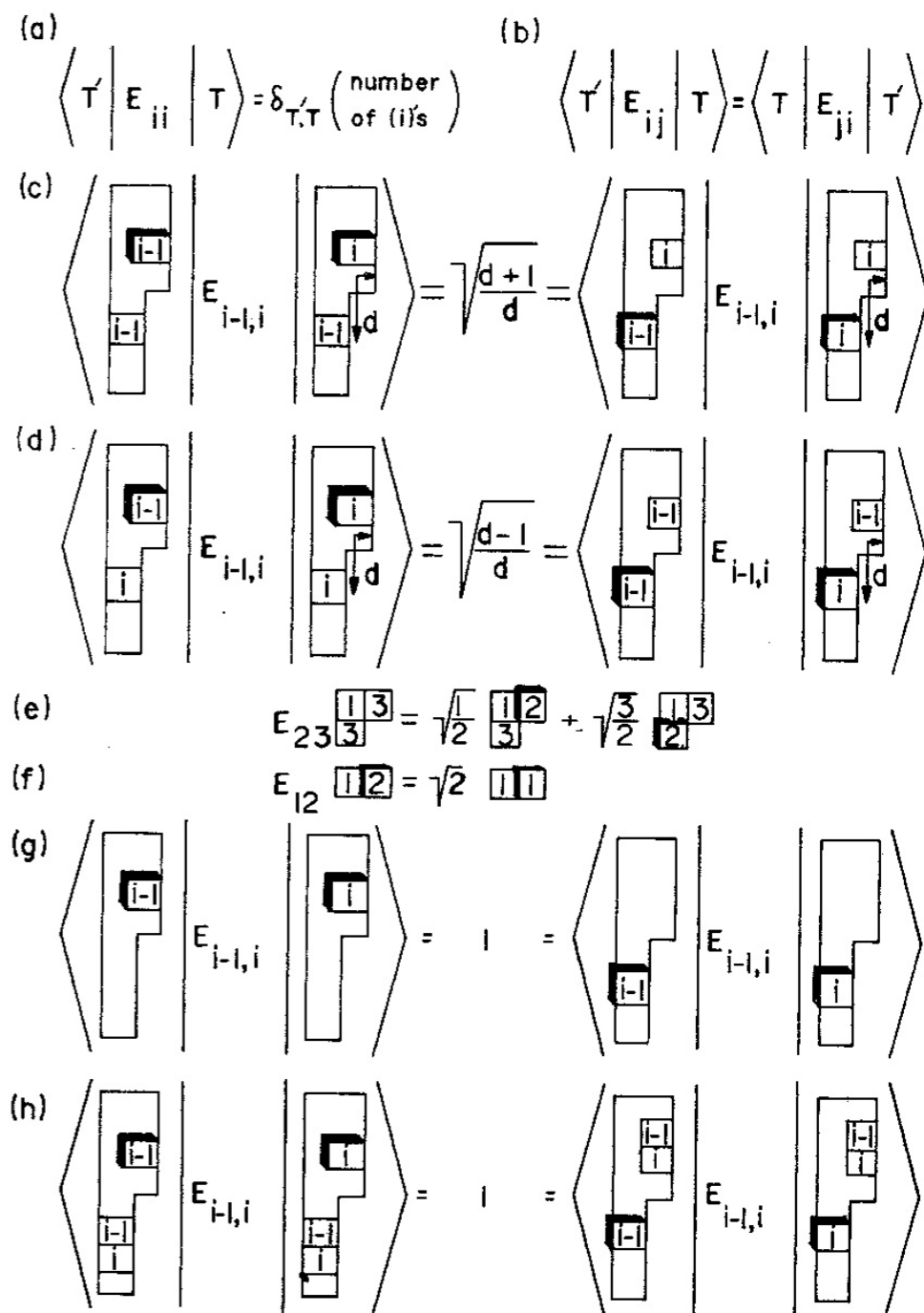
$$= E_{12} \sqrt{\frac{1}{2}} \begin{vmatrix} 12 \\ 2 \end{vmatrix} - E_{23} \sqrt{2} \begin{vmatrix} 11 \\ 3 \end{vmatrix}$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = ??$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$	$M=-2$	
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



## Sample applications of "Jawbone" formulae

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} - E_{23}E_{12} \quad (2\text{-jump } E_{i-2,i})$$

$$E_{13} \begin{vmatrix} 12 \\ 3 \end{vmatrix} = E_{12} E_{23} \begin{vmatrix} 12 \\ 3 \end{vmatrix} - E_{23} E_{12} \begin{vmatrix} 12 \\ 3 \end{vmatrix}$$

$$= E_{12} \sqrt{\frac{1}{2}} \begin{vmatrix} 12 \\ 2 \end{vmatrix} - E_{23} \sqrt{2} \begin{vmatrix} 11 \\ 3 \end{vmatrix}$$

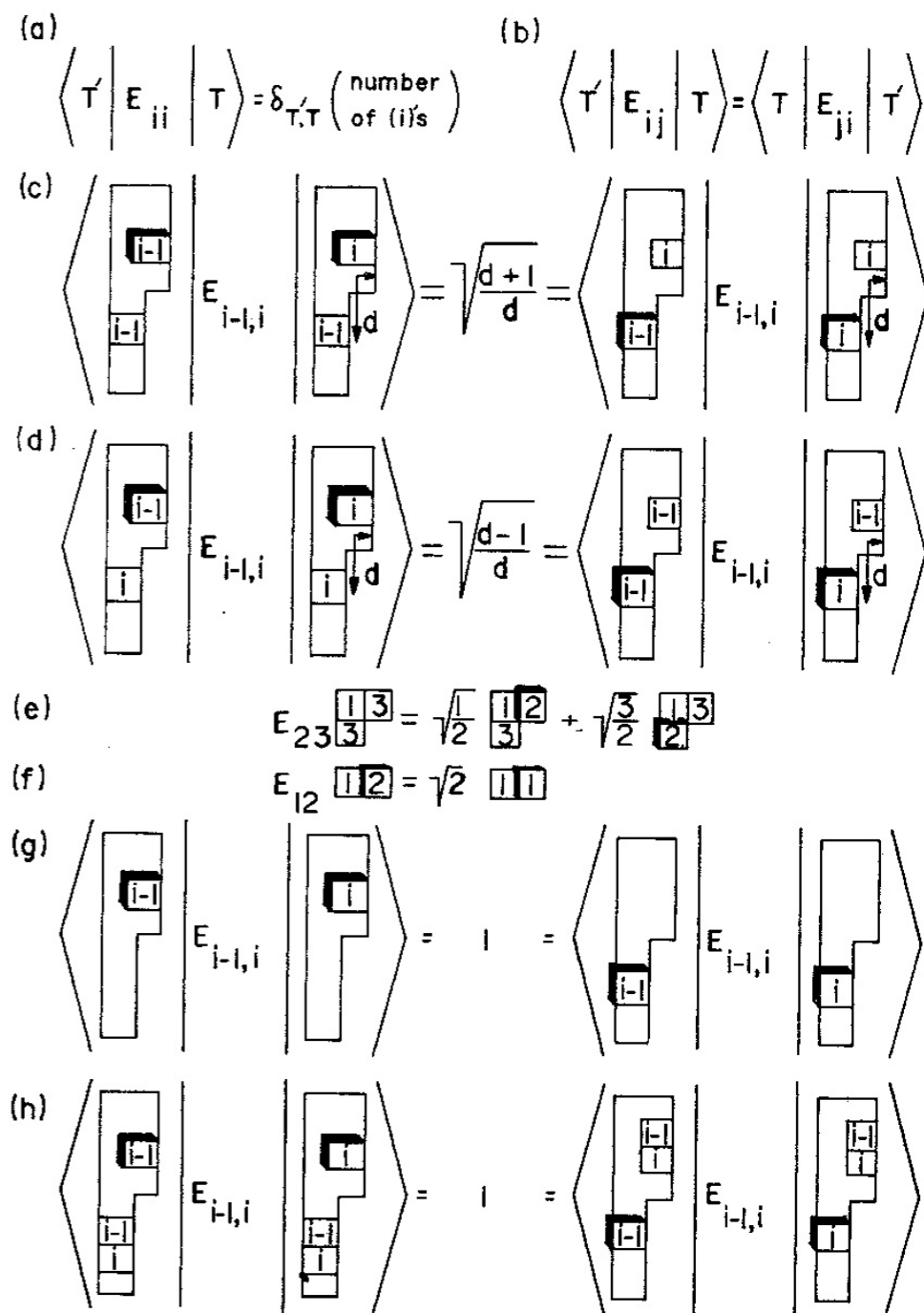
$$= 1 \sqrt{\frac{1}{2}} \begin{vmatrix} 11 \\ 2 \end{vmatrix} - 1 \sqrt{2} \begin{vmatrix} 11 \\ 2 \end{vmatrix}$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = ??$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$	$M=-2$	
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



## Sample applications of "Jawbone" formulae

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} - E_{23}E_{12} \quad (2\text{-jump } E_{i-2,i})$$

$$E_{13} \begin{vmatrix} 12 \\ 3 \end{vmatrix} = E_{12} E_{23} \begin{vmatrix} 12 \\ 3 \end{vmatrix} - E_{23} E_{12} \begin{vmatrix} 12 \\ 3 \end{vmatrix}$$

$$= E_{12} \sqrt{\frac{1}{2}} \begin{vmatrix} 12 \\ 2 \end{vmatrix} - E_{23} \sqrt{2} \begin{vmatrix} 11 \\ 3 \end{vmatrix}$$

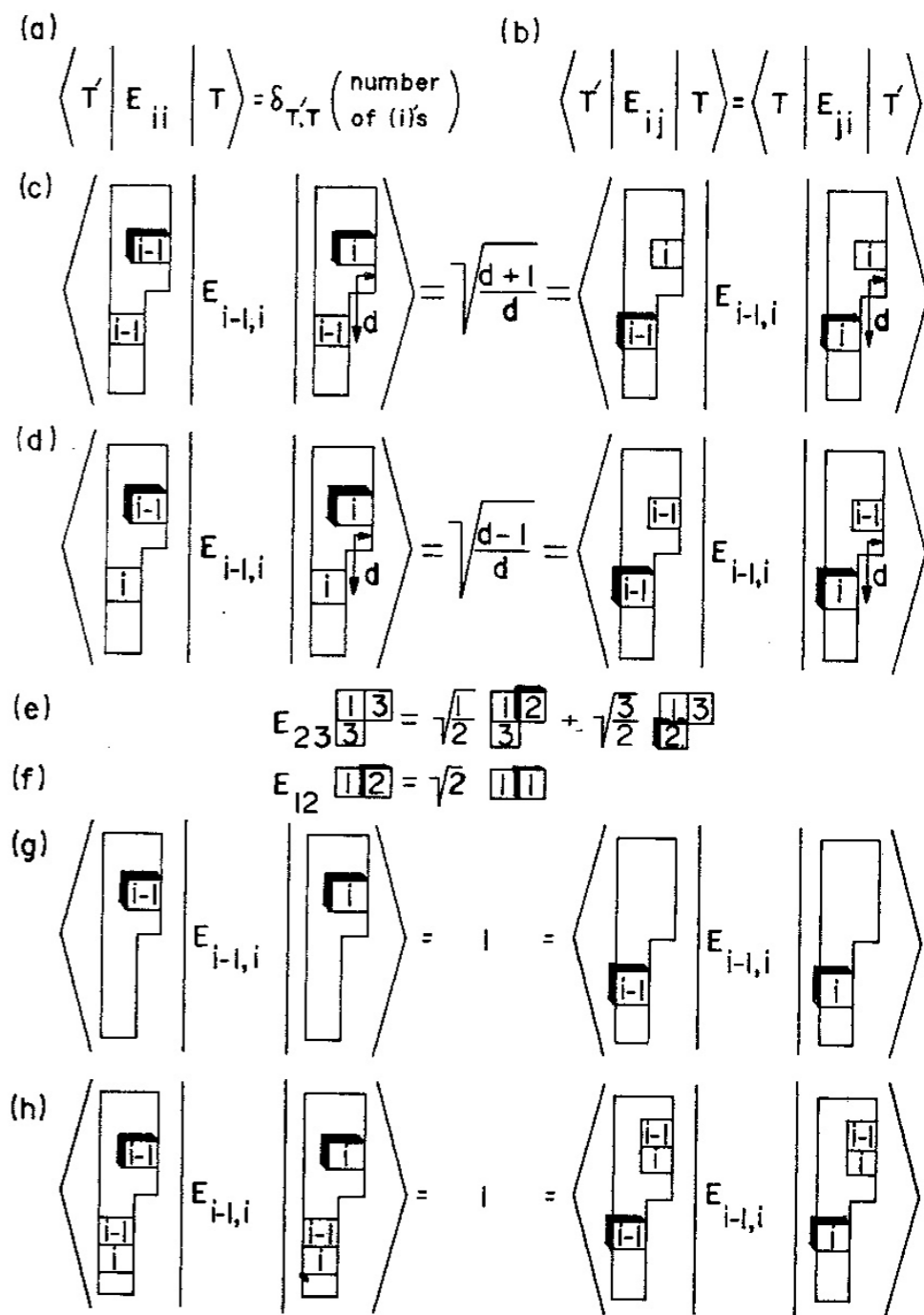
$$= 1 \sqrt{\frac{1}{2}} \begin{vmatrix} 11 \\ 2 \end{vmatrix} - 1 \sqrt{2} \begin{vmatrix} 11 \\ 2 \end{vmatrix}$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = ??$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$	$M=-2$	
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



## Sample applications of "Jawbone" formulae

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} - E_{23}E_{12} \quad (2\text{-jump } E_{i-2,i})$$

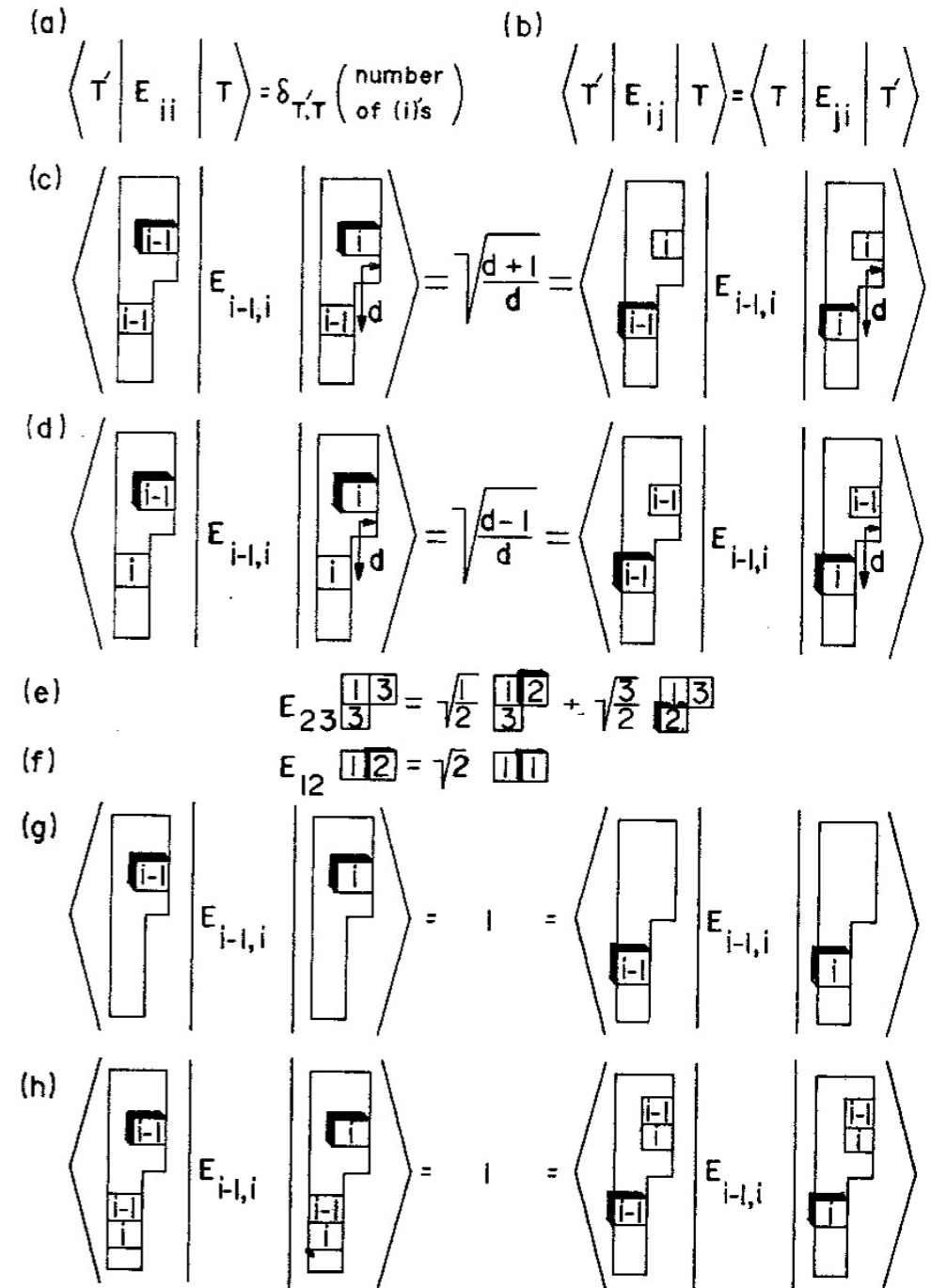
$$\begin{aligned} E_{13} \begin{vmatrix} 12 \\ 3 \end{vmatrix} &= E_{12} E_{23} \begin{vmatrix} 12 \\ 3 \end{vmatrix} - E_{23} E_{12} \begin{vmatrix} 12 \\ 3 \end{vmatrix} \\ &= E_{12} \sqrt{\frac{1}{2}} \begin{vmatrix} 12 \\ 2 \end{vmatrix} - E_{23} \sqrt{2} \begin{vmatrix} 11 \\ 3 \end{vmatrix} \\ &= 1 \sqrt{\frac{1}{2}} \begin{vmatrix} 11 \\ 2 \end{vmatrix} - 1 \sqrt{2} \begin{vmatrix} 11 \\ 2 \end{vmatrix} \end{aligned}$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 12 \\ 3 \end{vmatrix} \rangle = \sqrt{\frac{1}{2}} - \sqrt{2} = -\sqrt{\frac{1}{2}}$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$-\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $		.	$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\sqrt{2}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{2}$	$\sqrt{\frac{1}{2}}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $				.	$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\sqrt{\frac{3}{2}}$	.	$\sqrt{\frac{3}{2}}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $						.	$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



## Sample applications of "Jawbone" formulae

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} - E_{23}E_{12} \quad (2\text{-jump } E_{i-2,i})$$

$$E_{13} \begin{vmatrix} 13 \\ 2 \end{vmatrix} = E_{12}E_{23} \begin{vmatrix} 13 \\ 2 \end{vmatrix} - E_{23}E_{12} \begin{vmatrix} 13 \\ 2 \end{vmatrix}$$

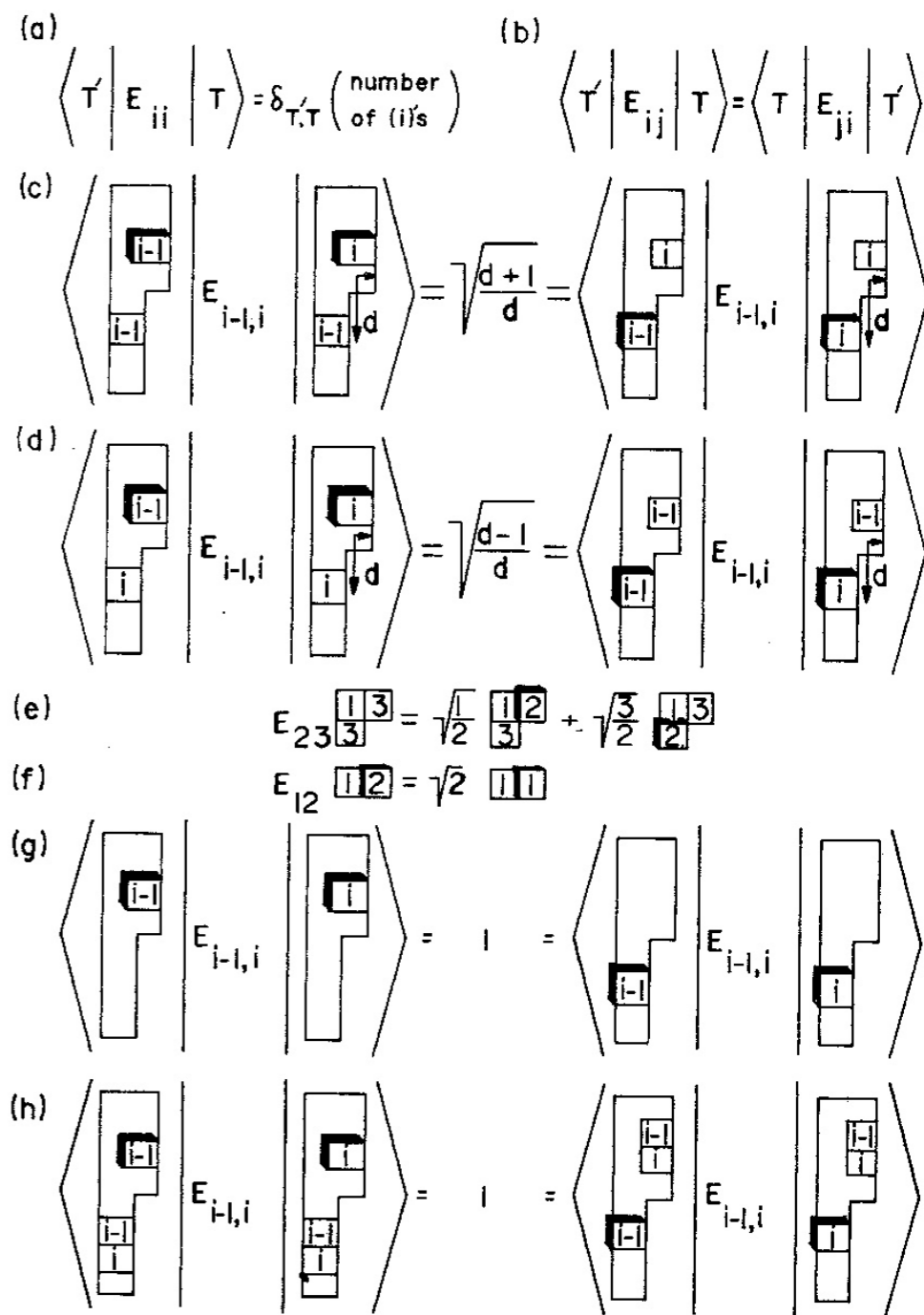
$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 13 \\ 2 \end{vmatrix} \rangle = ??$$



# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$-\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\sqrt{2}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{2}$	$\sqrt{\frac{1}{2}}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\sqrt{\frac{3}{2}}$	.	$\sqrt{\frac{3}{2}}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



## Sample applications of "Jawbone" formulae

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} - E_{23}E_{12} \quad (2\text{-jump } E_{i-2,i})$$

$$E_{13} \begin{vmatrix} 13 \\ 2 \end{vmatrix} = E_{12}E_{23} \begin{vmatrix} 13 \\ 2 \end{vmatrix} - E_{23}E_{12} \begin{vmatrix} 13 \\ 2 \end{vmatrix}$$

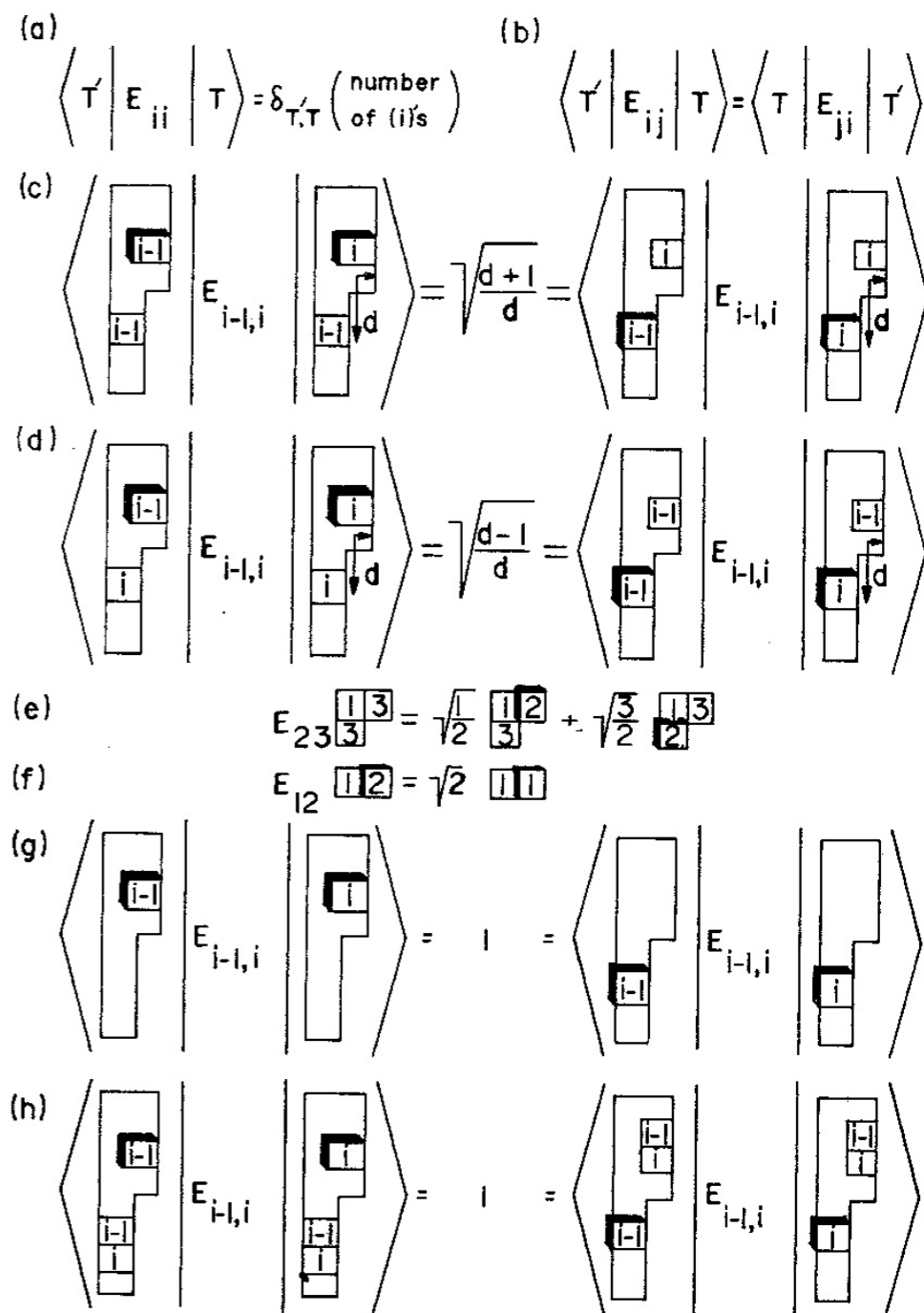
$$= E_{12} \sqrt{\frac{3}{2}} \begin{vmatrix} 12 \\ 2 \end{vmatrix} - E_{23} 0 \begin{vmatrix} 13 \\ 1 \end{vmatrix}$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 13 \\ 2 \end{vmatrix} \rangle = ??$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $	.	$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $	.	.	$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $	.	.	.	$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $	.	.	.	.	$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $	.	.	.	.	.	$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $	.	.	.	.	.	.	$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $	.	.	.	.	.	.	.	$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



## Sample applications of "Jawbone" formulae

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} - E_{23}E_{12} \quad (2\text{-jump } E_{i-2,i})$$

$$E_{13} \begin{vmatrix} 13 \\ 2 \end{vmatrix} = E_{12}E_{23} \begin{vmatrix} 13 \\ 2 \end{vmatrix} - E_{23}E_{12} \begin{vmatrix} 13 \\ 2 \end{vmatrix}$$

$$= E_{12} \sqrt{\frac{3}{2}} \begin{vmatrix} 12 \\ 2 \end{vmatrix} - E_{23} 0 \begin{vmatrix} 13 \\ 1 \end{vmatrix}$$

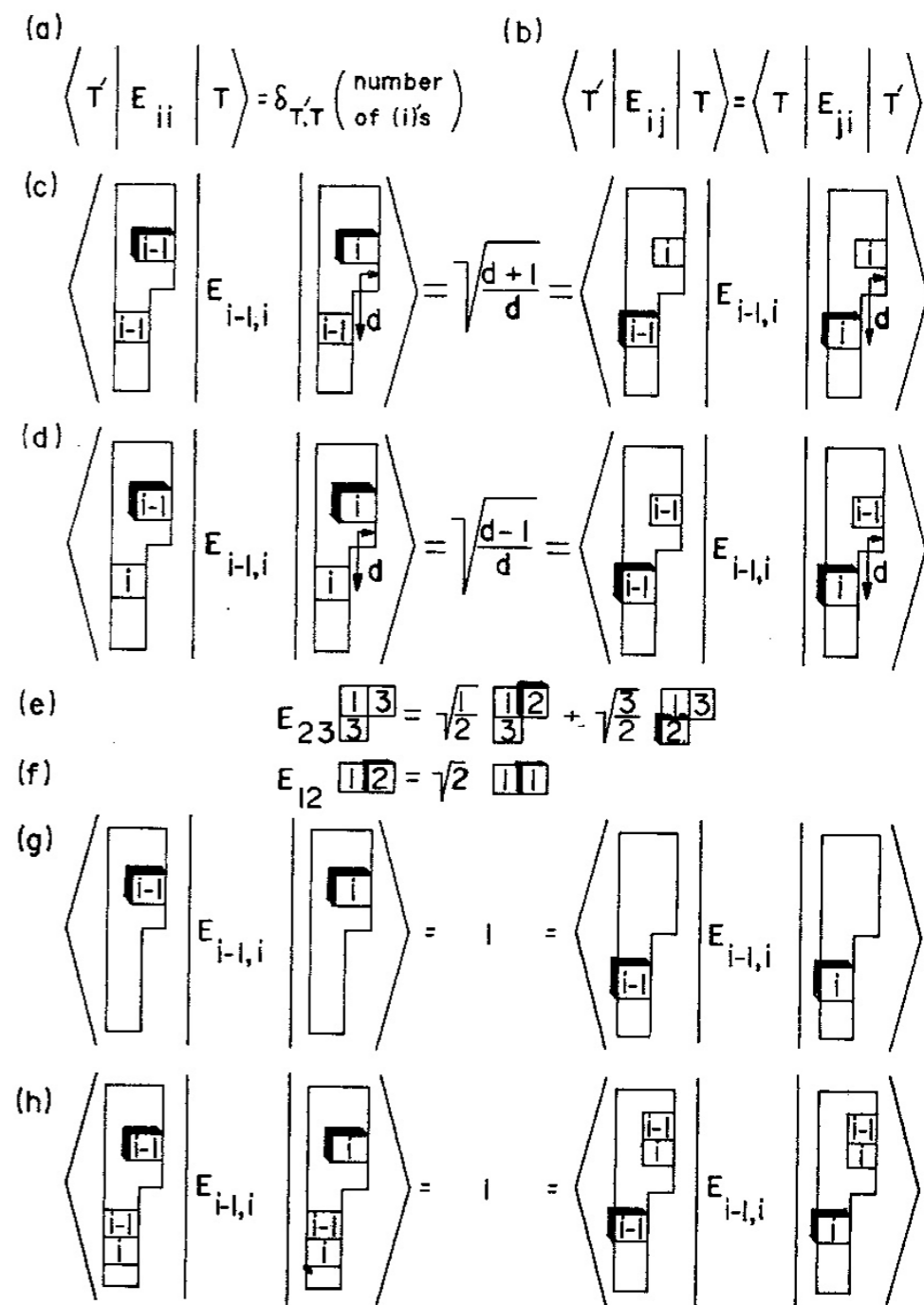
$$= 1 \sqrt{\frac{3}{2}} \begin{vmatrix} 11 \\ 2 \end{vmatrix} - 0$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 13 \\ 2 \end{vmatrix} \rangle = ??$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$-\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\sqrt{2}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{2}$	$\sqrt{\frac{1}{2}}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\sqrt{\frac{3}{2}}$	.	$\sqrt{\frac{3}{2}}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



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$$E_{13} \begin{vmatrix} 13 \\ 2 \end{vmatrix} = E_{12}E_{23} \begin{vmatrix} 13 \\ 2 \end{vmatrix} - E_{23}E_{12} \begin{vmatrix} 13 \\ 2 \end{vmatrix}$$

$$= E_{12} \sqrt{\frac{3}{2}} \begin{vmatrix} 12 \\ 2 \end{vmatrix} - E_{23} 0 \begin{vmatrix} 13 \\ 1 \end{vmatrix}$$

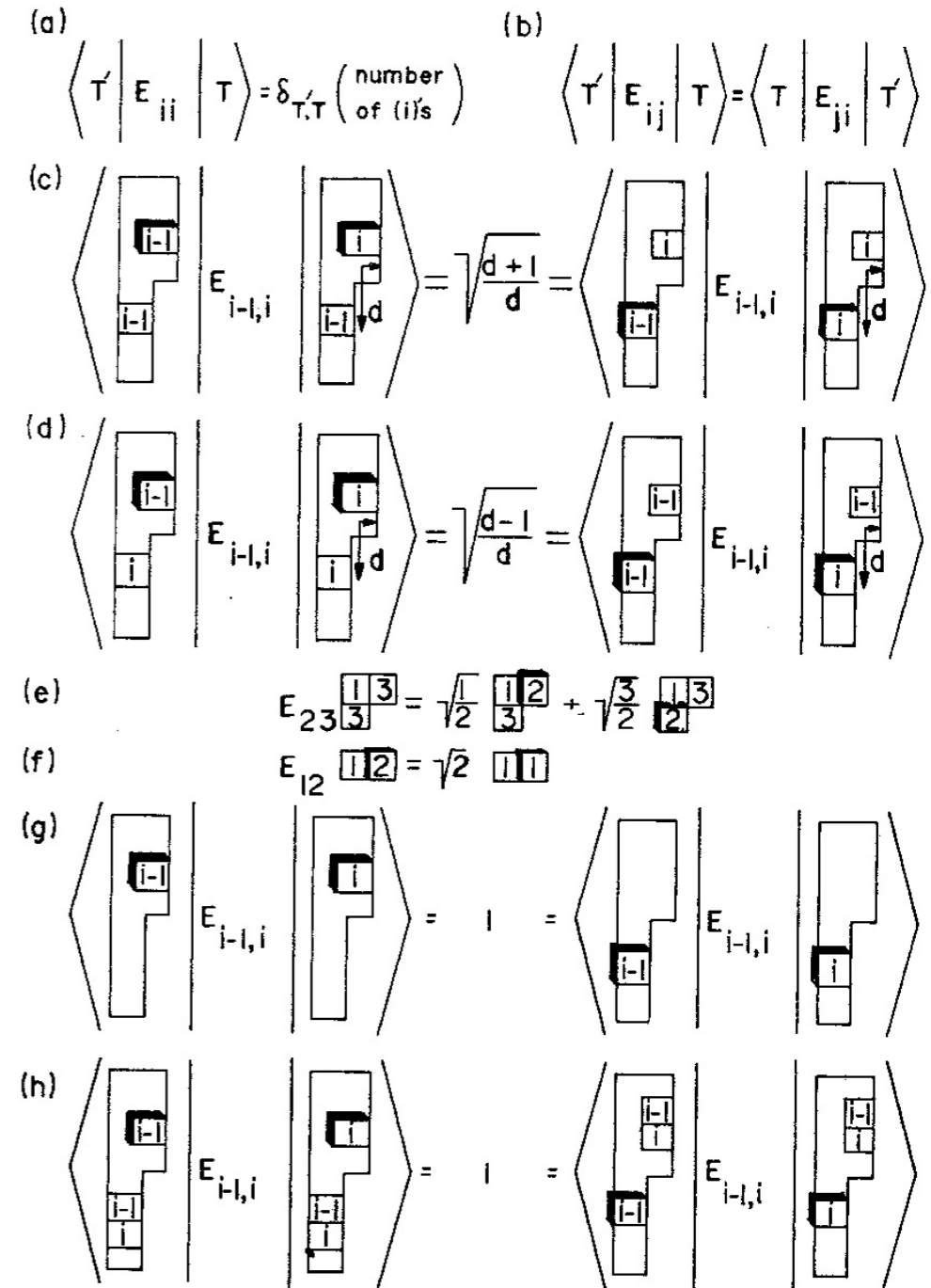
$$= 1 \sqrt{\frac{3}{2}} \begin{vmatrix} 11 \\ 2 \end{vmatrix} - 0$$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 13 \\ 2 \end{vmatrix} \rangle = \sqrt{\frac{3}{2}}$$

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	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



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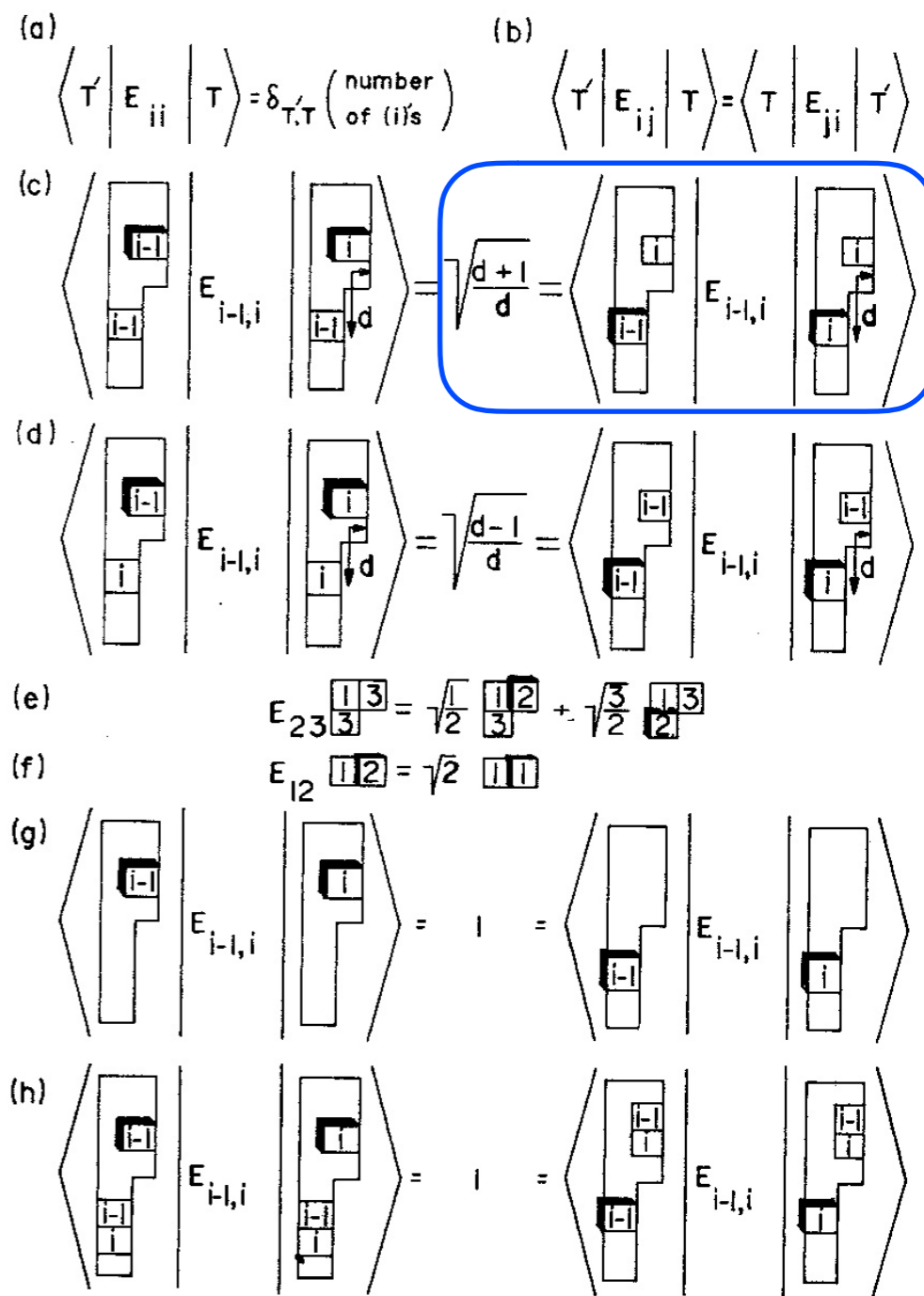
$$E_{13} \begin{vmatrix} 22 \\ 3 \end{vmatrix} = E_{12}E_{23} \begin{vmatrix} 22 \\ 3 \end{vmatrix} - E_{23}E_{12} \begin{vmatrix} 22 \\ 3 \end{vmatrix}$$

$$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 22 \\ 3 \end{vmatrix} \rangle = ??$$

# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
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$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
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$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$



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$$E_{13} \begin{vmatrix} 22 \\ 3 \end{vmatrix} = 0 - E_{23} \sqrt{2} \begin{vmatrix} 12 \\ 3 \end{vmatrix}$$

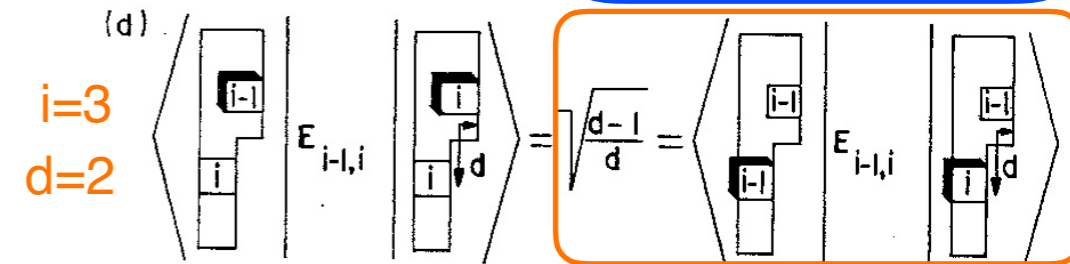
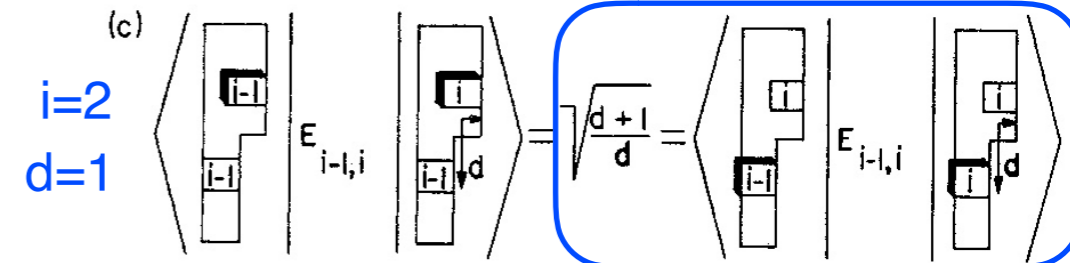
$$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 22 \\ 3 \end{vmatrix} \rangle = ??$$

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	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$-\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\sqrt{2}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{2}$	$\sqrt{\frac{1}{2}}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\sqrt{\frac{3}{2}}$	.	$\sqrt{\frac{3}{2}}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 22 \\ 3 \end{vmatrix}  $							$\begin{matrix} (22) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1+2 \end{matrix}$

$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$

(a)  $\langle T | E_{ii} | T \rangle = \delta_{T,T} \left( \begin{matrix} \text{number} \\ \text{of } (i)'s \end{matrix} \right)$       (b)  $\langle T | E_{ij} | T \rangle = \langle T | E_{ji} | T \rangle$



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$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} - E_{23}E_{12} \quad (2\text{-jump } E_{i-2,i})$$

$$E_{13} \begin{vmatrix} 12 \\ 2 \end{vmatrix} = E_{12}E_{23} \begin{vmatrix} 22 \\ 3 \end{vmatrix} - E_{23}E_{12} \begin{vmatrix} 22 \\ 3 \end{vmatrix}$$

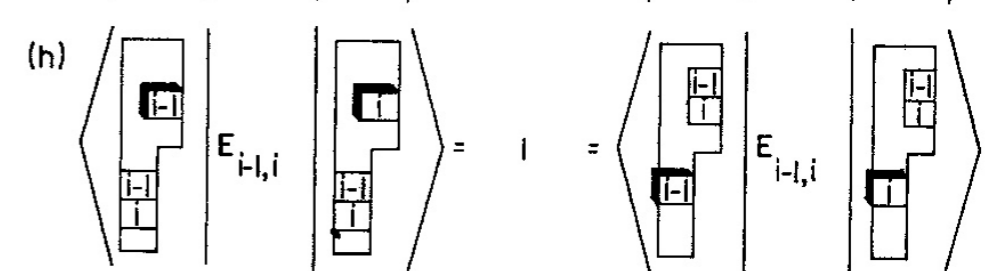
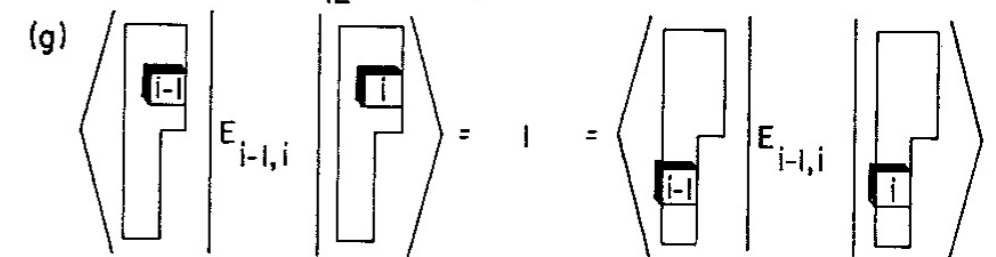
$$E_{13} \begin{vmatrix} 12 \\ 2 \end{vmatrix} = 0 - E_{23} \sqrt{2} \begin{vmatrix} 12 \\ 3 \end{vmatrix}$$

$$E_{13} \begin{vmatrix} 12 \\ 2 \end{vmatrix} = 0 - \frac{1}{\sqrt{2}} \sqrt{2} \begin{vmatrix} 12 \\ 2 \end{vmatrix}$$

$$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 22 \\ 3 \end{vmatrix} \rangle = ??$$

(e)  $E_{23} \begin{vmatrix} 13 \\ 3 \end{vmatrix} = \frac{1}{\sqrt{2}} \begin{vmatrix} 12 \\ 3 \end{vmatrix} + \frac{\sqrt{3}}{\sqrt{2}} \begin{vmatrix} 13 \\ 2 \end{vmatrix}$

(f)  $E_{12} \begin{vmatrix} 11 \\ 2 \end{vmatrix} = \sqrt{2} \begin{vmatrix} 11 \\ 1 \end{vmatrix}$

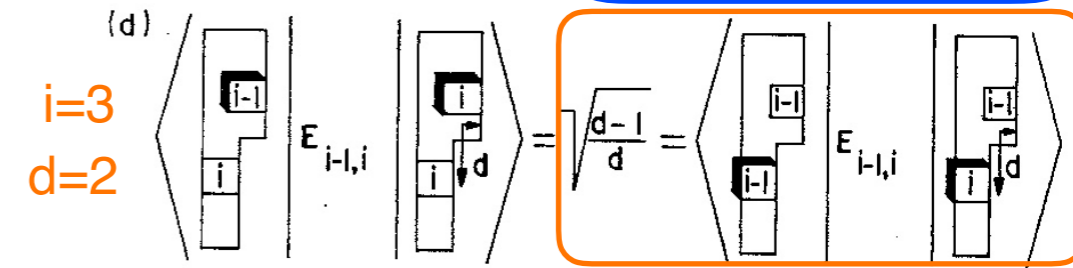
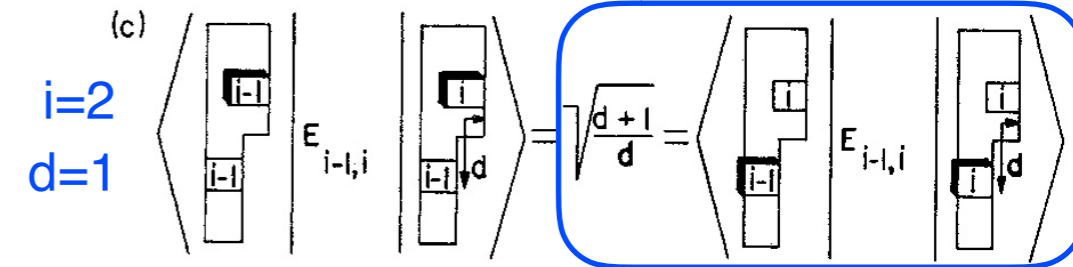


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	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{1/2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$	.	.	.
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ -1 \end{matrix}$	.
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $			$\begin{matrix} (11) & (33) \\ 2+1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	.	$\begin{matrix} (13) \\ 1 \end{matrix}$	.	.
$E_{jk} = \langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	.	$\begin{matrix} (23) \\ \sqrt{1/2} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{1/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 2 \end{vmatrix}  $					$\begin{matrix} (11) & (22) & (33) \\ 1+1+1 \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{3/2} \end{matrix}$	.	$\begin{matrix} (13) \\ \sqrt{3/2} \end{matrix}$
$\langle \begin{vmatrix} 13 \\ 3 \end{vmatrix}  $						$\begin{matrix} (11) & (33) \\ 1+2 \end{matrix}$	.	$\begin{matrix} (12) \\ 1 \end{matrix}$
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$$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{11} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 2 \quad \langle \begin{vmatrix} 11 \\ 2 \end{vmatrix} | E_{22} | \begin{vmatrix} 11 \\ 2 \end{vmatrix} \rangle = 1$$

(a)  $\langle T | E_{ii} | T \rangle = \delta_{T,T} \left( \begin{matrix} \text{number} \\ \text{of } (i\text{'s}) \end{matrix} \right)$       (b)  $\langle T | E_{ij} | T \rangle = \langle T | E_{ji} | T \rangle$



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$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} - E_{23}E_{12} \quad (2\text{-jump } E_{i-2,i})$$

$$E_{13} \begin{vmatrix} 12 \\ 2 \end{vmatrix} = E_{12}E_{23} \begin{vmatrix} 22 \\ 3 \end{vmatrix} - E_{23}E_{12} \begin{vmatrix} 22 \\ 3 \end{vmatrix}$$

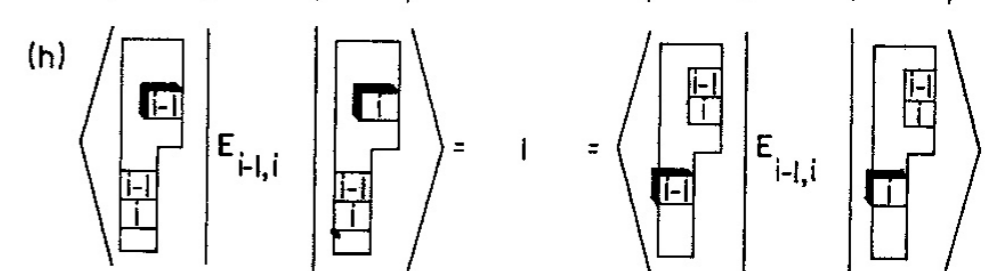
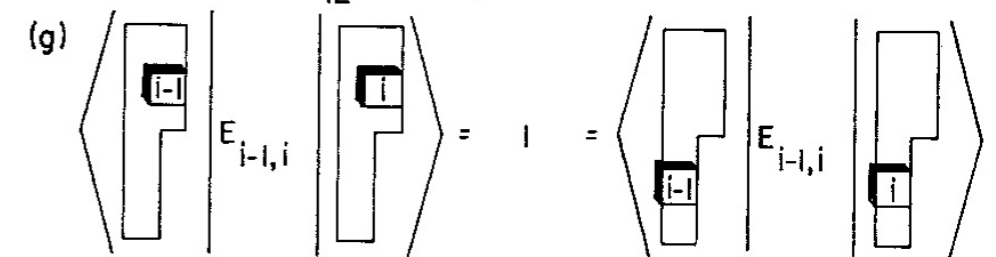
$$E_{13} \begin{vmatrix} 12 \\ 2 \end{vmatrix} = 0 - E_{23} \sqrt{2} \begin{vmatrix} 12 \\ 3 \end{vmatrix}$$

$$E_{13} \begin{vmatrix} 12 \\ 2 \end{vmatrix} = 0 - \frac{1}{\sqrt{2}} \sqrt{2} \begin{vmatrix} 12 \\ 2 \end{vmatrix}$$

$$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix} | E_{13} | \begin{vmatrix} 22 \\ 3 \end{vmatrix} \rangle = -1$$

(e)  $E_{23} \begin{vmatrix} 13 \\ 3 \end{vmatrix} = \frac{1}{\sqrt{2}} \begin{vmatrix} 12 \\ 3 \end{vmatrix} + \frac{\sqrt{3}}{\sqrt{2}} \begin{vmatrix} 13 \\ 2 \end{vmatrix}$

(f)  $E_{12} \begin{vmatrix} 11 \\ 2 \end{vmatrix} = \sqrt{2} \begin{vmatrix} 11 \\ 1 \end{vmatrix}$



# 4.16.18 class 23: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

## $(S_n)^*(U(m))$ shell model of electrostatic quadrupole-quadrupole-e interactions

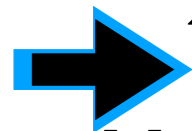
Complete set of  $E_{jk}$  matrix elements for the doublet (spin- $1/2$ )  $p^3$  orbits

Detailed sample applications of “Jawbone” formulae

Number operators

1-jump  $E_{i-1,i}$  operators

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Linear multipoles;  $P_1$ -dipole,  $P_2$ -quadrupole,  $P_3$ -octupole,...

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Tensor tables are  $(2\ell+1)$ -by- $(2\ell+1)$  arrays  $(p^k_q)$  giving  $V_q^k$  in terms of  $E_{p,q}$ .

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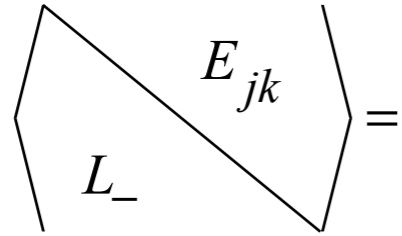
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# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$M=2$	$M=1$		$M=0$		$M=-1$	$M=-2$	
	$\begin{vmatrix} 11 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 11 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 12 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 2 \end{vmatrix}$	$\begin{vmatrix} 13 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 22 \\ 3 \end{vmatrix}$	$\begin{vmatrix} 23 \\ 3 \end{vmatrix}$
$\langle \begin{vmatrix} 11 \\ 2 \end{vmatrix}  $	$\begin{matrix} (11) & (22) \\ 2 + 1 \end{matrix}$	$\begin{matrix} (12) \\ 1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$	$\begin{matrix} (13) \\ -\sqrt{\frac{1}{2}} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{\frac{3}{2}} \end{matrix}$	$\cdot$	$\cdot$	$\cdot$
$\langle \begin{vmatrix} 12 \\ 2 \end{vmatrix}  $		$\begin{matrix} (11) & (22) \\ 1 + 2 \end{matrix}$	$\cdot$	$\begin{matrix} (23) \\ \sqrt{\frac{1}{2}} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{\frac{3}{2}} \end{matrix}$	$\cdot$	$\begin{matrix} (13) \\ -1 \end{matrix}$	$\cdot$
$\langle \begin{vmatrix} 11 \\ 3 \end{vmatrix}  $		$\cdot$	$\begin{matrix} (11) & (33) \\ 2 + 1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\cdot$	$\begin{matrix} (13) \\ 1 \end{matrix}$	$\cdot$	$\cdot$
$\langle \begin{vmatrix} 12 \\ 3 \end{vmatrix}  $				$\begin{matrix} (11) & (22) & (33) \\ 1 + 1 + 1 \end{matrix}$	$\cdot$	$\begin{matrix} (23) \\ \sqrt{\frac{1}{2}} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{\frac{1}{2}} \end{matrix}$
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$\langle \begin{vmatrix} 23 \\ 3 \end{vmatrix}  $								$\begin{matrix} (22) & (33) \\ 1 + 2 \end{matrix}$



Relating  $U(3)$  tableau states to angular momentum states begins with orbital operators

$$L_z \equiv \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} = (E_{11} - E_{33}) = \sqrt{2} \mathbf{v}_0^1$$

$$L_+ \equiv \sqrt{2} \begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} = \sqrt{2} (E_{12} + E_{23}) = L_x + iL_y, \quad L_- \equiv \sqrt{2} \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix} = \sqrt{2} (E_{21} + E_{32}) = L_x - iL_y.$$

$$L_x = \frac{1}{\sqrt{2}} \begin{pmatrix} \cdot & 1 & \cdot \\ 1 & \cdot & 1 \\ \cdot & 1 & \cdot \end{pmatrix} = \frac{L_+ + L_-}{2}, \quad L_y = \frac{1}{\sqrt{2}} \begin{pmatrix} \cdot & -i & \cdot \\ i & \cdot & -i \\ \cdot & i & \cdot \end{pmatrix} = \frac{L_+ - L_-}{2i}$$

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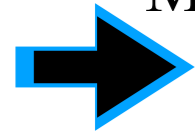
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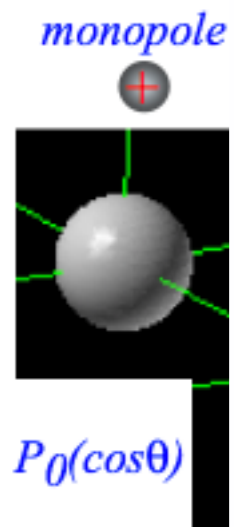
*Legendre polynomials*  $P_\ell$  defined by R(3) irep  $D^\ell$ :  $X_0^\ell = r^\ell D_{0,0}^\ell(\cdot, \theta, \cdot) = r^\ell P_\ell(\cos\theta)$

Derivatives of *monopole potential*  $V^{\text{monopole}}(r) = \frac{q}{r} = \frac{qP_0(\cos\theta)}{r}$

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# Multipole expansions and Coulomb (e-e)-electrostatic interaction

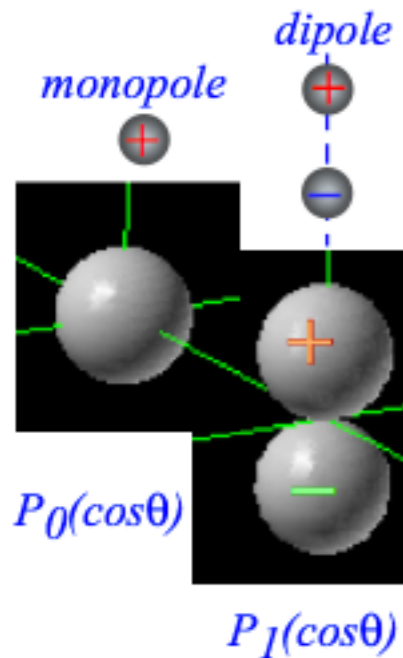
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*dipole potential*:

$$V^{\text{dipole}}(r) = -\frac{\partial}{\partial z} V^{\text{monopole}}(r) = \frac{qz}{r^3} = \frac{q \cos\theta}{r^2} = \frac{qP_1(\cos\theta)}{r^2}$$



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Derivatives of *monopole potential*

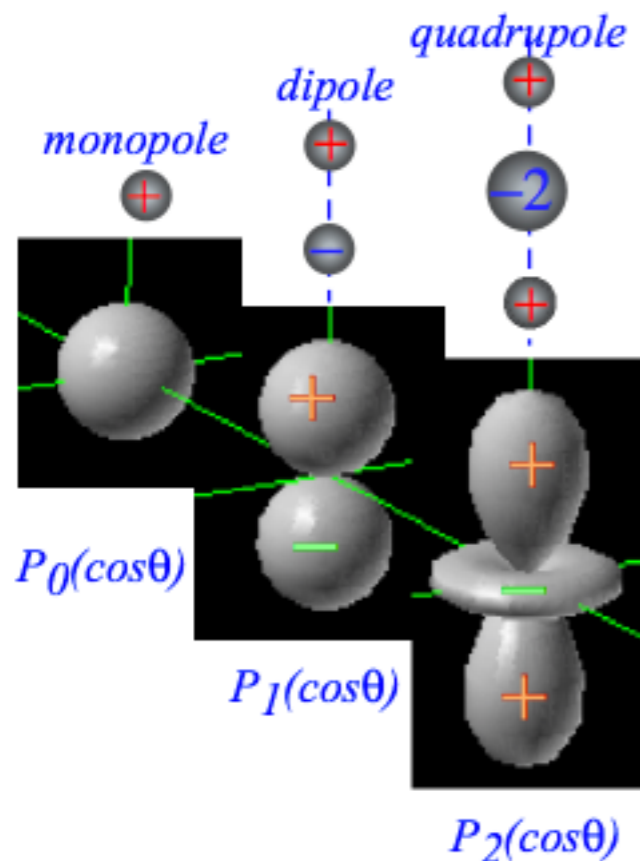
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QTCA Unit 8 *Wavefunctions* begins on p. 24

QTCA Unit 8 *Multipole functions* begins on p. 33

# Multipole expansions and Coulomb (e-e)-electrostatic interaction

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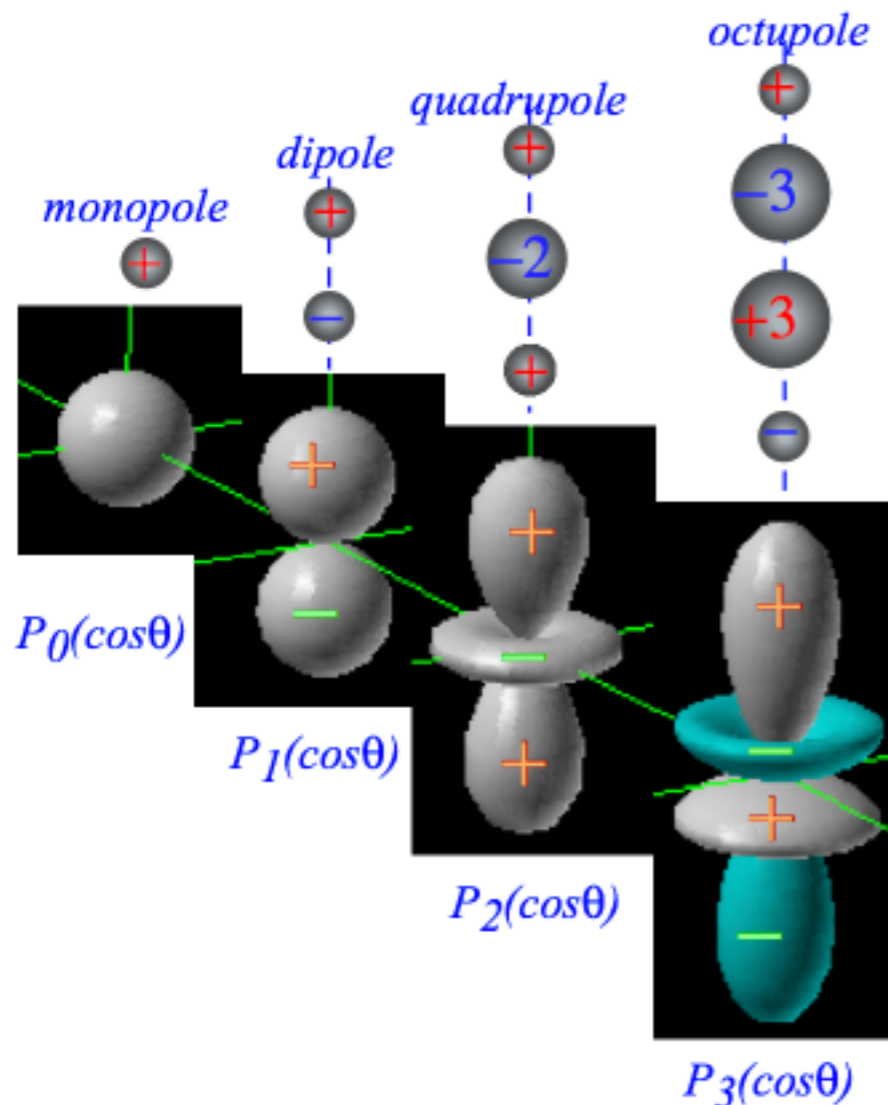
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*octupole potential:*

$$V^{\text{octupole}}(r) = \frac{-1}{3} \frac{\partial}{\partial z} V^{\text{quadrupole}}(r) = \frac{-1}{3} \frac{\partial}{\partial z} \frac{3z^2 - r^2}{2r^5} = q \frac{5z^3 - 3z}{2r^5} = \frac{qP_3(\cos\theta)}{r^4}$$



QTCA Unit 8 [Wavefunctions begins on p. 24](#)

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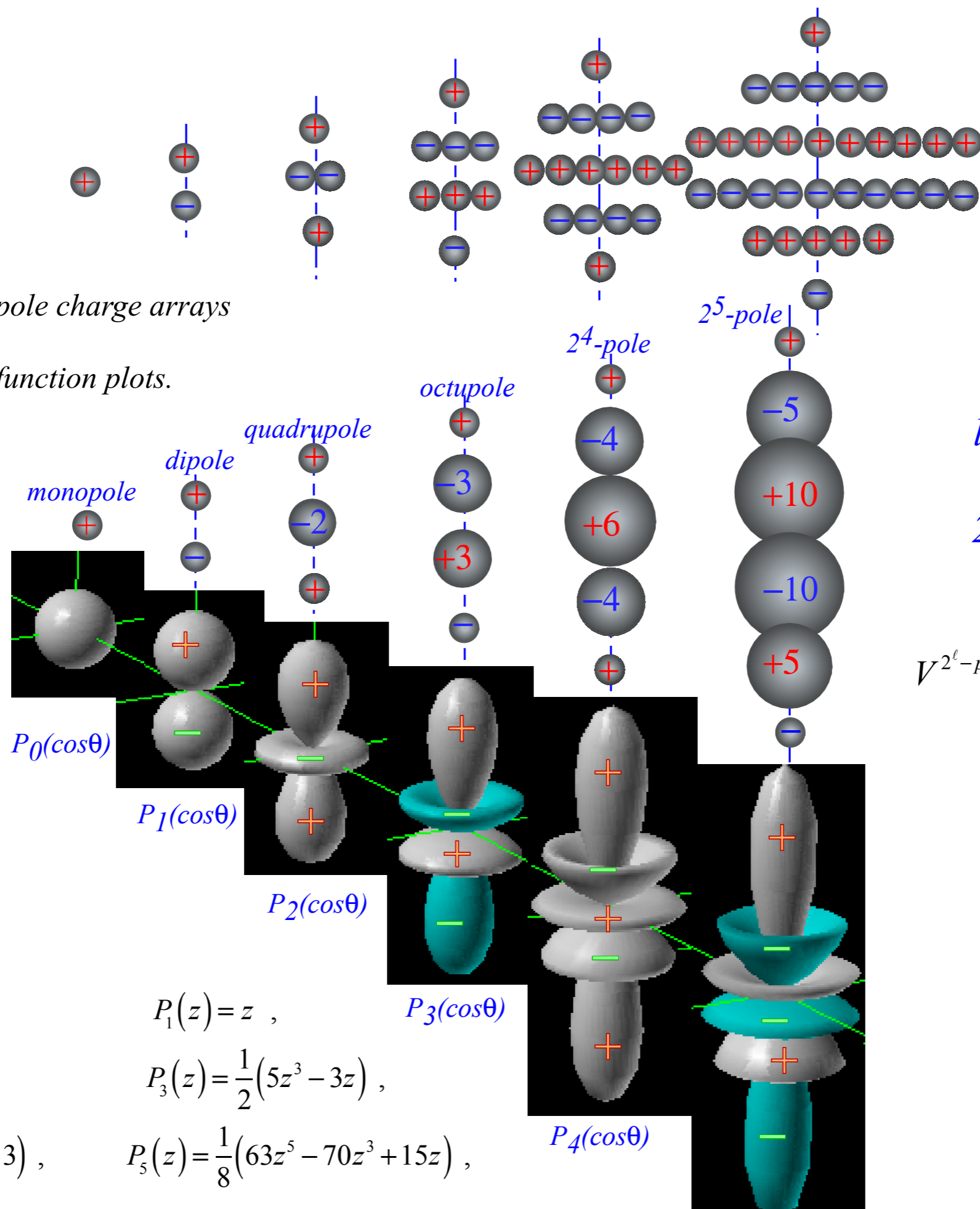
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*linear multi-pole or  $2^\ell$ -pole potential*  $V^{2^\ell\text{-pole}}(r) = \frac{(-1)^\ell}{\ell!} \frac{\partial^\ell}{\partial z^\ell} \left( \frac{q}{r} \right) = \frac{qP_\ell(\cos\theta)}{r^{\ell+1}}$



Fig. 23.3.4 Linear  $2^k$ -pole charge arrays and potential or wave function plots.



linear multi-pole  
or  
 $2^l$ -pole potential

$$V^{2^l\text{-pole}}(r) = \frac{(-1)^l}{l!} \frac{\partial^l}{\partial z^l} \left( \frac{q}{r} \right)$$

$$= \frac{qP_l(\cos\theta)}{r^{\ell+1}}$$

$$P_0(z) = 1,$$

$$P_2(z) = \frac{1}{2}(3z^2 - 1),$$

$$P_4(z) = \frac{1}{8}(35z^4 - 30z^2 + 3),$$

$$P_1(z) = z,$$

$$P_3(z) = \frac{1}{2}(5z^3 - 3z),$$

$$P_5(z) = \frac{1}{8}(63z^5 - 70z^3 + 15z),$$

$$P_3(\cos\theta)$$

$$P_4(\cos\theta)$$

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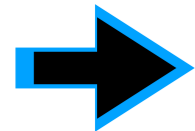
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Moving off-axis: On-z-axis linear multipole  $P_\ell(\cos\theta)$  wave expansion:

$$\begin{aligned}\frac{q}{|\mathbf{r}-\mathbf{r}'|} &= \frac{q}{r} - r' \frac{\partial}{\partial z} \left( \frac{q}{r} \right) + \frac{(r')^2}{2!} \frac{\partial^2}{\partial z^2} \left( \frac{q}{r} \right) - \frac{(r')^3}{3!} \frac{\partial^3}{\partial z^3} \left( \frac{q}{r} \right) + \dots + \frac{(-r')^\ell}{\ell!} \frac{\partial^\ell}{\partial z^\ell} \left( \frac{q}{r} \right) \dots \\ &= \frac{q}{r} + \frac{qr'}{r^2} P_1(\cos\theta) + \frac{q(r')^2}{r^3} P_2(\cos\theta) + \frac{q(r')^3}{r^4} P_3(\cos\theta) + \dots + \frac{q(r')^\ell}{r^{\ell+1}} P_\ell(\cos\theta) \dots\end{aligned}$$

Moving off-axis: On-z-axis linear multipole  $P_\ell(\cos\theta)$  wave expansion:

$$\begin{aligned} \frac{q}{|\mathbf{r}-\mathbf{r}'|} &= \frac{q}{r} - r' \frac{\partial}{\partial z} \left( \frac{q}{r} \right) + \frac{(r')^2}{2!} \frac{\partial^2}{\partial z^2} \left( \frac{q}{r} \right) - \frac{(r')^3}{3!} \frac{\partial^3}{\partial z^3} \left( \frac{q}{r} \right) + \dots + \frac{(-r')^\ell}{\ell!} \frac{\partial^\ell}{\partial z^\ell} \left( \frac{q}{r} \right) \dots \\ &= \frac{q}{r} + \frac{qr'}{r^2} P_1(\cos\theta) + \frac{q(r')^2}{r^3} P_2(\cos\theta) + \frac{q(r')^3}{r^4} P_3(\cos\theta) + \dots + \frac{q(r')^\ell}{r^{\ell+1}} P_\ell(\cos\theta) \dots \end{aligned}$$

Off-z-axis position state  $|\alpha, \beta, 0\rangle$  by Euler rotation:  $\mathbf{R}(\alpha, \beta, 0)|0, 0, 0\rangle = |\alpha, \beta, 0\rangle$

Off-z-axis  $P_\ell(\cos\theta)$  wave by Euler rotation: 
$$\begin{aligned} \left| \begin{matrix} \ell \\ 0 \end{matrix} \right\rangle_{(\alpha, \beta)} &= \mathbf{R}(\alpha, \beta, 0) \left| \begin{matrix} \ell \\ 0, 0 \end{matrix} \right\rangle \\ &= \sum_{m=-\ell}^{\ell} \left| \begin{matrix} \ell \\ m, 0 \end{matrix} \right\rangle D_{m,0}^\ell(\alpha, \beta, 0) = \sum_{m=-\ell}^{\ell} \left| \begin{matrix} \ell \\ m, 0 \end{matrix} \right\rangle Y_m^{\ell*}(\alpha, \beta) \sqrt{\frac{4\pi}{2\ell+1}} \end{aligned}$$

## Moving off-axis: On-z-axis linear multipole $P_\ell(\cos\theta)$ wave expansion:

$$\frac{q}{|\mathbf{r}-\mathbf{r}'|} = \frac{q}{r} - r' \frac{\partial}{\partial z} \left( \frac{q}{r} \right) + \frac{(r')^2}{2!} \frac{\partial^2}{\partial z^2} \left( \frac{q}{r} \right) - \frac{(r')^3}{3!} \frac{\partial^3}{\partial z^3} \left( \frac{q}{r} \right) + \dots + \frac{(-r')^\ell}{\ell!} \frac{\partial^\ell}{\partial z^\ell} \left( \frac{q}{r} \right) \dots$$

$$= \frac{q}{r} + \frac{qr'}{r^2} P_1(\cos\theta) + \frac{q(r')^2}{r^3} P_2(\cos\theta) + \frac{q(r')^3}{r^4} P_3(\cos\theta) + \dots + \frac{q(r')^\ell}{r^{\ell+1}} P_\ell(\cos\theta) \dots$$

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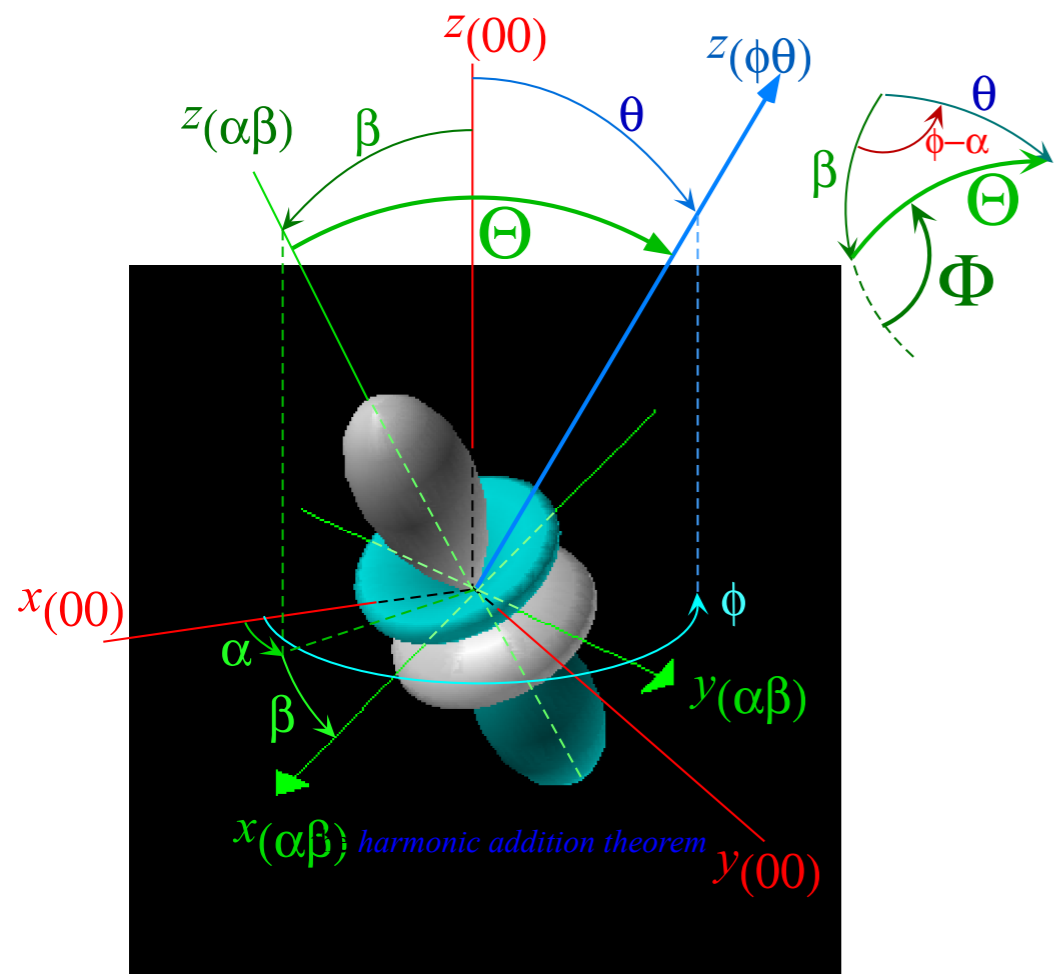
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$$= \sum_{m=-\ell}^{\ell} \left| \begin{smallmatrix} \ell \\ m, 0 \end{smallmatrix} \right\rangle D_{m,0}^\ell(\alpha, \beta, 0) = \sum_{m=-\ell}^{\ell} \left| \begin{smallmatrix} \ell \\ m, 0 \end{smallmatrix} \right\rangle Y_m^{\ell*}(\alpha, \beta) \sqrt{\frac{4\pi}{2\ell+1}}$$

Amplitude at polar position  $|\phi, \theta, 0\rangle$  of rotated  $P$ -wave:  $\langle \phi, \theta | \left| \begin{smallmatrix} \ell \\ 0 \end{smallmatrix} \right\rangle_{(\alpha, \beta)} = \langle \phi, \theta | \mathbf{R}(\alpha, \beta, 0) \left| \begin{smallmatrix} \ell \\ 0, 0 \end{smallmatrix} \right\rangle$

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$$= \sum_{m=-\ell}^{\ell} Y_m^\ell(\phi, \theta) Y_m^{\ell*}(\alpha, \beta) \frac{4\pi}{2\ell+1}$$



## Moving off-axis: On-z-axis linear multipole $P_\ell(\cos\theta)$ wave expansion:

$$\frac{q}{|\mathbf{r}-\mathbf{r}'|} = \frac{q}{r} - r' \frac{\partial}{\partial z} \left( \frac{q}{r} \right) + \frac{(r')^2}{2!} \frac{\partial^2}{\partial z^2} \left( \frac{q}{r} \right) - \frac{(r')^3}{3!} \frac{\partial^3}{\partial z^3} \left( \frac{q}{r} \right) + \dots + \frac{(-r')^\ell}{\ell!} \frac{\partial^\ell}{\partial z^\ell} \left( \frac{q}{r} \right) \dots$$

$$= \frac{q}{r} + \frac{qr'}{r^2} P_1(\cos\theta) + \frac{q(r')^2}{r^3} P_2(\cos\theta) + \frac{q(r')^3}{r^4} P_3(\cos\theta) + \dots + \frac{q(r')^\ell}{r^{\ell+1}} P_\ell(\cos\theta) \dots$$

Off-z-axis position state  $|\alpha, \beta, 0\rangle$  by Euler rotation:  $\mathbf{R}(\alpha, \beta, 0)|0, 0, 0\rangle = |\alpha, \beta, 0\rangle$

Off-z-axis  $P_\ell(\cos\theta)$  wave by Euler rotation:  $\left| \begin{smallmatrix} \ell \\ 0 \end{smallmatrix} \right\rangle_{(\alpha, \beta)} = \mathbf{R}(\alpha, \beta, 0) \left| \begin{smallmatrix} \ell \\ 0, 0 \end{smallmatrix} \right\rangle$

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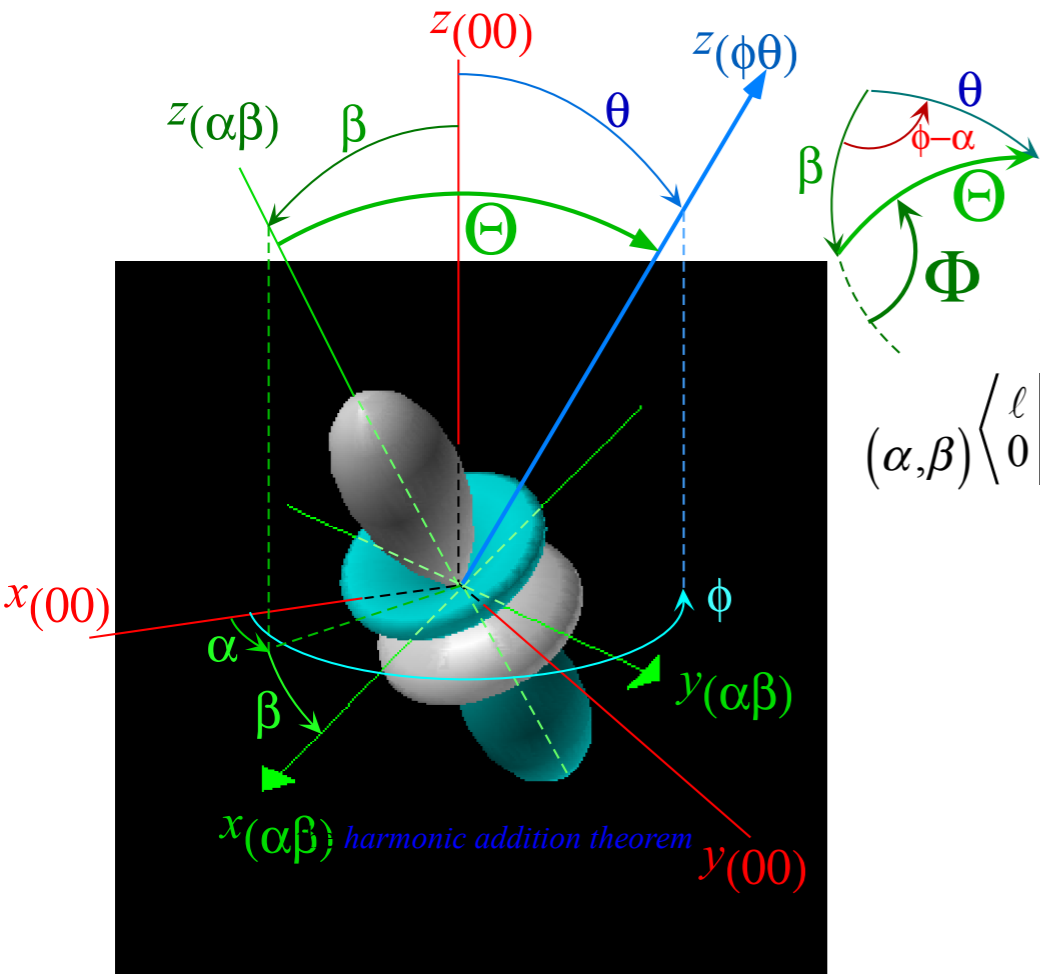
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$$= \sum_{m=-\ell}^{\ell} Y_m^\ell(\phi, \theta) Y_m^{\ell*}(\alpha, \beta) \frac{4\pi}{2\ell+1}$$

...representing a group product  $\mathbf{R}^\dagger(\alpha, \beta, 0)\mathbf{R}(\phi, \theta, 0) = \mathbf{R}(\Phi, \Theta, 0)$ .

$$(\alpha, \beta) \left\langle \begin{smallmatrix} \ell \\ 0 \end{smallmatrix} \middle| \begin{smallmatrix} \ell \\ 0 \end{smallmatrix} \right\rangle_{(\phi, \theta)} = \left\langle \begin{smallmatrix} \ell \\ 0 \end{smallmatrix} \middle| \mathbf{R}^\dagger(\alpha, \beta, 0)\mathbf{R}(\phi, \theta, 0) \left| \begin{smallmatrix} \ell \\ 0 \end{smallmatrix} \right\rangle = \left\langle \begin{smallmatrix} \ell \\ 0 \end{smallmatrix} \middle| \mathbf{R}(\Phi, \Theta, 0) \left| \begin{smallmatrix} \ell \\ 0 \end{smallmatrix} \right\rangle$$

$$= \sum_{m=-\ell}^{\ell} D_{0,m}^{\ell\dagger}(\alpha, \beta, 0) D_{m,0}^\ell(\phi, \theta, 0) = D_{0,0}^\ell(\Phi, \Theta, 0) = P_\ell(\cos\Theta)$$



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William G. Harter - University of Arkansas

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Complete set of E<sub>jk</sub> matrix elements for the doublet (spin-1/2) p<sup>3</sup> orbits

Detailed sample applications of “Jawbone” formulae

Number operators

1-jump E<sub>i-1,i</sub> operators

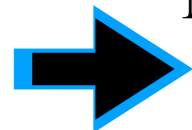
2-jump E<sub>i-2,i</sub> operators

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Multipole expansions and Coulomb (e-e)-electrostatic interaction

Linear multipoles; P<sub>1</sub>-dipole, P<sub>2</sub>-quadrupole, P<sub>3</sub>-octupole,...

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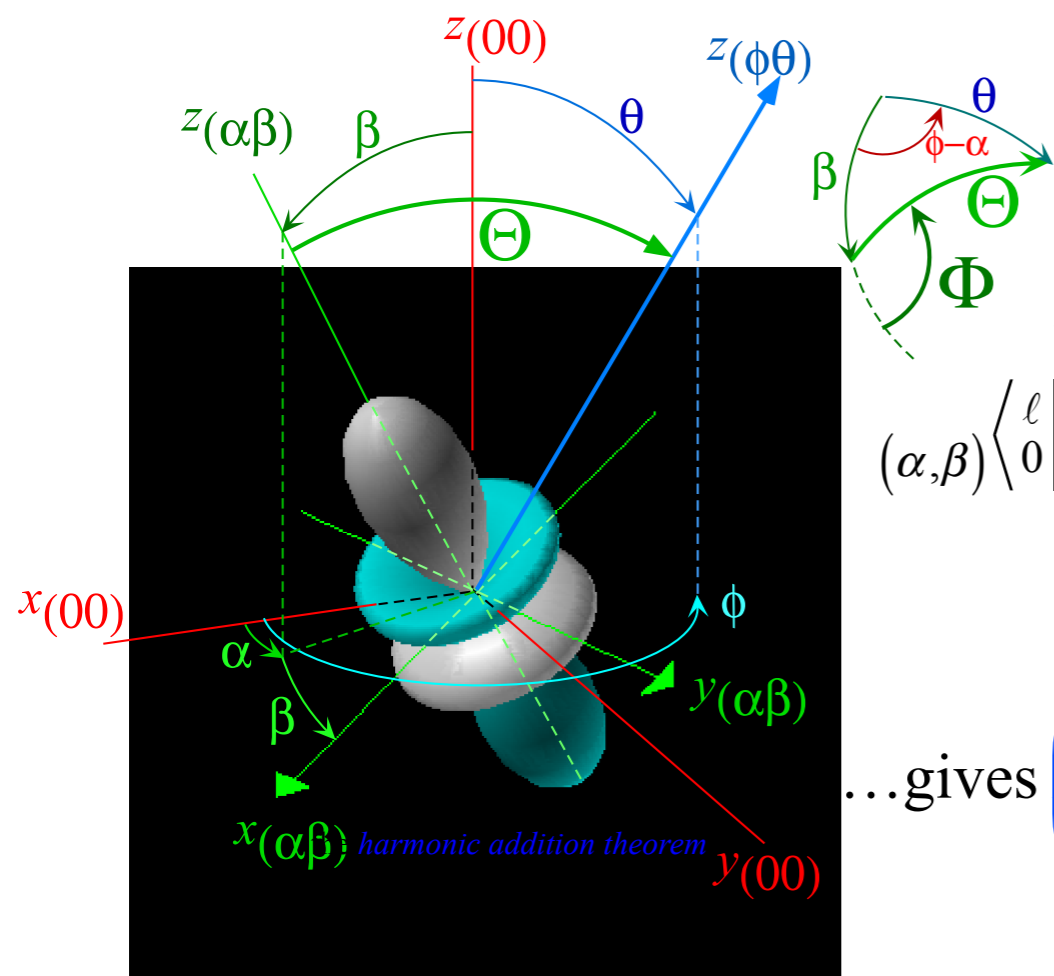
...representing a group product  $\mathbf{R}^\dagger(\alpha, \beta, 0)\mathbf{R}(\phi, \theta, 0) = \mathbf{R}(\Phi, \Theta, 0)$ .

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...gives **Multipole Addition Theorem**  $P_\ell(\cos\Theta) = \sum_{m=-\ell}^{\ell} Y_m^\ell(\phi, \theta) Y_m^{\ell*}(\alpha, \beta) \frac{4\pi}{2\ell+1}$

...but should be called the (group) **Multiplication Theorem**





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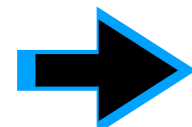
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# Coulomb (e-e)-electrostatic interaction and its Hamiltonian Matrix elements

$$\text{Multipole Addition Theorem } P_\ell(\cos\Theta) = \sum_{m=-\ell}^{\ell} Y_m^\ell(\phi, \theta) Y_m^{\ell*}(\alpha, \beta) \frac{4\pi}{2\ell+1}$$

$$\frac{e^2}{|\mathbf{r}_\alpha - \mathbf{r}_\beta|} = \sum_{\ell=0}^{\infty} \frac{e^2 r_{<}^\ell}{r_{>}^{\ell+1}} P_\ell(\cos\Theta_1) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{4\pi e^2 r_\alpha^\ell}{(2\ell+1)r_\beta^{\ell+1}} Y_m^{\ell*}(\phi_1, \theta_1) Y_m^\ell(\phi, \theta) \quad \text{for: } r_\alpha < r_\beta$$

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## Shorthand Tensor form of (e-e)-interaction

$$\frac{1}{|\mathbf{r}_{\alpha\beta}|} = \sum_{k=0}^{\infty} \sum_{q=-k}^k \frac{r_\alpha^k}{r_\beta^{k+1}} C_{-q}^k(\alpha) C_q^k(\beta) \quad \text{where: } C_q^k(\alpha) = \sqrt{\frac{4\pi}{2k+1}} Y_q^k(\phi_\alpha, \theta_\alpha)$$

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## (e-e)-interaction matrix (multi- $\ell$ -shell)

Given in terms of Slater radial integral(s):

$$F^k(\ell'_1 \ell'_2 \ell_1 \ell_2) = \int r_1^2 dr_1 \int r_2^2 dr_2 R_{\ell'_1}(r_1) R_{\ell'_2}(r_2) \frac{r_{<}^k}{r_{>}^{k+1}} R_{\ell_1}(r_1) R_{\ell_2}(r_2)$$

$$\left\langle \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right\rangle = \sum_{\substack{\ell'_1 \ell'_2 \ell_1 \ell_2 \\ m'_1 m'_2 m_1 m_2}} \left\langle \begin{matrix} \ell'_1 & \ell'_2 \\ m'_1 & m'_2 \end{matrix} \right| \left\langle \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right| \begin{matrix} \ell_1 & \ell_2 \\ m_1 & m_2 \end{matrix} \right\rangle$$

$$= \sum_{\substack{\ell'_1 \ell'_2 \ell_1 \ell_2 \\ m'_1 m'_2 m_1 m_2}} e_{\ell'_1 \ell_1}(\alpha) e_{\ell'_2 \ell_2}(\beta) \sum_k F^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \left[ \sum_q (-1)^{q+\Delta} \left\langle \begin{matrix} \ell'_1 \\ m'_1 \end{matrix} \right| C_{-q}^k(\alpha) \left| \begin{matrix} \ell_1 \\ m_1 \end{matrix} \right\rangle \left\langle \begin{matrix} \ell'_2 \\ m'_2 \end{matrix} \right| C_q^k(\beta) \left| \begin{matrix} \ell_2 \\ m_2 \end{matrix} \right\rangle \right]$$

$$\text{where parity requires: } \begin{cases} 1 = (-1)^{\ell'_1+k+\ell_1} = (-1)^{\ell'_2+k+\ell_2} \\ (-1)^\Delta = (-1)^{\ell'_1-\ell_1} = (-1)^{\ell'_2-\ell_2} \end{cases}$$

# Coulomb (e-e)-electrostatic interaction and its Hamiltonian Matrix elements

$$\text{Multipole Addition Theorem } P_\ell(\cos\Theta) = \sum_{m=-\ell}^{\ell} Y_m^\ell(\phi, \theta) Y_m^{\ell*}(\alpha, \beta) \frac{4\pi}{2\ell+1}$$

$$\frac{e^2}{|\mathbf{r}_\alpha - \mathbf{r}_\beta|} = \sum_{\ell=0}^{\infty} \frac{e^2 r_{<}^\ell}{r_{>}^{\ell+1}} P_\ell(\cos\Theta_1) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{4\pi e^2 r_\alpha^\ell}{(2\ell+1)r_\beta^{\ell+1}} Y_m^{\ell*}(\phi_1, \theta_1) Y_m^\ell(\phi, \theta) \quad \text{for: } r_\alpha < r_\beta$$

## Shorthand Tensor form of (e-e)-interaction

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$$= \sum_{\substack{\ell'_1 \ell'_2 \ell_1 \ell_2 \\ m'_1 m'_2 m_1 m_2}} e_{\ell'_1 \ell_1}(\alpha) e_{\ell'_2 \ell_2}(\beta) \sum_k F^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \left[ \sum_q (-1)^{q+\Delta} \left\langle \begin{matrix} \ell'_1 \\ m'_1 \end{matrix} \right| C_{-q}^k(\alpha) \left| \begin{matrix} \ell_1 \\ m_1 \end{matrix} \right\rangle \left\langle \begin{matrix} \ell'_2 \\ m'_2 \end{matrix} \right| C_q^k(\beta) \left| \begin{matrix} \ell_2 \\ m_2 \end{matrix} \right\rangle \right]$$

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## Elementary operator expressions for (e-e)-interaction matrix

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Corrected level diagrams Nitrogen  $p^3$

(Repeating from preceding page) *(e-e)-interaction matrix (multi- $\ell$ -shell)*

$$\left\langle \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right\rangle = \sum_{\substack{\ell'_1 \ell'_2 \ell_1 \ell_2 \\ m'_1 m'_2 m_1 m_2}} \left| \begin{matrix} \ell'_1 & \ell'_2 \\ m'_1 & m'_2 \end{matrix} \right\rangle \left\langle \begin{matrix} \ell'_1 & \ell'_2 \\ m'_1 & m'_2 \end{matrix} \left| \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right| \begin{matrix} \ell_1 & \ell_2 \\ m_1 & m_2 \end{matrix} \right\rangle \left\langle \begin{matrix} \ell_1 & \ell_2 \\ m_1 & m_2 \end{matrix} \right|$$

$$= \sum_{\substack{\ell'_1 \ell'_2 \ell_1 \ell_2 \\ m'_1 m'_2 m_1 m_2}} e_{\ell'_1 \ell_1}(\alpha) e_{\ell'_2 \ell_2}(\beta) \sum_k F^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \left[ \sum_q (-1)^{q+\Delta} \left\langle \begin{matrix} \ell'_1 \\ m'_1 \end{matrix} \left| C_{-q}^k(\alpha) \right| \begin{matrix} \ell_1 \\ m_1 \end{matrix} \right\rangle \left\langle \begin{matrix} \ell'_2 \\ m'_2 \end{matrix} \left| C_q^k(\beta) \right| \begin{matrix} \ell_2 \\ m_2 \end{matrix} \right\rangle \right]$$

where parity requires: 
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Shorthand  $\mathbf{e}_{jk}$  index labeling  $\mathbf{e}_{1'1}$  maps to momentum quanta:

$$1' \rightarrow \begin{matrix} \ell'_1 \\ m'_1 \end{matrix}, \quad 1 \rightarrow \begin{matrix} \ell_1 \\ m_1 \end{matrix}$$

$$2' \rightarrow \begin{matrix} \ell'_2 \\ m'_2 \end{matrix}, \quad 2 \rightarrow \begin{matrix} \ell_2 \\ m_2 \end{matrix}$$

2-particle elementary  $\mathbf{e}_{jk}$  operator expressions for *(e-e)-interaction matrix*

$$\left\langle \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right\rangle = \sum_{\substack{\ell'_1 \ell'_2 \ell_1 \ell_2 \\ m'_1 m'_2 m_1 m_2}} \sum_k A^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \left[ \sum_q (-1)^{q+\Delta} \begin{pmatrix} k \\ 1'1 \end{pmatrix} \mathbf{e}_{1'1}(\alpha) \begin{pmatrix} k \\ 2'2 \end{pmatrix} \mathbf{e}_{2'2}(\beta) \right]$$

with tensor factors:  $\begin{pmatrix} k \\ 1'1 \end{pmatrix} = C_{-q m_1 m_1 - q}^{k \ell_1 \ell'_1} \sqrt{\frac{2k+1}{2\ell'_1+1}}$  and  $\begin{pmatrix} k \\ 2'2 \end{pmatrix} = C_{-q m_2 m_2 - q}^{k \ell_2 \ell'_2} \sqrt{\frac{2k+1}{2\ell'_2+1}}$

and radial integral(s):  $A^k(\ell'_1 \ell'_2 \ell_1 \ell_2) = F^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \begin{pmatrix} k \ell_1 \ell'_1 \\ 0 0 0 \end{pmatrix} \begin{pmatrix} k \ell_2 \ell'_2 \\ 0 0 0 \end{pmatrix} \frac{\sqrt{(2\ell'_1+1)(2\ell'_2+1)(2\ell_1+1)(2\ell_2+1)}}{2k+1}$

(Repeating from preceding page) *(e-e)-interaction matrix (multi- $\ell$ -shell)*

$$\left\langle \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right\rangle = \sum_{\substack{\ell'_1 \ell'_2 \ell_1 \ell_2 \\ m'_1 m'_2 m_1 m_2}} \left| \begin{matrix} \ell'_1 & \ell'_2 \\ m'_1 & m'_2 \end{matrix} \right\rangle \left\langle \begin{matrix} \ell'_1 & \ell'_2 \\ m'_1 & m'_2 \end{matrix} \left| \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right| \begin{matrix} \ell_1 & \ell_2 \\ m_1 & m_2 \end{matrix} \right\rangle \left\langle \begin{matrix} \ell_1 & \ell_2 \\ m_1 & m_2 \end{matrix} \right|$$

$$= \sum_{\substack{\ell'_1 \ell'_2 \ell_1 \ell_2 \\ m'_1 m'_2 m_1 m_2}} e_{\ell'_1 \ell_1}(\alpha) e_{\ell'_2 \ell_2}(\beta) \sum_k F^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \left[ \sum_q (-1)^{q+\Delta} \left\langle \begin{matrix} \ell'_1 \\ m'_1 \end{matrix} \left| C_{-q}^k(\alpha) \right| \begin{matrix} \ell_1 \\ m_1 \end{matrix} \right\rangle \left\langle \begin{matrix} \ell'_2 \\ m'_2 \end{matrix} \left| C_q^k(\beta) \right| \begin{matrix} \ell_2 \\ m_2 \end{matrix} \right\rangle \right]$$

where parity requires: 
$$\begin{cases} 1 = (-1)^{\ell'_1+k+\ell_1} = (-1)^{\ell'_2+k+\ell_2} \\ (-1)^\Delta = (-1)^{\ell'_1-\ell_1} = (-1)^{\ell'_2-\ell_2} \end{cases}$$

Shorthand  $\mathbf{e}_{jk}$  index labeling  $\mathbf{e}_{1'1}$  maps to momentum quanta:

$$\begin{aligned} 1' &\rightarrow \begin{matrix} \ell'_1 \\ m'_1 \end{matrix}, & 1 &\rightarrow \begin{matrix} \ell_1 \\ m_1 \end{matrix} \\ 2' &\rightarrow \begin{matrix} \ell'_2 \\ m'_2 \end{matrix}, & 2 &\rightarrow \begin{matrix} \ell_2 \\ m_2 \end{matrix} \end{aligned}$$

2-particle elementary  $\mathbf{e}_{jk}$  operator expressions for *(e-e)-interaction matrix*

$$\left\langle \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right\rangle = \sum_{\substack{\ell'_1 \ell'_2 \ell_1 \ell_2 \\ m'_1 m'_2 m_1 m_2}} \sum_k A^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \left[ \sum_q (-1)^{q+\Delta} \begin{pmatrix} k \\ 1'1 \end{pmatrix} \mathbf{e}_{1'1}(\alpha) \begin{pmatrix} k \\ 2'2 \end{pmatrix} \mathbf{e}_{2'2}(\beta) \right]$$

with tensor factors:  $\begin{pmatrix} k \\ 1'1 \end{pmatrix} = C_{-q m'_1 m_1 - q}^{k \ell'_1 \ell_1} \sqrt{\frac{2k+1}{2\ell'_1+1}}$  and  $\begin{pmatrix} k \\ 2'2 \end{pmatrix} = C_{-q m'_2 m_2 - q}^{k \ell'_2 \ell_2} \sqrt{\frac{2k+1}{2\ell'_2+1}}$

and radial integral(s):  $A^k(\ell'_1 \ell'_2 \ell_1 \ell_2) = F^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \begin{pmatrix} k \ell_1 \ell'_1 \\ 0 0 0 \end{pmatrix} \begin{pmatrix} k \ell_2 \ell'_2 \\ 0 0 0 \end{pmatrix} \frac{\sqrt{(2\ell'_1+1)(2\ell'_2+1)(2\ell_1+1)(2\ell_2+1)}}{2k+1}$

*n*-particle elementary  $\mathbf{E}_{jk} = \sum_\alpha \mathbf{e}_{jk}(\alpha)$  summed operator expressions (Using  $\mathbf{e}_{ij}(\alpha) \mathbf{e}_{km}(\alpha) = \delta_{jk} \mathbf{e}_{im}(\alpha)$  )

$$\frac{1}{2} \sum_{\alpha \neq \beta} \left\langle \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right\rangle = \frac{1}{2} \sum_{\ell'_1 \ell'_2 \ell_1 \ell_2} \sum_k A^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \left[ \sum_{\substack{q \\ m_1, m_2}} (-1)^{q+\Delta} \begin{pmatrix} k \\ 1'1 \end{pmatrix} \mathbf{E}_{1'1} \begin{pmatrix} k \\ 2'2 \end{pmatrix} \mathbf{E}_{2'2} - \sum_{\substack{q \\ m_1, m_2}} (-1)^{q+\Delta} \begin{pmatrix} k \\ 1'1 \end{pmatrix} \begin{pmatrix} k \\ 2'2 \end{pmatrix} \delta_{2'1} \mathbf{E}_{1'2} \right]$$



(Repeating from preceding page) *(e-e)-interaction matrix (multi- $\ell$ -shell)*

$$\left\langle \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right\rangle = \sum_{\substack{\ell'_1 \ell'_2 \ell_1 \ell_2 \\ m'_1 m'_2 m_1 m_2}} \left| \begin{matrix} \ell'_1 & \ell'_2 \\ m'_1 & m'_2 \end{matrix} \right\rangle \left\langle \begin{matrix} \ell'_1 & \ell'_2 \\ m'_1 & m'_2 \end{matrix} \left| \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right| \begin{matrix} \ell_1 & \ell_2 \\ m_1 & m_2 \end{matrix} \right\rangle \left\langle \begin{matrix} \ell_1 & \ell_2 \\ m_1 & m_2 \end{matrix} \right|$$

$$= \sum_{\substack{\ell'_1 \ell'_2 \ell_1 \ell_2 \\ m'_1 m'_2 m_1 m_2}} e_{\ell'_1 \ell_1}(\alpha) e_{\ell'_2 \ell_2}(\beta) \sum_k F^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \left[ \sum_q (-1)^{q+\Delta} \left\langle \begin{matrix} \ell'_1 \\ m'_1 \end{matrix} \left| C_{-q}^k(\alpha) \right| \begin{matrix} \ell_1 \\ m_1 \end{matrix} \right\rangle \left\langle \begin{matrix} \ell'_2 \\ m'_2 \end{matrix} \left| C_q^k(\beta) \right| \begin{matrix} \ell_2 \\ m_2 \end{matrix} \right\rangle \right]$$

where parity requires: 
$$\begin{cases} 1 = (-1)^{\ell'_1+k+\ell_1} = (-1)^{\ell'_2+k+\ell_2} \\ (-1)^\Delta = (-1)^{\ell'_1-\ell_1} = (-1)^{\ell'_2-\ell_2} \end{cases}$$

Shorthand  $\mathbf{e}_{jk}$  index labeling  $\mathbf{e}_{r_1}$  maps to momentum quanta:

$$\begin{aligned} 1' &\rightarrow \begin{matrix} \ell'_1 \\ m'_1 \end{matrix}, & 1 &\rightarrow \begin{matrix} \ell_1 \\ m_1 \end{matrix} \\ 2' &\rightarrow \begin{matrix} \ell'_2 \\ m'_2 \end{matrix}, & 2 &\rightarrow \begin{matrix} \ell_2 \\ m_2 \end{matrix} \end{aligned}$$

2-particle elementary  $\mathbf{e}_{jk}$  operator expressions for *(e-e)-interaction matrix*

$$\left\langle \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right\rangle = \sum_{\substack{\ell'_1 \ell'_2 \ell_1 \ell_2 \\ m'_1 m'_2 m_1 m_2}} \sum_k A^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \left[ \sum_q (-1)^{q+\Delta} \begin{pmatrix} k \\ 1'1 \end{pmatrix} \mathbf{e}_{1'1}(\alpha) \begin{pmatrix} k \\ 2'2 \end{pmatrix} \mathbf{e}_{2'2}(\beta) \right]$$

with tensor factors:  $\begin{pmatrix} k \\ 1'1 \end{pmatrix} = C_{-q m_1 m_1 - q}^{k \ell_1 \ell'_1} \sqrt{\frac{2k+1}{2\ell'_1+1}}$  and  $\begin{pmatrix} k \\ 2'2 \end{pmatrix} = C_{-q m_2 m_2 - q}^{k \ell_2 \ell'_2} \sqrt{\frac{2k+1}{2\ell'_2+1}}$

and radial integral(s):  $A^k(\ell'_1 \ell'_2 \ell_1 \ell_2) = F^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \begin{pmatrix} k \ell_1 \ell'_1 \\ 0 0 0 \end{pmatrix} \begin{pmatrix} k \ell_2 \ell'_2 \\ 0 0 0 \end{pmatrix} \frac{\sqrt{(2\ell'_1+1)(2\ell'_2+1)(2\ell_1+1)(2\ell_2+1)}}{2k+1}$

*n*-particle elementary  $\mathbf{E}_{jk} = \sum_{\alpha} \mathbf{e}_{jk}(\alpha)$  summed operator expressions (Using  $\mathbf{e}_{ij}(\alpha) \mathbf{e}_{km}(\alpha) = \delta_{jk} \mathbf{e}_{im}(\alpha)$  )

$$\frac{1}{2} \sum_{\alpha \neq \beta} \left\langle \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right\rangle = \frac{1}{2} \sum_{\ell'_1 \ell'_2 \ell_1 \ell_2} \sum_k A^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \left[ \sum_{\substack{q \\ m_1, m_2}} (-1)^{q+\Delta} \begin{pmatrix} k \\ 1'1 \end{pmatrix} \mathbf{E}_{1'1} \begin{pmatrix} k \\ 2'2 \end{pmatrix} \mathbf{E}_{2'2} - \sum_{\substack{q \\ m_1, m_2}} (-1)^{q+\Delta} \begin{pmatrix} k \\ 1'1 \end{pmatrix} \begin{pmatrix} k \\ 2'2 \end{pmatrix} \delta_{2'1} \mathbf{E}_{1'2} \right]$$

$$= \frac{1}{2} \sum_{\ell'_1 \ell'_2 \ell_1 \ell_2} \sum_k A^k(\ell'_1 \ell'_2 \ell_1 \ell_2) \sum_{\substack{q \\ m_1, m_2}} (\ell'_1, \tilde{\mathbf{v}}_q^k \ell_1) (\ell'_2, \tilde{\mathbf{v}}_q^k \ell_2) - \frac{1}{2} \sum_{\ell_1 \ell_2} \sum_k A^k(\ell_1 \ell_2 \ell_1 \ell_2) \frac{2k+1}{2\ell_1+1} \sum_{m_1} \mathbf{E}_{11}$$



# 4.16.18 class 23: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

## (S<sub>n</sub>)\*(U(m)) shell model of electrostatic quadrupole-quadrupole-e interactions

Complete set of E<sub>jk</sub> matrix elements for the doublet (spin-1/2) p<sup>3</sup> orbits

Detailed sample applications of “Jawbone” formulae

Number operators

1-jump E<sub>i-1,i</sub> operators

2-jump E<sub>i-2,i</sub> operators

Angular momentum operators (for later application)

Multipole expansions and Coulomb (e-e)-electrostatic interaction

Linear multipoles; P<sub>1</sub>-dipole, P<sub>2</sub>-quadrupole, P<sub>3</sub>-octupole,...

Moving off-axis: On-z-axis linear multipole P<sub>ℓ</sub> (cosθ) wave expansion:

**Multipole Addition Theorem (should be called Group Multiplication Theorem)**

Coulomb (e-e)-electrostatic interaction and its Hamiltonian Matrix, Slater integrals

2-particle elementary e<sub>jk</sub> operator expressions for (e-e)-interaction matrix

➔ Tensor tables are (2ℓ+1)-by-(2ℓ+1) arrays (p<sup>k</sup><sub>q</sub>) giving V<sub>q</sub><sup>k</sup> in terms of E<sub>p,q</sub>.

Relating V<sub>q</sub><sup>k</sup> to E<sub>m',m</sub> by (m'<sup>k</sup><sub>m</sub>) arrays

Atomic p-shell ee-interaction in elementary operator form

[2,1] tableau basis (from p.29) and matrices of v<sup>1</sup> dipole and v<sup>1</sup>•v<sup>1</sup>=L•L

[2,1] tableau basis (from p.29) and matrices of v<sup>2</sup> and v<sup>2</sup>•v<sup>2</sup> quadrupole

<sup>4</sup>S, <sup>2</sup>P, and <sup>2</sup>D energy calculation of quartet and doublet (spin-1/2) p<sup>3</sup> orbits

Corrected level diagrams Nitrogen p<sup>3</sup>

Single- $\ell$  atomic shells  $p^n, d^n, f^n, \dots$

$n$ -particle pure shell  $ee$ -interaction reduces to:

$$\sum_{\alpha \neq \beta} \left\langle \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right\rangle = \sum_{\substack{k=0 \\ (\text{even } k)}} A^k(\ell) (\mathbf{V}^k \cdot \mathbf{V}^k) + \text{const.} \quad \text{where:} \quad \mathbf{V}^k \cdot \mathbf{V}^k = \sum_{q=-k}^k (-1)^q \mathbf{V}_{-q}^k \mathbf{V}_q^k = \sum_{q=-k}^k \tilde{\mathbf{V}}_q^k \mathbf{V}_q^k \quad (\tilde{\mathbf{V}}_q^k \text{ means transpose of } \mathbf{V}_q^k)$$

# Single- $\ell$ atomic shells $p^n, d^n, f^n, \dots$

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$$= (\mathbf{V}_0^k)^2 + \sum_{q=-k}^k (\tilde{\mathbf{V}}_q^k \mathbf{V}_q^k + \mathbf{V}_q^k \tilde{\mathbf{V}}_q^k)$$

Tensor tables are  $(2\ell+1)$ -by- $(2\ell+1)$  arrays  $(p^k_q)$  giving  $\mathbf{V}_q^k$  in terms of elementary operators  $\mathbf{E}_{p,q}$ .

$\ell=1$   $p$ -shell example:

$\langle \mathbf{v}_{-2}^2 \rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \end{pmatrix}$	$\langle \mathbf{v}_{-1}^2 \rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{pmatrix} \frac{1}{\sqrt{2}}$	$\langle \mathbf{v}_0^2 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & -2 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{6}}$	$\langle \mathbf{v}_{+1}^2 \rangle = \begin{pmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} \frac{1}{\sqrt{2}}$	$\langle \mathbf{v}_{+2}^2 \rangle = \begin{pmatrix} \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$
$\langle \mathbf{v}_{-1}^1 \rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix} \frac{1}{\sqrt{2}}$		$\langle \mathbf{v}_0^1 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} \frac{1}{\sqrt{2}}$	$\langle \mathbf{v}_{+1}^1 \rangle = \begin{pmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \\ \cdot & \cdot & \cdot \end{pmatrix} \frac{1}{\sqrt{2}}$	
$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$				

# Single- $\ell$ atomic shells $p^n, d^n, f^n, \dots$

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$$\sum_{\alpha \neq \beta} \left\langle \frac{1}{|\mathbf{r}_{\alpha\beta}|} \right\rangle = \sum_{\substack{k=0 \\ (\text{even } k)}} A^k(\ell) (\mathbf{V}^k \cdot \mathbf{V}^k) + \text{const.} \quad \text{where: } \mathbf{V}^k \cdot \mathbf{V}^k = \sum_{q=-k}^k (-1)^q \mathbf{V}_{-q}^k \mathbf{V}_q^k = \sum_{q=-k}^k \tilde{\mathbf{V}}_q^k \mathbf{V}_q^k \quad (\tilde{\mathbf{V}}_q^k \text{ means transpose of } \mathbf{V}_q^k)$$

$$= (\mathbf{V}_0^k)^2 + \sum_{q=-k}^k (\tilde{\mathbf{V}}_q^k \mathbf{V}_q^k + \mathbf{V}_q^k \tilde{\mathbf{V}}_q^k)$$

Tensor tables are  $(2\ell+1)$ -by- $(2\ell+1)$  arrays  $(p^k_q)$  giving  $\mathbf{V}_q^k$  in terms of elementary operators  $\mathbf{E}_{p,q}$ .

$\ell=1$   $p$ -shell example:

A compact format helps display.

$$\langle \mathbf{v}_{-2}^2 \rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \end{pmatrix} \quad \langle \mathbf{v}_{-1}^2 \rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{pmatrix} \frac{1}{\sqrt{2}} \quad \langle \mathbf{v}_0^2 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & -2 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{6}} \quad \langle \mathbf{v}_{+1}^2 \rangle = \begin{pmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} \frac{1}{\sqrt{2}} \quad \langle \mathbf{v}_{+2}^2 \rangle = \begin{pmatrix} \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$$

$$\langle \mathbf{v}_{-1}^1 \rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix} \frac{1}{\sqrt{2}} \quad \langle \mathbf{v}_0^1 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \quad \langle \mathbf{v}_{+1}^1 \rangle = \begin{pmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \\ \cdot & \cdot & \cdot \end{pmatrix} \frac{1}{\sqrt{2}}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

$$\langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} 1 & -1 & 1 \\ 1 & -2 & 1 \\ 1 & -1 & 1 \end{pmatrix} \begin{matrix} 1 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{matrix}$$

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

# Single- $\ell$ atomic shells $p^n, d^n, f^n, \dots$

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$$= (\mathbf{V}_0^k)^2 + \sum_{q=-k}^k (\tilde{\mathbf{V}}_q^k \mathbf{V}_q^k + \mathbf{V}_q^k \tilde{\mathbf{V}}_q^k)$$

Tensor tables are  $(2\ell+1)$ -by- $(2\ell+1)$  arrays  $(p^k_q)$  giving  $\mathbf{V}_q^k$  in terms of elementary operators  $\mathbf{E}_{p,q}$ .

$\ell=1$   $p$ -shell example:

A compact format helps display.

$$\langle \mathbf{v}_{-2}^2 \rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \end{pmatrix} \quad \langle \mathbf{v}_{-1}^2 \rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{pmatrix} \frac{1}{\sqrt{2}} \quad \langle \mathbf{v}_0^2 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & -2 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{6}} \quad \langle \mathbf{v}_{+1}^2 \rangle = \begin{pmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} \frac{1}{\sqrt{2}} \quad \langle \mathbf{v}_{+2}^2 \rangle = \begin{pmatrix} \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$$

$$\langle \mathbf{v}_{-1}^1 \rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix} \frac{1}{\sqrt{2}} \quad \langle \mathbf{v}_0^1 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \quad \langle \mathbf{v}_{+1}^1 \rangle = \begin{pmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \\ \cdot & \cdot & \cdot \end{pmatrix} \frac{1}{\sqrt{2}}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

A normalizing factor  $1/\sqrt{n}$  sits below each  $45^\circ$  line†

$$\langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} 1 & -1 & 1 \\ 1 & -2 & 1 \\ 1 & -1 & 1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{matrix}$$

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

# Single- $\ell$ atomic shells $p^n, d^n, f^n, \dots$

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$\ell=1$   $p$ -shell example:

A compact format helps display.

$\langle \mathbf{v}_{-2}^2 \rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \end{pmatrix}$ 
 $\langle \mathbf{v}_{-1}^2 \rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{pmatrix} \frac{1}{\sqrt{2}}$ 
 $\langle \mathbf{v}_0^2 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & -2 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{6}}$ 
 $\langle \mathbf{v}_{+1}^2 \rangle = \begin{pmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} \frac{1}{\sqrt{2}}$ 
 $\langle \mathbf{v}_{+2}^2 \rangle = \begin{pmatrix} \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$

$\langle \mathbf{v}_{-1}^1 \rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix} \frac{1}{\sqrt{2}}$ 
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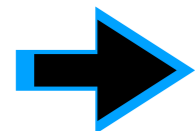
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Dirac notational derivation of  $\mathbf{V}_q^k$  to  $\mathbf{E}_{m',m}$  relation by  $\binom{k}{m' m}$  arrays:

$$\mathbf{V}_q^k = \sum_{m, m'} |m'\rangle \langle m'| \mathbf{V}_q^k |m\rangle \langle m| = \sum_{m, m'} \langle m'| \mathbf{V}_q^k |m\rangle |m'\rangle \langle m| = \sum_{m, m'} \langle m'| \mathbf{V}_q^k |m\rangle \mathbf{E}_{m'm} = \mu \sum_{m, m'} C_{q m m'=m+q}^{k \ell \ell} \mathbf{E}_{m'm}$$

$$= \mu \sum_{m, m'} \binom{k}{m' m} \mathbf{E}_{m'm} \quad \text{with proportionality constant: } \mu = (-1)^k \sqrt{\frac{2k+1}{2\ell+1}} \quad \dots \text{that won't vary with } (m', m)$$

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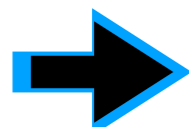
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$$\tilde{\mathbf{V}}_1^2 \mathbf{V}_1^2 = \frac{1}{2} \begin{array}{c|cc} & -E_{12} & +E_{23} \\ \hline -E_{21} & +E_{21}E_{12} & -E_{21}E_{23} \\ +E_{32} & -E_{32}E_{12} & +E_{32}E_{23} \end{array} \quad \mathbf{V}_1^2 \tilde{\mathbf{V}}_1^2 = \frac{1}{2} \begin{array}{c|cc} & -E_{12} & +E_{23} \\ \hline +E_{12}E_{21} & -E_{12}E_{32} \\ -E_{23}E_{12} & +E_{23}E_{32} \end{array}$$

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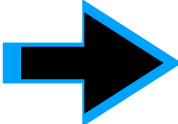
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$\begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} = [2,1]$  tableau basis and  $U(3)$  irep (from p. 29)

$M=2$        $M=1$        $M=0$        $M=-1$        $M=-2$

	$\begin{array}{ c } \hline \begin{array}{c} 11 \\ 2 \end{array} \\ \hline \end{array}$	$\begin{array}{ c c } \hline \begin{array}{c} 12 \\ 2 \end{array} & \begin{array}{c} 11 \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 12 \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 13 \\ 2 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 13 \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c c } \hline \begin{array}{c} 22 \\ 3 \end{array} & \begin{array}{c} 23 \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 23 \\ 3 \end{array} \\ \hline \end{array}$	
$\langle \begin{array}{ c } \hline \begin{array}{c} 11 \\ 2 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (11) (22) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ 1 \end{array}$ $\begin{array}{c} (23) \\ 1 \end{array}$	$\begin{array}{c} (13) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	.	
$\langle \begin{array}{ c } \hline \begin{array}{c} 12 \\ 2 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (11) (22) \\ 1+2 \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ -1 \end{array}$	.	
$\langle \begin{array}{ c } \hline \begin{array}{c} 11 \\ 3 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (32) \\ 1 \end{array}$	.	$\begin{array}{c} (11) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	.	$\begin{array}{c} (13) \\ 1 \end{array}$	.	
$\langle \begin{array}{ c } \hline \begin{array}{c} 12 \\ 3 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{1}{2}} \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 13 \\ 2 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 13 \\ 3 \end{array} \\ \hline \end{array}  $	.	.	$\begin{array}{c} (31) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (11) (33) \\ 1+2 \end{array}$	.	$\begin{array}{c} (12) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 22 \\ 3 \end{array} \\ \hline \end{array}  $	.	$\begin{array}{c} (31) \\ -1 \end{array}$	.	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	.	.	$\begin{array}{c} (22) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 23 \\ 3 \end{array} \\ \hline \end{array}  $	.	.	.	$\begin{array}{c} (31) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ 1 \end{array}$	$\begin{array}{c} (22) (33) \\ 1+2 \end{array}$

$$\langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} \begin{pmatrix} 2 \\ 11 \end{pmatrix} & \begin{pmatrix} 2 \\ 12 \end{pmatrix} & \begin{pmatrix} 2 \\ 13 \end{pmatrix} \\ \begin{pmatrix} 2 \\ 21 \end{pmatrix} & \begin{pmatrix} 2 \\ 22 \end{pmatrix} & \begin{pmatrix} 2 \\ 23 \end{pmatrix} \\ \begin{pmatrix} 2 \\ 31 \end{pmatrix} & \begin{pmatrix} 2 \\ 32 \end{pmatrix} & \begin{pmatrix} 2 \\ 33 \end{pmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} 1 & -1 & 1 \\ 1 & -2 & 1 \\ 1 & -1 & 1 \end{pmatrix} \begin{matrix} 1 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{matrix}$$

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{pmatrix} 1 \\ 11 \end{pmatrix} & \begin{pmatrix} 1 \\ 12 \end{pmatrix} & \cdot \\ \begin{pmatrix} 1 \\ 21 \end{pmatrix} & \begin{pmatrix} 1 \\ 22 \end{pmatrix} & \begin{pmatrix} 1 \\ 23 \end{pmatrix} \\ \cdot & \begin{pmatrix} 1 \\ 32 \end{pmatrix} & \begin{pmatrix} 1 \\ 33 \end{pmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \begin{pmatrix} 0 \\ 11 \end{pmatrix} & \cdot & \cdot \\ \cdot & \begin{pmatrix} 0 \\ 22 \end{pmatrix} & \cdot \\ \cdot & \cdot & \begin{pmatrix} 0 \\ 33 \end{pmatrix} \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

$\begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} = [2,1]$  tableau basis and matrices of  $\mathbf{v}^1$  dipole

$M=2$        $M=1$        $M=0$        $M=-1$        $M=-2$

	$\begin{array}{ c } \hline  11\rangle \\  2\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  12\rangle \\  2\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  11\rangle \\  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  12\rangle \\  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  13\rangle \\  2\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  13\rangle \\  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  22\rangle \\  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  23\rangle \\  3\rangle \\ \hline \end{array}$
$\langle \begin{array}{ c } \hline  11\rangle \\  2\rangle \\ \hline \end{array}  $	$\begin{array}{c} (11) (22) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ 1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$	$\begin{array}{c} (13) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	.
$\langle \begin{array}{ c } \hline  12\rangle \\  2\rangle \\ \hline \end{array}  $	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (11) (22) \\ 1+2 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ -1 \end{array}$	.
$\langle \begin{array}{ c } \hline  11\rangle \\  3\rangle \\ \hline \end{array}  $	$\begin{array}{c} (32) \\ 1 \end{array}$	.	$\begin{array}{c} (11) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	.	$\begin{array}{c} (13) \\ 1 \end{array}$	.	.
$E_{jk} = \langle \begin{array}{ c } \hline  12\rangle \\  3\rangle \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{1}{2}} \end{array}$
$\langle \begin{array}{ c } \hline  13\rangle \\  2\rangle \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$
$\langle \begin{array}{ c } \hline  13\rangle \\  3\rangle \\ \hline \end{array}  $	.	.	$\begin{array}{c} (31) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (11) (33) \\ 1+2 \end{array}$	.	$\begin{array}{c} (12) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline  22\rangle \\  3\rangle \\ \hline \end{array}  $	.	$\begin{array}{c} (31) \\ -1 \end{array}$	.	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	.	.	$\begin{array}{c} (22) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline  23\rangle \\  3\rangle \\ \hline \end{array}  $	.	.	.	$\begin{array}{c} (31) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ 1 \end{array}$	$\begin{array}{c} (22) (33) \\ 1+2 \end{array}$

dipole ( $k=1$ ) angular momentum  $\mathbf{L}$ -operators

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{array}{c} (1) \\ (11) \end{array} & \begin{array}{c} (1) \\ (12) \end{array} & \cdot \\ \begin{array}{c} (1) \\ (21) \end{array} & \begin{array}{c} (1) \\ (22) \end{array} & \begin{array}{c} (1) \\ (23) \end{array} \\ \cdot & \begin{array}{c} (1) \\ (32) \end{array} & \begin{array}{c} (1) \\ (33) \end{array} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \begin{array}{c} (0) \\ (11) \end{array} & \cdot & \cdot \\ \cdot & \begin{array}{c} (0) \\ (22) \end{array} & \cdot \\ \cdot & \cdot & \begin{array}{c} (0) \\ (33) \end{array} \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

$\begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \square \\ \hline \end{array} = [2,1]$  tableau basis and matrices of  $\mathbf{v}^1$  dipole

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{array}{ c } \hline \begin{array}{c} (11) \\ 2 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} (12) \\ 2 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} (11) \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} (12) \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} (13) \\ 2 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} (13) \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} (22) \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} (23) \\ 3 \end{array} \\ \hline \end{array}$
$E_{jk} = \langle \begin{array}{ c } \hline \begin{array}{c} (11) \\ 2 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (11) \ (22) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ 1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$	$\begin{array}{c} (13) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	.
$\langle \begin{array}{ c } \hline \begin{array}{c} (12) \\ 2 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (11) \ (22) \\ 1+2 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ -1 \end{array}$	.
$\langle \begin{array}{ c } \hline \begin{array}{c} (11) \\ 3 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (32) \\ 1 \end{array}$	.	$\begin{array}{c} (11) \ (33) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	.	$\begin{array}{c} (13) \\ 1 \end{array}$	.	.
$\langle \begin{array}{ c } \hline \begin{array}{c} (12) \\ 3 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (11) \ (22) \ (33) \\ 1+1+1 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{1}{2}} \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} (13) \\ 2 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	$\begin{array}{c} (11) \ (22) \ (33) \\ 1+1+1 \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} (13) \\ 3 \end{array} \\ \hline \end{array}  $	.	.	$\begin{array}{c} (31) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (11) \ (33) \\ 1+2 \end{array}$	.	$\begin{array}{c} (12) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} (22) \\ 3 \end{array} \\ \hline \end{array}  $	.	$\begin{array}{c} (31) \\ -1 \end{array}$	.	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	.	.	$\begin{array}{c} (22) \ (33) \\ 2+1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} (23) \\ 3 \end{array} \\ \hline \end{array}  $	.	.	.	$\begin{array}{c} (31) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ 1 \end{array}$	$\begin{array}{c} (22) \ (33) \\ 1+2 \end{array}$

$$L_z \equiv \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} = (E_{11} - E_{33}) = \sqrt{2} \mathbf{v}_0^1$$

dipole ( $k=1$ ) angular momentum  $\mathbf{L}$ -operators

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{array}{c} (1) \\ (11) \end{array} & \begin{array}{c} (1) \\ (12) \end{array} & \cdot \\ \begin{array}{c} (1) \\ (21) \end{array} & \begin{array}{c} (1) \\ (22) \end{array} & \begin{array}{c} (1) \\ (23) \end{array} \\ \cdot & \begin{array}{c} (1) \\ (32) \end{array} & \begin{array}{c} (1) \\ (33) \end{array} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \begin{array}{c} (0) \\ (11) \end{array} & \cdot & \cdot \\ \cdot & \begin{array}{c} (0) \\ (22) \end{array} & \cdot \\ \cdot & \cdot & \begin{array}{c} (0) \\ (33) \end{array} \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

$\begin{smallmatrix} \square & \square \\ \square & \end{smallmatrix} = [2,1]$  tableau basis and matrices of  $\mathbf{v}^1$  dipole

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{smallmatrix}  11\rangle \\  2 \end{smallmatrix}$	$\begin{smallmatrix}  12\rangle \\  2 \end{smallmatrix}$	$\begin{smallmatrix}  11\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  12\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  13\rangle \\  2 \end{smallmatrix}$	$\begin{smallmatrix}  13\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  22\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  23\rangle \\  3 \end{smallmatrix}$
$E_{jk} = \langle \begin{smallmatrix} 11 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (11) & (22) \\ 2+1 \end{smallmatrix}$	$\begin{smallmatrix} (12) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (13) \\ -\sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (13) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	.	.	.
$\langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (21) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (11) & (22) \\ 1+2 \end{smallmatrix}$	.	$\begin{smallmatrix} (23) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	.	$\begin{smallmatrix} (13) \\ -1 \end{smallmatrix}$	.
$\langle \begin{smallmatrix} 11 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} (32) \\ 1 \end{smallmatrix}$	.	$\begin{smallmatrix} (11) & (33) \\ 2+1 \end{smallmatrix}$	$\begin{smallmatrix} (12) \\ \sqrt{2} \end{smallmatrix}$	.	$\begin{smallmatrix} (13) \\ 1 \end{smallmatrix}$	.	.
$\langle \begin{smallmatrix} 12 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} (31) \\ -\sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (21) \\ \sqrt{2} \end{smallmatrix}$	$\begin{smallmatrix} (11) & (22) & (33) \\ 1+1+1 \end{smallmatrix}$	.	$\begin{smallmatrix} (23) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (12) \\ \sqrt{2} \end{smallmatrix}$	$\begin{smallmatrix} (13) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$
$\langle \begin{smallmatrix} 13 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (31) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	.	.	$\begin{smallmatrix} (11) & (22) & (33) \\ 1+1+1 \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	.	$\begin{smallmatrix} (13) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$
$\langle \begin{smallmatrix} 13 \\ 3 \end{smallmatrix}  $	.	.	$\begin{smallmatrix} (31) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (11) & (33) \\ 1+2 \end{smallmatrix}$	.	$\begin{smallmatrix} (12) \\ 1 \end{smallmatrix}$
$\langle \begin{smallmatrix} 22 \\ 3 \end{smallmatrix}  $	.	$\begin{smallmatrix} (31) \\ -1 \end{smallmatrix}$	.	$\begin{smallmatrix} (21) \\ \sqrt{2} \end{smallmatrix}$	.	.	$\begin{smallmatrix} (22) & (33) \\ 2+1 \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ 1 \end{smallmatrix}$
$\langle \begin{smallmatrix} 23 \\ 3 \end{smallmatrix}  $	.	.	.	$\begin{smallmatrix} (31) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (31) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (21) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (22) & (33) \\ 1+2 \end{smallmatrix}$

$$L_z \equiv \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} = (E_{11} - E_{33}) = \sqrt{2} \mathbf{v}_0^1$$

$$L_+ \equiv \sqrt{2} \begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} = \sqrt{2} (E_{12} + E_{23}) = L_x + iL_y = -\sqrt{2} \mathbf{v}_1^1$$

dipole ( $k=1$ ) angular momentum  $\mathbf{L}$ -operators

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{smallmatrix} (1) \\ (11) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (12) \end{smallmatrix} & \cdot \\ \begin{smallmatrix} (1) \\ (21) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (22) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (23) \end{smallmatrix} \\ \cdot & \begin{smallmatrix} (1) \\ (32) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (33) \end{smallmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \begin{smallmatrix} (0) \\ (11) \end{smallmatrix} & \cdot & \cdot \\ \cdot & \begin{smallmatrix} (0) \\ (22) \end{smallmatrix} & \cdot \\ \cdot & \cdot & \begin{smallmatrix} (0) \\ (33) \end{smallmatrix} \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

$\begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \square \\ \hline \end{array} = [2,1]$  tableau basis and matrices of  $\mathbf{v}^1$  dipole

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{array}{ c } \hline  11\rangle \\  2\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  12\rangle \\  2\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  11\rangle \\  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  12\rangle \\  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  13\rangle \\  2\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  13\rangle \\  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  22\rangle \\  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  23\rangle \\  3\rangle \\ \hline \end{array}$
$E_{jk} = \langle \begin{array}{ c } \hline  11\rangle \\  2\rangle \\ \hline \end{array}  $	$\begin{array}{c} (11) (22) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ 1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$	$\begin{array}{c} (13) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	.
$\langle \begin{array}{ c } \hline  12\rangle \\  2\rangle \\ \hline \end{array}  $	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (11) (22) \\ 1+2 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ -1 \end{array}$	.
$\langle \begin{array}{ c } \hline  11\rangle \\  3\rangle \\ \hline \end{array}  $	$\begin{array}{c} (32) \\ 1 \end{array}$	.	$\begin{array}{c} (11) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	.	$\begin{array}{c} (13) \\ 1 \end{array}$	.	.
$\langle \begin{array}{ c } \hline  12\rangle \\  3\rangle \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{1}{2}} \end{array}$
$\langle \begin{array}{ c } \hline  13\rangle \\  2\rangle \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$
$\langle \begin{array}{ c } \hline  13\rangle \\  3\rangle \\ \hline \end{array}  $	.	.	$\begin{array}{c} (31) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (11) (33) \\ 1+2 \end{array}$	.	$\begin{array}{c} (12) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline  22\rangle \\  3\rangle \\ \hline \end{array}  $	.	$\begin{array}{c} (31) \\ -1 \end{array}$	.	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	.	.	$\begin{array}{c} (22) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline  23\rangle \\  3\rangle \\ \hline \end{array}  $	.	.	.	$\begin{array}{c} (31) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ 1 \end{array}$	$\begin{array}{c} (22) (33) \\ 1+2 \end{array}$

$$L_z \equiv \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} = (E_{11} - E_{33}) = \sqrt{2} \mathbf{v}_0^1$$

$$L_+ \equiv \sqrt{2} \begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} = \sqrt{2} (E_{12} + E_{23}) = L_x + iL_y = -\sqrt{2} \mathbf{v}_1^1$$

$$L_- \equiv \sqrt{2} \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix} = \sqrt{2} (E_{21} + E_{32}) = L_x - iL_y = \sqrt{2} \mathbf{v}_{-1}^1$$

dipole ( $k=1$ ) angular momentum  $\mathbf{L}$ -operators

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{array}{c} (1) \\ (11) \end{array} & \begin{array}{c} (1) \\ (12) \end{array} & \cdot \\ \begin{array}{c} (1) \\ (21) \end{array} & \begin{array}{c} (1) \\ (22) \end{array} & \begin{array}{c} (1) \\ (23) \end{array} \\ \cdot & \begin{array}{c} (1) \\ (32) \end{array} & \begin{array}{c} (1) \\ (33) \end{array} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \begin{array}{c} (0) \\ (11) \end{array} & \cdot & \cdot \\ \cdot & \begin{array}{c} (0) \\ (22) \end{array} & \cdot \\ \cdot & \cdot & \begin{array}{c} (0) \\ (33) \end{array} \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

$\begin{array}{|c|} \hline \square \square \\ \hline \square \\ \hline \end{array} = [2,1]$  tableau basis and matrices of  $\mathbf{v}^1$  dipole

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{array}{ c } \hline  11\rangle \\  2\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  12\rangle \\  2\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  11\rangle \\  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  12\rangle \\  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  13\rangle \\  2\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  13\rangle \\  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  22\rangle \\  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  23\rangle \\  3\rangle \\ \hline \end{array}$
$E_{jk} = \langle \begin{array}{ c } \hline  11\rangle \\  2\rangle \\ \hline \end{array}  $	$\begin{array}{ c } \hline (11) (22) \\ 2+1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (12) \\ 1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (23) \\ 1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (13) \\ -\sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (13) \\ \sqrt{\frac{3}{2}} \\ \hline \end{array}$	.	.	.
$\langle \begin{array}{ c } \hline  12\rangle \\  2\rangle \\ \hline \end{array}  $	$\begin{array}{ c } \hline (21) \\ 1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (11) (22) \\ 1+2 \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (23) \\ \sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (23) \\ \sqrt{\frac{3}{2}} \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (13) \\ -1 \\ \hline \end{array}$	.
$\langle \begin{array}{ c } \hline  11\rangle \\  3\rangle \\ \hline \end{array}  $	$\begin{array}{ c } \hline (32) \\ 1 \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (11) (33) \\ 2+1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (12) \\ \sqrt{2} \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (13) \\ 1 \\ \hline \end{array}$	.	.
$\langle \begin{array}{ c } \hline  12\rangle \\  3\rangle \\ \hline \end{array}  $	$\begin{array}{ c } \hline (31) \\ -\sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (32) \\ \sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (21) \\ \sqrt{2} \\ \hline \end{array}$	$\begin{array}{ c } \hline (11) (22) (33) \\ 1+1+1 \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (23) \\ \sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (12) \\ \sqrt{2} \\ \hline \end{array}$	$\begin{array}{ c } \hline (13) \\ \sqrt{\frac{1}{2}} \\ \hline \end{array}$
$\langle \begin{array}{ c } \hline  13\rangle \\  2\rangle \\ \hline \end{array}  $	$\begin{array}{ c } \hline (31) \\ \sqrt{\frac{3}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (32) \\ \sqrt{\frac{3}{2}} \\ \hline \end{array}$	.	.	$\begin{array}{ c } \hline (11) (22) (33) \\ 1+1+1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (23) \\ \sqrt{\frac{3}{2}} \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (13) \\ \sqrt{\frac{3}{2}} \\ \hline \end{array}$
$\langle \begin{array}{ c } \hline  13\rangle \\  3\rangle \\ \hline \end{array}  $	.	.	$\begin{array}{ c } \hline (31) \\ 1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (32) \\ \sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (32) \\ \sqrt{\frac{3}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (11) (33) \\ 1+2 \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (12) \\ 1 \\ \hline \end{array}$
$\langle \begin{array}{ c } \hline  22\rangle \\  3\rangle \\ \hline \end{array}  $	.	$\begin{array}{ c } \hline (31) \\ -1 \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (21) \\ \sqrt{2} \\ \hline \end{array}$	.	.	$\begin{array}{ c } \hline (22) (33) \\ 2+1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (23) \\ 1 \\ \hline \end{array}$
$\langle \begin{array}{ c } \hline  23\rangle \\  3\rangle \\ \hline \end{array}  $	.	.	.	$\begin{array}{ c } \hline (31) \\ \sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (31) \\ \sqrt{\frac{3}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (21) \\ 1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (32) \\ 1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (22) (33) \\ 1+2 \\ \hline \end{array}$

$$\begin{aligned} \langle \begin{array}{|c|} \hline |11\rangle \\ |2\rangle \\ \hline \end{array} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{array}{|c|} \hline |11\rangle \\ |2\rangle \\ \hline \end{array} \rangle &= \left( 2\binom{1}{11} + \binom{1}{22} \right)^2 + \binom{1}{21}^2 + \binom{1}{23}^2 + 2\binom{1}{13}^2 \\ &= \frac{1}{2} (2 \cdot 1 - 0)^2 + \left(\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}}\right)^2 + 2\left(\frac{1}{\sqrt{2}}\right)^2 = 3 \end{aligned}$$

$$L_z \equiv \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} = (E_{11} - E_{33}) = \sqrt{2} \mathbf{v}_0^1$$

$$L_+ \equiv \sqrt{2} \begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} = \sqrt{2} (E_{12} + E_{23}) = L_x + iL_y = -\sqrt{2} \mathbf{v}_1^1$$

$$L_- \equiv \sqrt{2} \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix} = \sqrt{2} (E_{21} + E_{32}) = L_x - iL_y = \sqrt{2} \mathbf{v}_{-1}^1$$

dipole ( $k=1$ ) angular momentum  $\mathbf{L}$ -operators

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \binom{1}{11} & \binom{1}{12} & \cdot \\ \binom{1}{21} & \binom{1}{22} & \binom{1}{23} \\ \cdot & \binom{1}{32} & \binom{1}{33} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

Squared angular momentum  $\mathbf{L} \cdot \mathbf{L}$ -operators

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \binom{0}{11} & \binom{0}{12} & \cdot \\ \cdot & \binom{0}{22} & \cdot \\ \cdot & \cdot & \binom{0}{33} \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

$\begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \square \\ \hline \end{array} = [2,1]$  tableau basis and matrices of  $\mathbf{v}^1$  dipole

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{array}{ c } \hline  11\rangle \\ \hline  2\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  12\rangle \\ \hline  2\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  11\rangle \\ \hline  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  12\rangle \\ \hline  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  13\rangle \\ \hline  2\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  13\rangle \\ \hline  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  22\rangle \\ \hline  3\rangle \\ \hline \end{array}$	$\begin{array}{ c } \hline  23\rangle \\ \hline  3\rangle \\ \hline \end{array}$
$E_{jk} = \langle \begin{array}{ c } \hline  11\rangle \\ \hline  2\rangle \\ \hline \end{array}  $	$\begin{array}{c} (11) (22) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ 1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$	$\begin{array}{c} (13) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	.
$\langle \begin{array}{ c } \hline  12\rangle \\ \hline  2\rangle \\ \hline \end{array}  $	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (11) (22) \\ 1+2 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ -1 \end{array}$	.
$\langle \begin{array}{ c } \hline  11\rangle \\ \hline  3\rangle \\ \hline \end{array}  $	$\begin{array}{c} (32) \\ 1 \end{array}$	.	$\begin{array}{c} (11) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	.	$\begin{array}{c} (13) \\ 1 \end{array}$	.	.
$\langle \begin{array}{ c } \hline  12\rangle \\ \hline  3\rangle \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{1}{2}} \end{array}$
$\langle \begin{array}{ c } \hline  13\rangle \\ \hline  2\rangle \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$
$\langle \begin{array}{ c } \hline  13\rangle \\ \hline  3\rangle \\ \hline \end{array}  $	.	.	$\begin{array}{c} (31) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (11) (33) \\ 1+2 \end{array}$	.	$\begin{array}{c} (12) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline  22\rangle \\ \hline  3\rangle \\ \hline \end{array}  $	.	$\begin{array}{c} (31) \\ -1 \end{array}$	.	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	.	.	$\begin{array}{c} (22) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline  23\rangle \\ \hline  3\rangle \\ \hline \end{array}  $	.	.	.	$\begin{array}{c} (31) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ 1 \end{array}$	$\begin{array}{c} (22) (33) \\ 1+2 \end{array}$

$$L_z \equiv \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} = (E_{11} - E_{33}) = \sqrt{2} \mathbf{v}_0^1$$

$$L_+ \equiv \sqrt{2} \begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} = \sqrt{2}(E_{12} + E_{23}) = L_x + iL_y = -\sqrt{2} \mathbf{v}_1^1$$

$$L_- \equiv \sqrt{2} \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix} = \sqrt{2}(E_{21} + E_{32}) = L_x - iL_y = \sqrt{2} \mathbf{v}_{-1}^1$$

dipole ( $k=1$ ) angular momentum  $\mathbf{L}$ -operators

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{array}{c} (1) \\ (11) \end{array} & \begin{array}{c} (1) \\ (12) \end{array} & \cdot \\ \begin{array}{c} (1) \\ (21) \end{array} & \begin{array}{c} (1) \\ (22) \end{array} & \begin{array}{c} (1) \\ (23) \end{array} \\ \cdot & \begin{array}{c} (1) \\ (32) \end{array} & \begin{array}{c} (1) \\ (33) \end{array} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

Squared angular momentum  $\mathbf{L} \cdot \mathbf{L}$ -operators

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \cdot & \begin{array}{c} (0) \\ (22) \end{array} & \cdot \\ \cdot & \cdot & \begin{array}{c} (0) \\ (33) \end{array} \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

$$\begin{aligned} \langle \begin{array}{|c|} \hline |11\rangle \\ \hline |2\rangle \\ \hline \end{array} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{array}{|c|} \hline |11\rangle \\ \hline |2\rangle \\ \hline \end{array} \rangle &= \left( 2 \binom{1}{11} + \binom{1}{22} \right)^2 + \binom{1}{21}^2 + \binom{1}{23}^2 + 2 \binom{1}{13}^2 \\ &= \frac{1}{2} (2 \cdot 1 - 0)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 = 3 \end{aligned}$$

$$\begin{aligned} \langle \begin{array}{|c|} \hline |12\rangle \\ \hline |2\rangle \\ \hline \end{array} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{array}{|c|} \hline |12\rangle \\ \hline |2\rangle \\ \hline \end{array} \rangle &= \left( \binom{1}{11} + 2 \binom{1}{22} \right)^2 + \binom{1}{21}^2 + 2 \binom{1}{23}^2 + \binom{1}{13}^2 \\ &= \frac{1}{2} (1 \cdot 1 + 2 \cdot 0)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 + 0 \\ &= \frac{1}{2} + \frac{1}{2} + 1 + 0 = 2 \end{aligned}$$

$\begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \end{array} = [2,1]$  tableau basis and matrices of  $\mathbf{v}^1$  dipole

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{array}{ c } \hline 11 \\ \hline 2 \\ \hline \end{array}$	$\begin{array}{ c } \hline 12 \\ \hline 2 \\ \hline \end{array}$	$\begin{array}{ c } \hline 11 \\ \hline 3 \\ \hline \end{array}$	$\begin{array}{ c } \hline 12 \\ \hline 3 \\ \hline \end{array}$	$\begin{array}{ c } \hline 13 \\ \hline 2 \\ \hline \end{array}$	$\begin{array}{ c } \hline 13 \\ \hline 3 \\ \hline \end{array}$	$\begin{array}{ c } \hline 22 \\ \hline 3 \\ \hline \end{array}$	$\begin{array}{ c } \hline 23 \\ \hline 3 \\ \hline \end{array}$
$E_{jk} = \langle \begin{array}{ c } \hline 11 \\ \hline 2 \\ \hline \end{array}  $	$\begin{array}{c} (11) (22) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ 1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$	$\begin{array}{c} (13) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	.
$\langle \begin{array}{ c } \hline 12 \\ \hline 2 \\ \hline \end{array}  $	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (11) (22) \\ 1+2 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ -1 \end{array}$	.
$\langle \begin{array}{ c } \hline 11 \\ \hline 3 \\ \hline \end{array}  $	$\begin{array}{c} (32) \\ 1 \end{array}$	.	$\begin{array}{c} (11) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	.	$\begin{array}{c} (13) \\ 1 \end{array}$	.	.
$\langle \begin{array}{ c } \hline 12 \\ \hline 3 \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{1}{2}} \end{array}$
$\langle \begin{array}{ c } \hline 13 \\ \hline 2 \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$
$\langle \begin{array}{ c } \hline 13 \\ \hline 3 \\ \hline \end{array}  $	.	.	$\begin{array}{c} (31) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (11) (33) \\ 1+2 \end{array}$	.	$\begin{array}{c} (12) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline 22 \\ \hline 3 \\ \hline \end{array}  $	.	$\begin{array}{c} (31) \\ -1 \end{array}$	.	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	.	.	$\begin{array}{c} (22) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline 23 \\ \hline 3 \\ \hline \end{array}  $	.	.	.	$\begin{array}{c} (31) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ 1 \end{array}$	$\begin{array}{c} (22) (33) \\ 1+2 \end{array}$

$$L_z \equiv \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} = (E_{11} - E_{33}) = \sqrt{2} \mathbf{v}_0^1$$

$$L_+ \equiv \sqrt{2} \begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} = \sqrt{2}(E_{12} + E_{23}) = L_x + iL_y = -\sqrt{2} \mathbf{v}_1^1$$

$$L_- \equiv \sqrt{2} \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix} = \sqrt{2}(E_{21} + E_{32}) = L_x - iL_y = \sqrt{2} \mathbf{v}_{-1}^1$$

dipole ( $k=1$ ) angular momentum  $\mathbf{L}$ -operators

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{array}{|c|} \hline (1) \\ \hline (11) \end{array} & \begin{array}{|c|} \hline (1) \\ \hline (12) \end{array} & \cdot \\ \begin{array}{|c|} \hline (1) \\ \hline (21) \end{array} & \begin{array}{|c|} \hline (1) \\ \hline (22) \end{array} & \begin{array}{|c|} \hline (1) \\ \hline (23) \end{array} \\ \cdot & \begin{array}{|c|} \hline (1) \\ \hline (32) \end{array} & \begin{array}{|c|} \hline (1) \\ \hline (33) \end{array} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

Squared angular momentum  $\mathbf{L} \cdot \mathbf{L}$ -operators

$$\begin{aligned} \langle \begin{array}{|c|} \hline 11 \\ \hline 2 \\ \hline \end{array} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{array}{|c|} \hline 11 \\ \hline 2 \\ \hline \end{array} \rangle &= \left( 2 \binom{1}{11} + \binom{1}{22} \right)^2 + \binom{1}{21}^2 + \binom{1}{23}^2 + 2 \binom{1}{13}^2 \\ &= \frac{1}{2} (2 \cdot 1 - 0)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 = 3 \end{aligned}$$

$$\begin{aligned} \langle \begin{array}{|c|} \hline 12 \\ \hline 2 \\ \hline \end{array} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{array}{|c|} \hline 12 \\ \hline 2 \\ \hline \end{array} \rangle &= \left( \binom{1}{11} + 2 \binom{1}{22} \right)^2 + \binom{1}{21}^2 + 2 \binom{1}{23}^2 + \binom{1}{13}^2 \\ &= \frac{1}{2} (1 \cdot 1 + 2 \cdot 0)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 + 0 \\ &= \frac{1}{2} + \frac{1}{2} + 1 + 0 = 2 \end{aligned}$$

$$\begin{aligned} \langle \begin{array}{|c|} \hline 11 \\ \hline 3 \\ \hline \end{array} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{array}{|c|} \hline 11 \\ \hline 3 \\ \hline \end{array} \rangle &= \left( 2 \binom{1}{11} + \binom{1}{33} \right)^2 + 2 \binom{1}{21}^2 + \binom{1}{23}^2 + \binom{1}{13}^2 \\ &= \frac{1}{2} (2 \cdot 1 - 1 \cdot 1)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 0 \\ &= \frac{1}{2} + 1 + \frac{1}{2} + 0 = 2 \end{aligned}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \cdot & \binom{0}{22} & \cdot \\ \cdot & \cdot & \binom{0}{33} \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$



$\begin{matrix} \square & \square \\ \square & \end{matrix} = [2,1]$  tableau basis and matrices of  $\mathbf{v}^1$  dipole

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{matrix}  11\rangle \\  2\rangle \end{matrix}$	$\begin{matrix}  12\rangle \\  2\rangle \end{matrix}$	$\begin{matrix}  11\rangle \\  3\rangle \end{matrix}$	$\begin{matrix}  12\rangle \\  3\rangle \end{matrix}$	$\begin{matrix}  13\rangle \\  2\rangle \end{matrix}$	$\begin{matrix}  13\rangle \\  3\rangle \end{matrix}$	$\begin{matrix}  22\rangle \\  3\rangle \end{matrix}$	$\begin{matrix}  23\rangle \\  3\rangle \end{matrix}$
$E_{jk} = \langle \begin{matrix} 11 \\ 2 \end{matrix}  $	$\begin{matrix} (11) & (22) \\ 2 & +1 \end{matrix}$	$\begin{matrix} (12) & (23) \\ 1 & 1 \end{matrix}$		$\begin{matrix} (13) \\ -\sqrt{\frac{1}{2}} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{\frac{3}{2}} \end{matrix}$			
$\langle \begin{matrix} 12 \\ 2 \end{matrix}  $	$\begin{matrix} (21) \\ 1 \end{matrix}$	$\begin{matrix} (11) & (22) \\ 1 & +2 \end{matrix}$		$\begin{matrix} (23) \\ \sqrt{\frac{1}{2}} \end{matrix}$	$\begin{matrix} (23) \\ \sqrt{\frac{3}{2}} \end{matrix}$		$\begin{matrix} (13) \\ -1 \end{matrix}$	
$\langle \begin{matrix} 11 \\ 3 \end{matrix}  $	$\begin{matrix} (32) \\ 1 \end{matrix}$		$\begin{matrix} (11) & (33) \\ 2 & +1 \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$			$\begin{matrix} (13) \\ 1 \end{matrix}$	
$\langle \begin{matrix} 12 \\ 3 \end{matrix}  $	$\begin{matrix} (31) \\ -\sqrt{\frac{1}{2}} \end{matrix}$	$\begin{matrix} (32) \\ \sqrt{\frac{1}{2}} \end{matrix}$	$\begin{matrix} (21) \\ \sqrt{2} \end{matrix}$	$\begin{matrix} (11) & (22) & (33) \\ 1 & +1 & +1 \end{matrix}$			$\begin{matrix} (23) \\ \sqrt{\frac{1}{2}} \end{matrix}$	$\begin{matrix} (12) \\ \sqrt{2} \end{matrix}$
$\langle \begin{matrix} 13 \\ 2 \end{matrix}  $	$\begin{matrix} (31) \\ \sqrt{\frac{3}{2}} \end{matrix}$	$\begin{matrix} (32) \\ \sqrt{\frac{3}{2}} \end{matrix}$			$\begin{matrix} (11) & (22) & (33) \\ 1 & +1 & +1 \end{matrix}$		$\begin{matrix} (23) \\ \sqrt{\frac{3}{2}} \end{matrix}$	$\begin{matrix} (13) \\ \sqrt{\frac{3}{2}} \end{matrix}$
$\langle \begin{matrix} 13 \\ 3 \end{matrix}  $			$\begin{matrix} (31) \\ 1 \end{matrix}$	$\begin{matrix} (32) \\ \sqrt{\frac{1}{2}} \end{matrix}$	$\begin{matrix} (32) \\ \sqrt{\frac{3}{2}} \end{matrix}$	$\begin{matrix} (11) & (33) \\ 1 & +2 \end{matrix}$		$\begin{matrix} (12) \\ 1 \end{matrix}$
$\langle \begin{matrix} 22 \\ 3 \end{matrix}  $		$\begin{matrix} (31) \\ -1 \end{matrix}$		$\begin{matrix} (21) \\ \sqrt{2} \end{matrix}$			$\begin{matrix} (22) & (33) \\ 2 & +1 \end{matrix}$	$\begin{matrix} (23) \\ 1 \end{matrix}$
$\langle \begin{matrix} 23 \\ 3 \end{matrix}  $				$\begin{matrix} (31) \\ \sqrt{\frac{1}{2}} \end{matrix}$	$\begin{matrix} (31) \\ \sqrt{\frac{3}{2}} \end{matrix}$	$\begin{matrix} (21) & (32) \\ 1 & 1 \end{matrix}$		$\begin{matrix} (22) & (33) \\ 1 & +2 \end{matrix}$

$$L_z \equiv \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} = (E_{11} - E_{33}) = \sqrt{2} \mathbf{v}_0^1$$

$$L_+ \equiv \sqrt{2} \begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} = \sqrt{2}(E_{12} + E_{23}) = L_x + iL_y = -\sqrt{2} \mathbf{v}_1^1$$

$$L_- \equiv \sqrt{2} \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix} = \sqrt{2}(E_{21} + E_{32}) = L_x - iL_y = \sqrt{2} \mathbf{v}_{-1}^1$$

dipole ( $k=1$ ) angular momentum  $\mathbf{L}$ -operators

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{matrix} (1) & (1) & \cdot \\ (11) & (12) & \cdot \end{matrix} \\ \begin{matrix} (1) & (1) & (1) \\ (21) & (22) & (23) \end{matrix} \\ \cdot & \begin{matrix} (1) & (1) \\ (32) & (33) \end{matrix} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

Squared angular momentum  $\mathbf{L} \cdot \mathbf{L}$ -operators

$$\begin{aligned} \langle \begin{matrix} 11 \\ 2 \end{matrix} | \mathcal{V}^1 \cdot \mathcal{V}^1 | \begin{matrix} 11 \\ 2 \end{matrix} \rangle &= \left( 2 \binom{1}{11} + \binom{1}{22} \right)^2 + \binom{1}{21}^2 + \binom{1}{23}^2 + 2 \binom{1}{13}^2 \\ &= \frac{1}{2} (2 \cdot 1 - 0)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 = 3 \end{aligned}$$

$$\begin{aligned} \langle \begin{matrix} 12 \\ 2 \end{matrix} | \mathcal{V}^1 \cdot \mathcal{V}^1 | \begin{matrix} 12 \\ 2 \end{matrix} \rangle &= \left( \binom{1}{11} + 2 \binom{1}{22} \right)^2 + \binom{1}{21}^2 + 2 \binom{1}{23}^2 + \binom{1}{13}^2 \\ &= \frac{1}{2} (1 \cdot 1 + 2 \cdot 0)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 + 0 \\ &= \frac{1}{2} + \frac{1}{2} + 1 + 0 = 2 \end{aligned}$$

$$\begin{aligned} \langle \begin{matrix} 11 \\ 3 \end{matrix} | \mathcal{V}^1 \cdot \mathcal{V}^1 | \begin{matrix} 11 \\ 3 \end{matrix} \rangle &= \left( 2 \binom{1}{11} + \binom{1}{33} \right)^2 + 2 \binom{1}{21}^2 + \binom{1}{23}^2 + \binom{1}{13}^2 \\ &= \frac{1}{2} (2 \cdot 1 - 1 \cdot 1)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 0 \\ &= \frac{1}{2} + 1 + \frac{1}{2} + 0 = 2 \end{aligned}$$

$$\begin{aligned} \langle \begin{matrix} 12 \\ 2 \end{matrix} | \mathcal{V}^1 \cdot \mathcal{V}^1 | \begin{matrix} 11 \\ 3 \end{matrix} \rangle &= + \binom{1}{21} \binom{1}{32} + \binom{1}{23} \binom{1}{13} \\ &= \frac{1}{2} (1 \cdot 1 + 1 \cdot 1) = -1 \end{aligned}$$

# $\begin{smallmatrix} \square & \square \\ \square \end{smallmatrix} = [2,1]$ tableau basis and matrices of $\mathbf{v}^1$ dipole

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{smallmatrix}  11\rangle \\  2\rangle \end{smallmatrix}$	$\begin{smallmatrix}  12\rangle \\  2\rangle \end{smallmatrix}$	$\begin{smallmatrix}  11\rangle \\  3\rangle \end{smallmatrix}$	$\begin{smallmatrix}  12\rangle \\  3\rangle \end{smallmatrix}$	$\begin{smallmatrix}  13\rangle \\  2\rangle \end{smallmatrix}$	$\begin{smallmatrix}  13\rangle \\  3\rangle \end{smallmatrix}$	$\begin{smallmatrix}  22\rangle \\  3\rangle \end{smallmatrix}$	$\begin{smallmatrix}  23\rangle \\  3\rangle \end{smallmatrix}$
$E_{jk} = \langle \begin{smallmatrix} 11 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (11) & (22) \\ 2+1 \end{smallmatrix}$	$\begin{smallmatrix} (12) & (23) \\ 1 & 1 \end{smallmatrix}$	$\begin{smallmatrix} (13) & (13) \\ -\sqrt{\frac{1}{2}} & \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (21) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (11) & (22) \\ 1+2 \end{smallmatrix}$	$\begin{smallmatrix} (23) & (23) \\ \sqrt{\frac{1}{2}} & \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\cdot$	$\begin{smallmatrix} (13) \\ -1 \end{smallmatrix}$	$\cdot$	$\cdot$	$\cdot$
$\langle \begin{smallmatrix} 11 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} (32) \\ 1 \end{smallmatrix}$	$\cdot$	$\begin{smallmatrix} (11) & (33) \\ 2+1 \end{smallmatrix}$	$\begin{smallmatrix} (12) \\ \sqrt{2} \end{smallmatrix}$	$\cdot$	$\begin{smallmatrix} (13) \\ 1 \end{smallmatrix}$	$\cdot$	$\cdot$
$\langle \begin{smallmatrix} 12 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} (31) \\ -\sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (21) \\ \sqrt{2} \end{smallmatrix}$	$\begin{smallmatrix} (11) & (22) & (33) \\ 1+1+1 \end{smallmatrix}$	$\cdot$	$\begin{smallmatrix} (23) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (12) \\ \sqrt{2} \end{smallmatrix}$	$\begin{smallmatrix} (13) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$
$\langle \begin{smallmatrix} 13 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (31) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\cdot$	$\cdot$	$\begin{smallmatrix} (11) & (22) & (33) \\ 1+1+1 \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\cdot$	$\begin{smallmatrix} (13) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$
$\langle \begin{smallmatrix} 13 \\ 3 \end{smallmatrix}  $	$\cdot$	$\cdot$	$\begin{smallmatrix} (31) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (11) & (33) \\ 1+2 \end{smallmatrix}$	$\cdot$	$\begin{smallmatrix} (12) \\ 1 \end{smallmatrix}$
$\langle \begin{smallmatrix} 22 \\ 3 \end{smallmatrix}  $	$\cdot$	$\begin{smallmatrix} (31) \\ -1 \end{smallmatrix}$	$\cdot$	$\begin{smallmatrix} (21) \\ \sqrt{2} \end{smallmatrix}$	$\cdot$	$\cdot$	$\begin{smallmatrix} (22) & (33) \\ 2+1 \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ 1 \end{smallmatrix}$
$\langle \begin{smallmatrix} 23 \\ 3 \end{smallmatrix}  $	$\cdot$	$\cdot$	$\cdot$	$\begin{smallmatrix} (31) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (31) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (21) & (32) \\ 1 & 1 \end{smallmatrix}$	$\begin{smallmatrix} (22) & (33) \\ 1+2 \end{smallmatrix}$	$\begin{smallmatrix} (22) & (33) \\ 1+2 \end{smallmatrix}$

$$L_z \equiv \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} = (E_{11} - E_{33}) = \sqrt{2} \mathbf{v}_0^1$$

$$L_+ \equiv \sqrt{2} \begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} = \sqrt{2}(E_{12} + E_{23}) = L_x + iL_y = -\sqrt{2} \mathbf{v}_1^1$$

$$L_- \equiv \sqrt{2} \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix} = \sqrt{2}(E_{21} + E_{32}) = L_x - iL_y = \sqrt{2} \mathbf{v}_{-1}^1$$

## dipole ( $k=1$ ) angular momentum $\mathbf{L}$ -operators

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{smallmatrix} (1) & (1) & \cdot \\ (11) & (12) & \cdot \end{smallmatrix} \\ \begin{smallmatrix} (1) & (1) & (1) \\ (21) & (22) & (23) \end{smallmatrix} \\ \cdot & \begin{smallmatrix} (1) & (1) \\ (32) & (33) \end{smallmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

## Squared angular momentum $\mathbf{L} \cdot \mathbf{L}$ -operators

$$\langle \begin{smallmatrix} 11 \\ 2 \end{smallmatrix} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{smallmatrix} 11 \\ 2 \end{smallmatrix} \rangle = \left( 2 \binom{1}{11} + \binom{1}{22} \right)^2 + \binom{1}{21}^2 + \binom{1}{23}^2 + 2 \binom{1}{13}^2$$

$$= \frac{1}{2} (2 \cdot 1 - 0)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 = 3$$

$$\langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{smallmatrix} 12 \\ 2 \end{smallmatrix} \rangle = \left( \binom{1}{11} + 2 \binom{1}{22} \right)^2 + \binom{1}{21}^2 + 2 \binom{1}{23}^2 + \binom{1}{13}^2$$

$$= \frac{1}{2} (1 \cdot 1 + 2 \cdot 0)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 + 0$$

$$= \frac{1}{2} + \frac{1}{2} + 1 + 0 = 2$$

$$\langle \begin{smallmatrix} 11 \\ 3 \end{smallmatrix} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{smallmatrix} 11 \\ 3 \end{smallmatrix} \rangle = \left( 2 \binom{1}{11} + \binom{1}{33} \right)^2 + 2 \binom{1}{21}^2 + \binom{1}{23}^2 + \binom{1}{13}^2$$

$$= \frac{1}{2} (2 \cdot 1 - 1 \cdot 1)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 0$$

$$= \frac{1}{2} + 1 + \frac{1}{2} + 0 = 2$$

$$\langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{smallmatrix} 11 \\ 3 \end{smallmatrix} \rangle = + \binom{1}{21} \binom{1}{32} + \binom{1}{23} \binom{1}{13}$$

$$= \frac{1}{2} (1 \cdot 1 + 1 \cdot 1) = -1$$

$\begin{smallmatrix} \square & \square \\ \square \end{smallmatrix}$	$\begin{smallmatrix} \square & \square \\ 2 \end{smallmatrix}$		
$\begin{smallmatrix} \square & \square \\ \square \end{smallmatrix}$	3	$\begin{smallmatrix} \square & \square \\ 2 \end{smallmatrix}$	$\begin{smallmatrix} \square & \square \\ 3 \end{smallmatrix}$
$\begin{smallmatrix} \square & \square \\ \square \end{smallmatrix}$	$\begin{smallmatrix} \square & \square \\ 2 \end{smallmatrix}$	2	-1
$\begin{smallmatrix} \square & \square \\ \square \end{smallmatrix}$	$\begin{smallmatrix} \square & \square \\ 3 \end{smallmatrix}$	-1	2

# $\begin{smallmatrix} \square & \square \\ \square \end{smallmatrix} = [2,1]$ tableau basis and matrices of $\mathbf{v}^1$ dipole

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{smallmatrix} 11 \\ 2 \end{smallmatrix}$	$\begin{smallmatrix} 12 \\ 2 \end{smallmatrix}$	$\begin{smallmatrix} 11 \\ 3 \end{smallmatrix}$	$\begin{smallmatrix} 12 \\ 3 \end{smallmatrix}$	$\begin{smallmatrix} 13 \\ 2 \end{smallmatrix}$	$\begin{smallmatrix} 13 \\ 3 \end{smallmatrix}$	$\begin{smallmatrix} 22 \\ 3 \end{smallmatrix}$	$\begin{smallmatrix} 23 \\ 3 \end{smallmatrix}$
$E_{jk} = \langle \begin{smallmatrix} 11 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (11) & (22) \\ 2 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (12) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ 1 \end{smallmatrix}$	$-\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	.	.
$\langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (21) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (11) & (22) \\ 1 & +2 \end{smallmatrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	.	$\begin{smallmatrix} (13) \\ -1 \end{smallmatrix}$	.
$\langle \begin{smallmatrix} 11 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} (32) \\ 1 \end{smallmatrix}$	.	$\begin{smallmatrix} (11) & (33) \\ 2 & +1 \end{smallmatrix}$	$\sqrt{2}$	.	$\begin{smallmatrix} (13) \\ 1 \end{smallmatrix}$	.	.
$\langle \begin{smallmatrix} 12 \\ 3 \end{smallmatrix}  $	$-\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	$\sqrt{2}$	$\begin{smallmatrix} (11) & (22) & (33) \\ 1 & +1 & +1 \end{smallmatrix}$	.	$\sqrt{\frac{1}{2}}$	$\sqrt{2}$	$\sqrt{\frac{1}{2}}$
$\langle \begin{smallmatrix} 13 \\ 2 \end{smallmatrix}  $	$\sqrt{\frac{3}{2}}$	$\sqrt{\frac{3}{2}}$	.	.	$\begin{smallmatrix} (11) & (22) & (33) \\ 1 & +1 & +1 \end{smallmatrix}$	$\sqrt{\frac{3}{2}}$	.	$\sqrt{\frac{3}{2}}$
$\langle \begin{smallmatrix} 13 \\ 3 \end{smallmatrix}  $	.	.	$\begin{smallmatrix} (31) \\ 1 \end{smallmatrix}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	$\begin{smallmatrix} (11) & (33) \\ 1 & +2 \end{smallmatrix}$	.	$\begin{smallmatrix} (12) \\ 1 \end{smallmatrix}$
$\langle \begin{smallmatrix} 22 \\ 3 \end{smallmatrix}  $	.	$\begin{smallmatrix} (31) \\ -1 \end{smallmatrix}$	.	$\sqrt{2}$	.	.	$\begin{smallmatrix} (22) & (33) \\ 2 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ 1 \end{smallmatrix}$
$\langle \begin{smallmatrix} 23 \\ 3 \end{smallmatrix}  $	.	.	.	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	$\begin{smallmatrix} (21) & (32) \\ 1 & 1 \end{smallmatrix}$	$\begin{smallmatrix} (22) & (33) \\ 1 & +2 \end{smallmatrix}$	.

$$L_z \equiv \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} = (E_{11} - E_{33}) = \sqrt{2} \mathbf{v}_0^1$$

$$L_+ \equiv \sqrt{2} \begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} = \sqrt{2}(E_{12} + E_{23}) = L_x + iL_y = -\sqrt{2} \mathbf{v}_1^1$$

$$L_- \equiv \sqrt{2} \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix} = \sqrt{2}(E_{21} + E_{32}) = L_x - iL_y = \sqrt{2} \mathbf{v}_{-1}^1$$

## dipole ( $k=1$ ) angular momentum $\mathbf{L}$ -operators

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{smallmatrix} (1) & (1) & \cdot \\ (11) & (12) & \cdot \end{smallmatrix} \\ \begin{smallmatrix} (1) & (1) & (1) \\ (21) & (22) & (23) \end{smallmatrix} \\ \cdot & \begin{smallmatrix} (1) & (1) \\ (32) & (33) \end{smallmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

## Squared angular momentum $\mathbf{L} \cdot \mathbf{L}$ -operators

$$\langle \begin{smallmatrix} 11 \\ 2 \end{smallmatrix} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{smallmatrix} 11 \\ 2 \end{smallmatrix} \rangle = \left( 2 \binom{1}{11} + \binom{1}{22} \right)^2 + \binom{1}{21}^2 + \binom{1}{23}^2 + 2 \binom{1}{13}^2$$

$$= \frac{1}{2} (2 \cdot 1 - 0)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 = 3$$

$$\langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{smallmatrix} 12 \\ 2 \end{smallmatrix} \rangle = \left( \binom{1}{11} + 2 \binom{1}{22} \right)^2 + \binom{1}{21}^2 + 2 \binom{1}{23}^2 + \binom{1}{13}^2$$

$$= \frac{1}{2} (1 \cdot 1 + 2 \cdot 0)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 + 0$$

$$= \frac{1}{2} + \frac{1}{2} + 1 + 0 = 2$$

$$\langle \begin{smallmatrix} 11 \\ 3 \end{smallmatrix} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{smallmatrix} 11 \\ 3 \end{smallmatrix} \rangle = \left( 2 \binom{1}{11} + \binom{1}{33} \right)^2 + 2 \binom{1}{21}^2 + \binom{1}{23}^2 + \binom{1}{13}^2$$

$$= \frac{1}{2} (2 \cdot 1 - 1 \cdot 1)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 0$$

$$= \frac{1}{2} + 1 + \frac{1}{2} + 0 = 2$$

$$\langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{smallmatrix} 11 \\ 3 \end{smallmatrix} \rangle = + \binom{1}{21} \binom{1}{32} + \binom{1}{23} \binom{1}{13}$$

$$= \frac{1}{2} (1 \cdot 1 + 1 \cdot 1) = -1$$

$\begin{smallmatrix} 11 \\ 2 \end{smallmatrix}$	$\begin{smallmatrix} 11 \\ 2 \end{smallmatrix}$			eigenvalues	
$\begin{smallmatrix} 11 \\ 2 \end{smallmatrix}$	3	$\begin{smallmatrix} 12 \\ 2 \end{smallmatrix}$	$\begin{smallmatrix} 11 \\ 3 \end{smallmatrix}$		3
$\begin{smallmatrix} 11 \\ 2 \end{smallmatrix}$	$\begin{smallmatrix} 12 \\ 2 \end{smallmatrix}$	2	-1		1 0
$\begin{smallmatrix} 11 \\ 3 \end{smallmatrix}$	$\begin{smallmatrix} 11 \\ 3 \end{smallmatrix}$	-1	2	0 3	

$\begin{array}{|c|} \hline \square\square \\ \hline \square \\ \hline \end{array} = [2,1]$  tableau basis and matrices of  $\mathbf{v}^1$  dipole

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\begin{array}{ c } \hline 11 \\ \hline 2 \\ \hline \end{array}$	$\begin{array}{ c } \hline 12 \\ \hline 2 \\ \hline \end{array}$	$\begin{array}{ c } \hline 11 \\ \hline 3 \\ \hline \end{array}$	$\begin{array}{ c } \hline 12 \\ \hline 3 \\ \hline \end{array}$	$\begin{array}{ c } \hline 13 \\ \hline 2 \\ \hline \end{array}$	$\begin{array}{ c } \hline 13 \\ \hline 3 \\ \hline \end{array}$	$\begin{array}{ c } \hline 22 \\ \hline 3 \\ \hline \end{array}$	$\begin{array}{ c } \hline 23 \\ \hline 3 \\ \hline \end{array}$
$E_{jk} = \langle \begin{array}{ c } \hline 11 \\ \hline 2 \\ \hline \end{array}  $	$\begin{array}{ c } \hline (11) (22) \\ \hline 2+1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (12) \\ \hline 1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (23) \\ \hline 1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (13) \\ \hline -\sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (13) \\ \hline \sqrt{\frac{3}{2}} \\ \hline \end{array}$	.	.	.
$\langle \begin{array}{ c } \hline 12 \\ \hline 2 \\ \hline \end{array}  $	$\begin{array}{ c } \hline (21) \\ \hline 1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (11) (22) \\ \hline 1+2 \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (23) \\ \hline \sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (23) \\ \hline \sqrt{\frac{3}{2}} \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (13) \\ \hline -1 \\ \hline \end{array}$	.
$\langle \begin{array}{ c } \hline 11 \\ \hline 3 \\ \hline \end{array}  $	$\begin{array}{ c } \hline (32) \\ \hline 1 \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (11) (33) \\ \hline 2+1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (12) \\ \hline \sqrt{2} \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (13) \\ \hline 1 \\ \hline \end{array}$	.	.
$\langle \begin{array}{ c } \hline 12 \\ \hline 3 \\ \hline \end{array}  $	$\begin{array}{ c } \hline (31) \\ \hline -\sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (32) \\ \hline \sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (21) \\ \hline \sqrt{2} \\ \hline \end{array}$	$\begin{array}{ c } \hline (11) (22) (33) \\ \hline 1+1+1 \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (23) \\ \hline \sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (12) \\ \hline \sqrt{2} \\ \hline \end{array}$	$\begin{array}{ c } \hline (13) \\ \hline \sqrt{\frac{1}{2}} \\ \hline \end{array}$
$\langle \begin{array}{ c } \hline 13 \\ \hline 2 \\ \hline \end{array}  $	$\begin{array}{ c } \hline (31) \\ \hline \sqrt{\frac{3}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (32) \\ \hline \sqrt{\frac{3}{2}} \\ \hline \end{array}$	.	.	$\begin{array}{ c } \hline (11) (22) (33) \\ \hline 1+1+1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (23) \\ \hline \sqrt{\frac{3}{2}} \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (13) \\ \hline \sqrt{\frac{3}{2}} \\ \hline \end{array}$
$\langle \begin{array}{ c } \hline 13 \\ \hline 3 \\ \hline \end{array}  $	.	.	$\begin{array}{ c } \hline (31) \\ \hline 1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (32) \\ \hline \sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (32) \\ \hline \sqrt{\frac{3}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (11) (33) \\ \hline 1+2 \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (12) \\ \hline 1 \\ \hline \end{array}$
$\langle \begin{array}{ c } \hline 22 \\ \hline 3 \\ \hline \end{array}  $	.	$\begin{array}{ c } \hline (31) \\ \hline -1 \\ \hline \end{array}$	.	$\begin{array}{ c } \hline (21) \\ \hline \sqrt{2} \\ \hline \end{array}$	.	.	$\begin{array}{ c } \hline (22) (33) \\ \hline 2+1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (23) \\ \hline 1 \\ \hline \end{array}$
$\langle \begin{array}{ c } \hline 23 \\ \hline 3 \\ \hline \end{array}  $	.	.	.	$\begin{array}{ c } \hline (31) \\ \hline \sqrt{\frac{1}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (31) \\ \hline \sqrt{\frac{3}{2}} \\ \hline \end{array}$	$\begin{array}{ c } \hline (21) \\ \hline 1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (32) \\ \hline 1 \\ \hline \end{array}$	$\begin{array}{ c } \hline (22) (33) \\ \hline 1+2 \\ \hline \end{array}$

$$L_z \equiv \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} = (E_{11} - E_{33}) = \sqrt{2} \mathbf{v}_0^1$$

$$L_+ \equiv \sqrt{2} \begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix} = \sqrt{2}(E_{12} + E_{23}) = L_x + iL_y = -\sqrt{2} \mathbf{v}_1^1$$

$$L_- \equiv \sqrt{2} \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix} = \sqrt{2}(E_{21} + E_{32}) = L_x - iL_y = \sqrt{2} \mathbf{v}_{-1}^1$$

dipole ( $k=1$ ) angular momentum  $\mathbf{L}$ -operators

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{array}{|c|} \hline (1) \\ \hline (11) \\ \hline \end{array} & \begin{array}{|c|} \hline (1) \\ \hline (12) \\ \hline \end{array} & \begin{array}{|c|} \hline (1) \\ \hline (13) \\ \hline \end{array} \\ \begin{array}{|c|} \hline (1) \\ \hline (21) \\ \hline \end{array} & \begin{array}{|c|} \hline (1) \\ \hline (22) \\ \hline \end{array} & \begin{array}{|c|} \hline (1) \\ \hline (23) \\ \hline \end{array} \\ \cdot & \begin{array}{|c|} \hline (1) \\ \hline (32) \\ \hline \end{array} & \begin{array}{|c|} \hline (1) \\ \hline (33) \\ \hline \end{array} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

Squared angular momentum  $\mathbf{L} \cdot \mathbf{L}$ -operators

$$\langle \begin{array}{|c|} \hline 11 \\ \hline 2 \\ \hline \end{array} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{array}{|c|} \hline 11 \\ \hline 2 \\ \hline \end{array} \rangle = \left( 2 \binom{1}{11} + \binom{1}{22} \right)^2 + \binom{1}{21}^2 + \binom{1}{23}^2 + 2 \binom{1}{13}^2$$

$$= \frac{1}{2} (2 \cdot 1 - 0)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 = 3$$

$$\langle \begin{array}{|c|} \hline 12 \\ \hline 2 \\ \hline \end{array} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{array}{|c|} \hline 12 \\ \hline 2 \\ \hline \end{array} \rangle = \left( \binom{1}{11} + 2 \binom{1}{22} \right)^2 + \binom{1}{21}^2 + 2 \binom{1}{23}^2 + \binom{1}{13}^2$$

$$= \frac{1}{2} (1 \cdot 1 + 2 \cdot 0)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 + 0$$

$$= \frac{1}{2} + \frac{1}{2} + 1 + 0 = 2$$

$$\langle \begin{array}{|c|} \hline 11 \\ \hline 3 \\ \hline \end{array} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{array}{|c|} \hline 11 \\ \hline 3 \\ \hline \end{array} \rangle = \left( 2 \binom{1}{11} + \binom{1}{33} \right)^2 + 2 \binom{1}{21}^2 + \binom{1}{23}^2 + \binom{1}{13}^2$$

$$= \frac{1}{2} (2 \cdot 1 - 1 \cdot 1)^2 + 2 \left( \frac{1}{\sqrt{2}} \right)^2 + \left( \frac{1}{\sqrt{2}} \right)^2 + 0$$

$$= \frac{1}{2} + 1 + \frac{1}{2} + 0 = 2$$

$$\langle \begin{array}{|c|} \hline 12 \\ \hline 2 \\ \hline \end{array} | \mathbf{V}^1 \cdot \mathbf{V}^1 | \begin{array}{|c|} \hline 11 \\ \hline 3 \\ \hline \end{array} \rangle = + \binom{1}{21} \binom{1}{32} + \binom{1}{23} \binom{1}{13}$$

$$= \frac{1}{2} (1 \cdot 1 + 1 \cdot 1) = -1$$

$\begin{array}{ c } \hline \square\square \\ \hline \square \\ \hline \end{array}$		eigenvalues	$\mathbf{L} \cdot \mathbf{L}$ eigenvalues
			$j(j+1)$
$\begin{array}{ c } \hline \square\square \\ \hline 2 \\ \hline \end{array}$	3	3	6 ( $j=2$ )
$\begin{array}{ c } \hline \square\square \\ \hline 2 \\ \hline \end{array}$	2	1	2 ( $j=1$ )
$\begin{array}{ c } \hline \square\square \\ \hline 3 \\ \hline \end{array}$	-1	0	0 ( $j=0$ )
$\begin{array}{ c } \hline \square\square \\ \hline 3 \\ \hline \end{array}$	2	0	0 ( $j=0$ )

# 4.16.18 class 23: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

## $(S_n)^*(U(m))$ shell model of electrostatic quadrupole-quadrupole-e interactions

Complete set of  $E_{jk}$  matrix elements for the doublet (spin- $1/2$ )  $p^3$  orbits

Detailed sample applications of “Jawbone” formulae

Number operators

1-jump  $E_{i-1,i}$  operators

2-jump  $E_{i-2,i}$  operators

Angular momentum operators (for later application)

Multipole expansions and Coulomb (e-e)-electrostatic interaction

Linear multipoles;  $P_1$ -dipole,  $P_2$ -quadrupole,  $P_3$ -octupole,...

Moving off-axis: On-z-axis linear multipole  $P_\ell (\cos\theta)$  wave expansion:

**Multipole Addition Theorem (should be called Group Multiplication Theorem)**

Coulomb (e-e)-electrostatic interaction and its Hamiltonian Matrix, Slater integrals

2-particle elementary  $e_{jk}$  operator expressions for (e-e)-interaction matrix

Tensor tables are  $(2\ell+1)$ -by- $(2\ell+1)$  arrays  $(p^k_q)$  giving  $V_q^k$  in terms of  $E_{p,q}$ .

Relating  $V_q^k$  to  $E_{m',m}$  by  $(m'^k_m)$  arrays

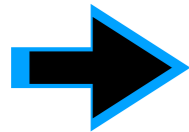
Atomic p-shell ee-interaction in elementary operator form

[2,1] tableau basis (from p.29) and matrices of  $v^1$  dipole and  $v^1 \cdot v^1 = L \cdot L$

[2,1] tableau basis (from p.29) and matrices of  $v^2$  and  $v^2 \cdot v^2$  quadrupole

$^4S, ^2P$ , and  $^2D$  energy calculation of quartet and doublet (spin- $1/2$ )  $p^3$  orbits

Corrected level diagrams Nitrogen  $p^3$



$\begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \square \\ \hline \end{array} = [2,1]$  tableau basis and  $U(3)$  irep (from p. 29)

$M=2$        $M=1$        $M=0$        $M=-1$        $M=-2$

	$\begin{array}{ c } \hline 11 \\ \hline 2 \\ \hline \end{array}$	$\begin{array}{ c } \hline 12 \\ \hline 2 \\ \hline \end{array}$	$\begin{array}{ c } \hline 11 \\ \hline 3 \\ \hline \end{array}$	$\begin{array}{ c } \hline 12 \\ \hline 3 \\ \hline \end{array}$	$\begin{array}{ c } \hline 13 \\ \hline 2 \\ \hline \end{array}$	$\begin{array}{ c } \hline 13 \\ \hline 3 \\ \hline \end{array}$	$\begin{array}{ c } \hline 22 \\ \hline 3 \\ \hline \end{array}$	$\begin{array}{ c } \hline 23 \\ \hline 3 \\ \hline \end{array}$
$\langle \begin{array}{ c } \hline 11 \\ \hline 2 \\ \hline \end{array}  $	$\begin{array}{c} (11) (22) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ 1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$	$\begin{array}{c} (13) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	.
$\langle \begin{array}{ c } \hline 12 \\ \hline 2 \\ \hline \end{array}  $	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (11) (22) \\ 1+2 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ -1 \end{array}$	.
$\langle \begin{array}{ c } \hline 11 \\ \hline 3 \\ \hline \end{array}  $	$\begin{array}{c} (32) \\ 1 \end{array}$	.	$\begin{array}{c} (11) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	.	$\begin{array}{c} (13) \\ 1 \end{array}$	.	.
$E_{jk} = \langle \begin{array}{ c } \hline 12 \\ \hline 3 \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{1}{2}} \end{array}$
$\langle \begin{array}{ c } \hline 13 \\ \hline 2 \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$
$\langle \begin{array}{ c } \hline 13 \\ \hline 3 \\ \hline \end{array}  $	.	.	$\begin{array}{c} (31) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (11) (33) \\ 1+2 \end{array}$	.	$\begin{array}{c} (12) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline 22 \\ \hline 3 \\ \hline \end{array}  $	.	$\begin{array}{c} (31) \\ -1 \end{array}$	.	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	.	.	$\begin{array}{c} (22) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline 23 \\ \hline 3 \\ \hline \end{array}  $	.	.	.	$\begin{array}{c} (31) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ 1 \end{array}$	$\begin{array}{c} (22) (33) \\ 1+2 \end{array}$

$\ell=1$   
(condensed  
format)

$$\langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} \begin{pmatrix} 2 \\ 11 \end{pmatrix} & \begin{pmatrix} 2 \\ 12 \end{pmatrix} & \begin{pmatrix} 2 \\ 13 \end{pmatrix} \\ \begin{pmatrix} 2 \\ 21 \end{pmatrix} & \begin{pmatrix} 2 \\ 22 \end{pmatrix} & \begin{pmatrix} 2 \\ 23 \end{pmatrix} \\ \begin{pmatrix} 2 \\ 31 \end{pmatrix} & \begin{pmatrix} 2 \\ 32 \end{pmatrix} & \begin{pmatrix} 2 \\ 33 \end{pmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} 1 & -1 & 1 \\ 1 & -2 & 1 \\ 1 & -1 & 1 \end{pmatrix} \begin{matrix} 1 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{matrix}$$

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{pmatrix} 1 \\ 11 \end{pmatrix} & \begin{pmatrix} 1 \\ 12 \end{pmatrix} & \cdot \\ \begin{pmatrix} 1 \\ 21 \end{pmatrix} & \begin{pmatrix} 1 \\ 22 \end{pmatrix} & \begin{pmatrix} 1 \\ 23 \end{pmatrix} \\ \cdot & \begin{pmatrix} 1 \\ 32 \end{pmatrix} & \begin{pmatrix} 1 \\ 33 \end{pmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \begin{pmatrix} 0 \\ 11 \end{pmatrix} & \cdot & \cdot \\ \cdot & \begin{pmatrix} 0 \\ 22 \end{pmatrix} & \cdot \\ \cdot & \cdot & \begin{pmatrix} 0 \\ 33 \end{pmatrix} \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

# $\begin{array}{|c|} \hline \square \square \\ \hline \square \\ \hline \end{array} = [2,1]$ tableau basis and matrices of $\mathbf{v}^2$ quadrupole

$M=2$        $M=1$        $M=0$        $M=-1$        $M=-2$

	$\begin{array}{ c } \hline \begin{array}{c} 11 \\ 2 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 12 \\ 2 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 11 \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 12 \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 13 \\ 2 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 13 \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 22 \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 23 \\ 3 \end{array} \\ \hline \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 11 \\ 2 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (11) (22) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ 1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$	$\begin{array}{c} (13) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	.
$\langle \begin{array}{ c } \hline \begin{array}{c} 12 \\ 2 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (11) (22) \\ 1+2 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ -1 \end{array}$	.
$\langle \begin{array}{ c } \hline \begin{array}{c} 11 \\ 3 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (32) \\ 1 \end{array}$	.	$\begin{array}{c} (11) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	.	$\begin{array}{c} (13) \\ 1 \end{array}$	.	.
$E_{jk} = \langle \begin{array}{ c } \hline \begin{array}{c} 12 \\ 3 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{1}{2}} \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 13 \\ 2 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 13 \\ 3 \end{array} \\ \hline \end{array}  $	.	.	$\begin{array}{c} (31) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (11) (33) \\ 1+2 \end{array}$	.	$\begin{array}{c} (12) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 22 \\ 3 \end{array} \\ \hline \end{array}  $	.	$\begin{array}{c} (31) \\ -1 \end{array}$	.	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	.	.	$\begin{array}{c} (22) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 23 \\ 3 \end{array} \\ \hline \end{array}  $	.	.	.	$\begin{array}{c} (31) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ 1 \end{array}$	$\begin{array}{c} (22) (33) \\ 1+2 \end{array}$

$\ell=1$   
(condensed  
format)

$$\langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} \begin{pmatrix} 2 \\ 11 \end{pmatrix} & \begin{pmatrix} 2 \\ 12 \end{pmatrix} & \begin{pmatrix} 2 \\ 13 \end{pmatrix} \\ \begin{pmatrix} 2 \\ 21 \end{pmatrix} & \begin{pmatrix} 2 \\ 22 \end{pmatrix} & \begin{pmatrix} 2 \\ 23 \end{pmatrix} \\ \begin{pmatrix} 2 \\ 31 \end{pmatrix} & \begin{pmatrix} 2 \\ 32 \end{pmatrix} & \begin{pmatrix} 2 \\ 33 \end{pmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} 1 & -1 & 1 \\ 1 & -2 & 1 \\ 1 & -1 & 1 \end{pmatrix} \begin{matrix} 1 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{matrix}$$

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{pmatrix} 1 \\ 11 \end{pmatrix} & \begin{pmatrix} 1 \\ 12 \end{pmatrix} & \cdot \\ \begin{pmatrix} 1 \\ 21 \end{pmatrix} & \begin{pmatrix} 1 \\ 22 \end{pmatrix} & \begin{pmatrix} 1 \\ 23 \end{pmatrix} \\ \cdot & \begin{pmatrix} 1 \\ 32 \end{pmatrix} & \begin{pmatrix} 1 \\ 33 \end{pmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \begin{pmatrix} 0 \\ 11 \end{pmatrix} & \cdot & \cdot \\ \cdot & \begin{pmatrix} 0 \\ 22 \end{pmatrix} & \cdot \\ \cdot & \cdot & \begin{pmatrix} 0 \\ 33 \end{pmatrix} \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

$$\begin{aligned} \langle \begin{array}{|c|} \hline \begin{array}{c} 11 \\ 2 \end{array} \\ \hline \end{array} | \mathcal{V}^2 \cdot \mathcal{V}^2 | \begin{array}{|c|} \hline \begin{array}{c} 11 \\ 2 \end{array} \\ \hline \end{array} \rangle &= \left( 2 \binom{2}{11} + \binom{2}{22} \right)^2 + \binom{2}{21} \binom{2}{12} + \binom{2}{32} \binom{2}{23} + 2 \binom{2}{31} \binom{2}{13} \\ &= \frac{1}{6} (2 \cdot 1 - 2)^2 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 2 \cdot 1 \cdot 1 = 3 \end{aligned}$$

# $\begin{array}{|c|} \hline \square \square \\ \hline \square \\ \hline \end{array} = [2,1]$ tableau basis and matrices of $\mathbf{v}^2$ quadrupole

$M=2$        $M=1$        $M=0$        $M=-1$        $M=-2$

	$\begin{array}{ c } \hline \begin{array}{c} 11 \\ 2 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 12 \\ 2 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 11 \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 12 \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 13 \\ 2 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 13 \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 22 \\ 3 \end{array} \\ \hline \end{array}$	$\begin{array}{ c } \hline \begin{array}{c} 23 \\ 3 \end{array} \\ \hline \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 11 \\ 2 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (11) (22) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ 1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$	$\begin{array}{c} (13) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	.
$\langle \begin{array}{ c } \hline \begin{array}{c} 12 \\ 2 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (11) (22) \\ 1+2 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ -1 \end{array}$	.
$\langle \begin{array}{ c } \hline \begin{array}{c} 11 \\ 3 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (32) \\ 1 \end{array}$	.	$\begin{array}{c} (11) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	.	$\begin{array}{c} (13) \\ 1 \end{array}$	.	.
$E_{jk} = \langle \begin{array}{ c } \hline \begin{array}{c} 12 \\ 3 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	.	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{1}{2}} \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 13 \\ 2 \end{array} \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	.	.	$\begin{array}{c} (11) (22) (33) \\ 1+1+1 \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	.	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 13 \\ 3 \end{array} \\ \hline \end{array}  $	.	.	$\begin{array}{c} (31) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (11) (33) \\ 1+2 \end{array}$	.	$\begin{array}{c} (12) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 22 \\ 3 \end{array} \\ \hline \end{array}  $	.	$\begin{array}{c} (31) \\ -1 \end{array}$	.	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	.	.	$\begin{array}{c} (22) (33) \\ 2+1 \end{array}$	$\begin{array}{c} (23) \\ 1 \end{array}$
$\langle \begin{array}{ c } \hline \begin{array}{c} 23 \\ 3 \end{array} \\ \hline \end{array}  $	.	.	.	$\begin{array}{c} (31) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (32) \\ 1 \end{array}$	$\begin{array}{c} (22) (33) \\ 1+2 \end{array}$

$\ell=1$   
(condensed  
format)

$$\langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} \binom{2}{11} & \binom{2}{12} & \binom{2}{13} \\ \binom{2}{21} & \binom{2}{22} & \binom{2}{23} \\ \binom{2}{31} & \binom{2}{32} & \binom{2}{33} \end{pmatrix} \quad \langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} 1 & -1 & 1 \\ 1 & -2 & 1 \\ 1 & -1 & 1 \end{pmatrix} \begin{matrix} 1 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{matrix}$$

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \binom{1}{11} & \binom{1}{12} & \cdot \\ \binom{1}{21} & \binom{1}{22} & \binom{1}{23} \\ \cdot & \binom{1}{32} & \binom{1}{33} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \binom{0}{11} & \cdot & \cdot \\ \cdot & \binom{0}{22} & \cdot \\ \cdot & \cdot & \binom{0}{33} \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

$$\begin{aligned} \langle \begin{array}{|c|} \hline \begin{array}{c} 11 \\ 2 \end{array} \\ \hline \end{array} | \mathcal{V}^2 \cdot \mathcal{V}^2 | \begin{array}{|c|} \hline \begin{array}{c} 11 \\ 2 \end{array} \\ \hline \end{array} \rangle &= \left( 2\binom{2}{11} + \binom{2}{22} \right)^2 + \binom{2}{21}\binom{2}{12} + \binom{2}{32}\binom{2}{23} + 2\binom{2}{31}\binom{2}{13} \\ &= \frac{1}{6} (2 \cdot 1 - 2)^2 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 2 \cdot 1 \cdot 1 = 3 \end{aligned}$$

$$\begin{aligned} \langle \begin{array}{|c|} \hline \begin{array}{c} 12 \\ 2 \end{array} \\ \hline \end{array} | \mathcal{V}^2 \cdot \mathcal{V}^2 | \begin{array}{|c|} \hline \begin{array}{c} 12 \\ 2 \end{array} \\ \hline \end{array} \rangle &= \left( \binom{2}{11} + 2\binom{2}{22} \right)^2 + \binom{2}{21}\binom{2}{12} + 2\binom{2}{32}\binom{2}{23} + \binom{2}{31}\binom{2}{13} \\ &= \frac{1}{6} (1 \cdot 1 - 2 \cdot 2)^2 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 2 \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 1 \cdot 1 \\ &= \frac{3}{2} + \frac{1}{2} + 1 + 1 = 4 \end{aligned}$$



# $\begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} = [2,1]$ tableau basis and matrices of $\mathbf{v}^2$ quadrupole

$M=2$        $M=1$        $M=0$        $M=-1$        $M=-2$

	$\begin{array}{ c } \hline  11\rangle \\ \hline  2 \\ \hline \end{array}$	$\begin{array}{ c c } \hline  12\rangle &  11\rangle \\ \hline  2 &  3 \\ \hline \end{array}$	$\begin{array}{ c c } \hline  12\rangle &  13\rangle \\ \hline  3 &  2 \\ \hline \end{array}$	$\begin{array}{ c c } \hline  13\rangle &  22\rangle \\ \hline  3 &  3 \\ \hline \end{array}$	$\begin{array}{ c } \hline  23\rangle \\ \hline  3 \\ \hline \end{array}$		
$\langle \begin{array}{ c } \hline  11\rangle \\ \hline  2 \\ \hline \end{array}  $	$\begin{array}{c} (11) \ (22) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \ (23) \\ 1 \quad 1 \end{array}$	$\begin{array}{c} (13) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} \cdot \\ \cdot \\ \cdot \end{array}$		
$\langle \begin{array}{ c } \hline  12\rangle \\ \hline  2 \\ \hline \end{array}  $	$\begin{array}{c} (21) \\ 1 \end{array}$	$\begin{array}{c} (11) \ (22) \\ 1+2 \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} \cdot \\ (13) \\ -1 \end{array}$		
$\langle \begin{array}{ c } \hline  11\rangle \\ \hline  3 \\ \hline \end{array}  $	$\begin{array}{c} (32) \\ 1 \end{array}$	$\begin{array}{c} \cdot \\ (11) \ (33) \\ 2+1 \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	$\begin{array}{c} \cdot \\ (13) \\ 1 \end{array}$	$\begin{array}{c} \cdot \\ \cdot \\ \cdot \end{array}$		
$E_{jk} = \langle \begin{array}{ c } \hline  12\rangle \\ \hline  3 \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ -\sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (11) \ (22) \ (33) \\ 1+1+1 \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (12) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (13) \\ \sqrt{\frac{1}{2}} \end{array}$
$\langle \begin{array}{ c } \hline  13\rangle \\ \hline  2 \\ \hline \end{array}  $	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} \cdot \\ (11) \ (22) \ (33) \\ 1+1+1 \end{array}$	$\begin{array}{c} (23) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} \cdot \\ (13) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} \cdot \\ \cdot \\ \cdot \end{array}$	
$\langle \begin{array}{ c } \hline  13\rangle \\ \hline  3 \\ \hline \end{array}  $	$\begin{array}{c} \cdot \\ (31) \\ 1 \end{array}$	$\begin{array}{c} \cdot \\ (32) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (31) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} (32) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (11) \ (33) \\ 1+2 \end{array}$	$\begin{array}{c} \cdot \\ (12) \\ 1 \end{array}$	
$\langle \begin{array}{ c } \hline  22\rangle \\ \hline  3 \\ \hline \end{array}  $	$\begin{array}{c} \cdot \\ (31) \\ -1 \end{array}$	$\begin{array}{c} \cdot \\ (32) \\ \sqrt{2} \end{array}$	$\begin{array}{c} (21) \\ \sqrt{2} \end{array}$	$\begin{array}{c} \cdot \\ (22) \ (33) \\ 2+1 \end{array}$	$\begin{array}{c} \cdot \\ (23) \\ 1 \end{array}$	$\begin{array}{c} \cdot \\ \cdot \\ \cdot \end{array}$	
$\langle \begin{array}{ c } \hline  23\rangle \\ \hline  3 \\ \hline \end{array}  $	$\begin{array}{c} \cdot \\ (31) \\ \sqrt{\frac{1}{2}} \end{array}$	$\begin{array}{c} \cdot \\ (32) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} \cdot \\ (21) \\ 1 \end{array}$	$\begin{array}{c} (31) \\ \sqrt{\frac{3}{2}} \end{array}$	$\begin{array}{c} (21) \ (32) \\ 1 \quad 1 \end{array}$	$\begin{array}{c} (22) \ (33) \\ 1+2 \end{array}$	

$\ell=1$   
(condensed  
format)

$$\langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} \binom{2}{11} & \binom{2}{12} & \binom{2}{13} \\ \binom{2}{21} & \binom{2}{22} & \binom{2}{23} \\ \binom{2}{31} & \binom{2}{32} & \binom{2}{33} \end{pmatrix} \quad \langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} 1 & -1 & 1 \\ 1 & -2 & 1 \\ 1 & -1 & 1 \end{pmatrix} \begin{matrix} 1 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{matrix}$$

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \binom{1}{11} & \binom{1}{12} & \cdot \\ \binom{1}{21} & \binom{1}{22} & \binom{1}{23} \\ \cdot & \binom{1}{32} & \binom{1}{33} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \binom{0}{11} & \cdot & \cdot \\ \cdot & \binom{0}{22} & \cdot \\ \cdot & \cdot & \binom{0}{33} \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

$$\begin{aligned} \langle \begin{array}{|c|} \hline |11\rangle \\ \hline |2 \\ \hline \end{array} | V^2 \cdot V^2 | \begin{array}{|c|} \hline |11\rangle \\ \hline |2 \\ \hline \end{array} \rangle &= \left( 2\binom{2}{11} + \binom{2}{22} \right)^2 + \binom{2}{21}\binom{2}{12} + \binom{2}{32}\binom{2}{23} + 2\binom{2}{31}\binom{2}{13} \\ &= \frac{1}{6} (2 \cdot 1 - 2)^2 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 2 \cdot 1 \cdot 1 = 3 \end{aligned}$$

$$\begin{aligned} \langle \begin{array}{|c|} \hline |12\rangle \\ \hline |2 \\ \hline \end{array} | V^2 \cdot V^2 | \begin{array}{|c|} \hline |12\rangle \\ \hline |2 \\ \hline \end{array} \rangle &= \left( \binom{2}{11} + 2\binom{2}{22} \right)^2 + \binom{2}{21}\binom{2}{12} + 2\binom{2}{32}\binom{2}{23} + \binom{2}{31}\binom{2}{13} \\ &= \frac{1}{6} (1 \cdot 1 - 2 \cdot 2)^2 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 2 \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 1 \cdot 1 \\ &= \frac{3}{2} + \frac{1}{2} + 1 + 1 = 4 \end{aligned}$$

$$\begin{aligned} \langle \begin{array}{|c|} \hline |11\rangle \\ \hline |3 \\ \hline \end{array} | V^2 \cdot V^2 | \begin{array}{|c|} \hline |11\rangle \\ \hline |3 \\ \hline \end{array} \rangle &= \left( 2\binom{2}{11} + \binom{2}{33} \right)^2 + \binom{2}{21}\binom{2}{12} + 2\binom{2}{32}\binom{2}{23} + \binom{2}{31}\binom{2}{13} \\ &= \frac{1}{6} (2 \cdot 1 + 1 \cdot 1)^2 + 2 \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 1 \cdot 1 \\ &= \frac{3}{2} + 1 + \frac{1}{2} + 1 = 4 \end{aligned}$$

# $\begin{smallmatrix} \square & \square \\ \square \end{smallmatrix} = [2,1]$ tableau basis and matrices of $\mathbf{v}^2$ quadrupole

$M=2$        $M=1$        $M=0$        $M=-1$        $M=-2$

	$\begin{smallmatrix}  11\rangle \\  2 \end{smallmatrix}$	$\begin{smallmatrix}  12\rangle \\  2 \end{smallmatrix}$	$\begin{smallmatrix}  11\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  12\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  13\rangle \\  2 \end{smallmatrix}$	$\begin{smallmatrix}  13\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  22\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  23\rangle \\  3 \end{smallmatrix}$
$\langle \begin{smallmatrix} 11 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (11) & (22) \\ 2 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (12) & (23) \\ 1 & 1 \end{smallmatrix}$		$\begin{smallmatrix} (13) & (13) \\ -\sqrt{\frac{1}{2}} & \sqrt{\frac{3}{2}} \end{smallmatrix}$				
$\langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (21) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (11) & (22) \\ 1 & +2 \end{smallmatrix}$		$\begin{smallmatrix} (23) & (23) \\ \sqrt{\frac{1}{2}} & \sqrt{\frac{3}{2}} \end{smallmatrix}$			$\begin{smallmatrix} (13) \\ -1 \end{smallmatrix}$	
$\langle \begin{smallmatrix} 11 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} (32) \\ 1 \end{smallmatrix}$		$\begin{smallmatrix} (11) & (33) \\ 2 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (12) \\ \sqrt{2} \end{smallmatrix}$		$\begin{smallmatrix} (13) \\ 1 \end{smallmatrix}$		
$E_{jk} = \langle \begin{smallmatrix} 12 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} (31) \\ -\sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (21) \\ \sqrt{2} \end{smallmatrix}$	$\begin{smallmatrix} (11) & (22) & (33) \\ 1 & +1 & +1 \end{smallmatrix}$		$\begin{smallmatrix} (23) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (12) \\ \sqrt{2} \end{smallmatrix}$	$\begin{smallmatrix} (13) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$
$\langle \begin{smallmatrix} 13 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (31) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$			$\begin{smallmatrix} (11) & (22) & (33) \\ 1 & +1 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$		$\begin{smallmatrix} (13) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$
$\langle \begin{smallmatrix} 13 \\ 3 \end{smallmatrix}  $			$\begin{smallmatrix} (31) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (11) & (33) \\ 1 & +2 \end{smallmatrix}$		$\begin{smallmatrix} (12) \\ 1 \end{smallmatrix}$
$\langle \begin{smallmatrix} 22 \\ 3 \end{smallmatrix}  $		$\begin{smallmatrix} (31) \\ -1 \end{smallmatrix}$		$\begin{smallmatrix} (21) \\ \sqrt{2} \end{smallmatrix}$			$\begin{smallmatrix} (22) & (33) \\ 2 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ 1 \end{smallmatrix}$
$\langle \begin{smallmatrix} 23 \\ 3 \end{smallmatrix}  $				$\begin{smallmatrix} (31) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (31) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (21) & (32) \\ 1 & 1 \end{smallmatrix}$		$\begin{smallmatrix} (22) & (33) \\ 1 & +2 \end{smallmatrix}$

$\ell=1$   
(condensed  
format)

$$\langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} \binom{2}{11} & \binom{2}{12} & \binom{2}{13} \\ \binom{2}{21} & \binom{2}{22} & \binom{2}{23} \\ \binom{2}{31} & \binom{2}{32} & \binom{2}{33} \end{pmatrix} \quad \langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} 1 & -1 & 1 \\ 1 & -2 & 1 \\ 1 & -1 & 1 \end{pmatrix} \begin{matrix} 1 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{matrix}$$

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \binom{1}{11} & \binom{1}{12} & \cdot \\ \binom{1}{21} & \binom{1}{22} & \binom{1}{23} \\ \cdot & \binom{1}{32} & \binom{1}{33} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{matrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{matrix}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \binom{0}{11} & \cdot & \cdot \\ \cdot & \binom{0}{22} & \cdot \\ \cdot & \cdot & \binom{0}{33} \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

$$\begin{aligned} \langle \begin{smallmatrix} 11 \\ 2 \end{smallmatrix} | V^2 \cdot V^2 | \begin{smallmatrix} 11 \\ 2 \end{smallmatrix} \rangle &= \left( 2\binom{2}{11} + \binom{2}{22} \right)^2 + \binom{2}{21}\binom{2}{12} + \binom{2}{32}\binom{2}{23} + 2\binom{2}{31}\binom{2}{13} \\ &= \frac{1}{6} (2 \cdot 1 - 2)^2 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 2 \cdot 1 \cdot 1 = 3 \end{aligned}$$

$$\begin{aligned} \langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix} | V^2 \cdot V^2 | \begin{smallmatrix} 12 \\ 2 \end{smallmatrix} \rangle &= \left( \binom{2}{11} + 2\binom{2}{22} \right)^2 + \binom{2}{21}\binom{2}{12} + 2\binom{2}{32}\binom{2}{23} + \binom{2}{31}\binom{2}{13} \\ &= \frac{1}{6} (1 \cdot 1 - 2 \cdot 2)^2 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 2 \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 1 \cdot 1 \\ &= \frac{3}{2} + \frac{1}{2} + 1 + 1 = 4 \end{aligned}$$

$$\begin{aligned} \langle \begin{smallmatrix} 11 \\ 3 \end{smallmatrix} | V^2 \cdot V^2 | \begin{smallmatrix} 11 \\ 3 \end{smallmatrix} \rangle &= \left( 2\binom{2}{11} + \binom{2}{33} \right)^2 + \binom{2}{21}\binom{2}{12} + 2\binom{2}{32}\binom{2}{23} + \binom{2}{31}\binom{2}{13} \\ &= \frac{1}{6} (2 \cdot 1 + 1 \cdot 1)^2 + 2 \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 1 \cdot 1 \\ &= \frac{3}{2} + 1 + \frac{1}{2} + 1 = 4 \end{aligned}$$

$$\begin{aligned} \langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix} | V^2 \cdot V^2 | \begin{smallmatrix} 11 \\ 3 \end{smallmatrix} \rangle &= +\binom{2}{21}\binom{2}{32} + \binom{2}{23}\binom{2}{12} \\ &= \frac{-1}{2} (1 \cdot 1 + 1 \cdot 1) = -1 \end{aligned}$$



# $\begin{smallmatrix} \square & \square \\ \square \end{smallmatrix} = [2,1]$ tableau basis and matrices of $\mathbf{v}^2$ quadrupole

$M=2$        $M=1$        $M=0$        $M=-1$        $M=-2$

	$\begin{smallmatrix}  11\rangle \\  2 \end{smallmatrix}$	$\begin{smallmatrix}  12\rangle \\  2 \end{smallmatrix}$	$\begin{smallmatrix}  11\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  12\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  13\rangle \\  2 \end{smallmatrix}$	$\begin{smallmatrix}  13\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  22\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  23\rangle \\  3 \end{smallmatrix}$
$\langle \begin{smallmatrix} 11 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (11) & (22) \\ 2 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (12) & (23) \\ 1 & 1 \end{smallmatrix}$		$\begin{smallmatrix} (13) \\ -\sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (13) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$			
$\langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (21) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (11) & (22) \\ 1 & +2 \end{smallmatrix}$		$\begin{smallmatrix} (23) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$		$\begin{smallmatrix} (13) \\ -1 \end{smallmatrix}$	
$\langle \begin{smallmatrix} 11 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} (32) \\ 1 \end{smallmatrix}$		$\begin{smallmatrix} (11) & (33) \\ 2 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (12) \\ \sqrt{2} \end{smallmatrix}$		$\begin{smallmatrix} (13) \\ 1 \end{smallmatrix}$		
$E_{jk} = \langle \begin{smallmatrix} 12 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} (31) \\ -\sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (21) \\ \sqrt{2} \end{smallmatrix}$	$\begin{smallmatrix} (11) & (22) & (33) \\ 1 & +1 & +1 \end{smallmatrix}$		$\begin{smallmatrix} (23) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (12) \\ \sqrt{2} \end{smallmatrix}$	$\begin{smallmatrix} (13) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$
$\langle \begin{smallmatrix} 13 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (31) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$			$\begin{smallmatrix} (11) & (22) & (33) \\ 1 & +1 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$		$\begin{smallmatrix} (13) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$
$\langle \begin{smallmatrix} 13 \\ 3 \end{smallmatrix}  $			$\begin{smallmatrix} (31) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (11) & (33) \\ 1 & +2 \end{smallmatrix}$		$\begin{smallmatrix} (12) \\ 1 \end{smallmatrix}$
$\langle \begin{smallmatrix} 22 \\ 3 \end{smallmatrix}  $		$\begin{smallmatrix} (31) \\ -1 \end{smallmatrix}$		$\begin{smallmatrix} (21) \\ \sqrt{2} \end{smallmatrix}$			$\begin{smallmatrix} (22) & (33) \\ 2 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ 1 \end{smallmatrix}$
$\langle \begin{smallmatrix} 23 \\ 3 \end{smallmatrix}  $				$\begin{smallmatrix} (31) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (31) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (21) & (32) \\ 1 & 1 \end{smallmatrix}$		$\begin{smallmatrix} (22) & (33) \\ 1 & +2 \end{smallmatrix}$

$$\langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} \begin{smallmatrix} (2) \\ (11) \end{smallmatrix} & \begin{smallmatrix} (2) \\ (12) \end{smallmatrix} & \begin{smallmatrix} (2) \\ (13) \end{smallmatrix} \\ \begin{smallmatrix} (2) \\ (21) \end{smallmatrix} & \begin{smallmatrix} (2) \\ (22) \end{smallmatrix} & \begin{smallmatrix} (2) \\ (23) \end{smallmatrix} \\ \begin{smallmatrix} (2) \\ (31) \end{smallmatrix} & \begin{smallmatrix} (2) \\ (32) \end{smallmatrix} & \begin{smallmatrix} (2) \\ (33) \end{smallmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} 1 & -1 & 1 \\ 1 & -2 & 1 \\ 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{pmatrix}$$

$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{smallmatrix} (1) \\ (11) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (12) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (13) \end{smallmatrix} \\ \begin{smallmatrix} (1) \\ (21) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (22) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (23) \end{smallmatrix} \\ \begin{smallmatrix} (1) \\ (31) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (32) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (33) \end{smallmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{smallmatrix} 1 \\ (11) \end{smallmatrix} \\ \begin{smallmatrix} 1 \\ (21) \end{smallmatrix} \\ \begin{smallmatrix} 1 \\ (31) \end{smallmatrix} \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{2}}$$

$$\langle \mathbf{v}_q^0 \rangle = \begin{pmatrix} \begin{smallmatrix} (0) \\ (11) \end{smallmatrix} & \begin{smallmatrix} (0) \\ (22) \end{smallmatrix} & \begin{smallmatrix} (0) \\ (33) \end{smallmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^0 \rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{3}}$$

$$|{}^2D_{M=2}\rangle = \begin{smallmatrix} |11\rangle \\ |2 \end{smallmatrix}$$

$$|{}^2D_{M=1}\rangle = \frac{1}{\sqrt{2}} \begin{smallmatrix} |12\rangle \\ |2 \end{smallmatrix} + \frac{1}{\sqrt{2}} \begin{smallmatrix} |11\rangle \\ |3 \end{smallmatrix}$$

$$|{}^2P_{M=1}\rangle = \frac{1}{\sqrt{2}} \begin{smallmatrix} |12\rangle \\ |2 \end{smallmatrix} - \frac{1}{\sqrt{2}} \begin{smallmatrix} |11\rangle \\ |3 \end{smallmatrix}$$

$$\langle \begin{smallmatrix} 11 \\ 2 \end{smallmatrix} | V^2 \cdot V^2 | \begin{smallmatrix} 11 \\ 2 \end{smallmatrix} \rangle = \left( 2 \binom{2}{11} + \binom{2}{22} \right)^2 + \binom{2}{21} \binom{2}{12} + \binom{2}{32} \binom{2}{23} + 2 \binom{2}{31} \binom{2}{13}$$

$$= \frac{1}{6} (2 \cdot 1 - 2)^2 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 2 \cdot 1 \cdot 1 = 3$$

$$\langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix} | V^2 \cdot V^2 | \begin{smallmatrix} 12 \\ 2 \end{smallmatrix} \rangle = \left( \binom{2}{11} + 2 \binom{2}{22} \right)^2 + \binom{2}{21} \binom{2}{12} + 2 \binom{2}{32} \binom{2}{23} + \binom{2}{31} \binom{2}{13}$$

$$= \frac{1}{6} (1 \cdot 1 - 2 \cdot 2)^2 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 2 \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 1 \cdot 1$$

$$= \frac{3}{2} + \frac{1}{2} + 1 + 1 = 4$$

$$\langle \begin{smallmatrix} 11 \\ 3 \end{smallmatrix} | V^2 \cdot V^2 | \begin{smallmatrix} 11 \\ 3 \end{smallmatrix} \rangle = \left( 2 \binom{2}{11} + \binom{2}{33} \right)^2 + \binom{2}{21} \binom{2}{12} + 2 \binom{2}{32} \binom{2}{23} + \binom{2}{31} \binom{2}{13}$$

$$= \frac{1}{6} (2 \cdot 1 + 1 \cdot 1)^2 + 2 \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 1 \cdot 1$$

$$= \frac{3}{2} + 1 + \frac{1}{2} + 1 = 4$$

$\begin{smallmatrix}  11\rangle \\  2 \end{smallmatrix}$		
3	$\begin{smallmatrix}  12\rangle \\  2 \end{smallmatrix}$	$\begin{smallmatrix}  11\rangle \\  3 \end{smallmatrix}$
$\begin{smallmatrix}  12\rangle \\  2 \end{smallmatrix}$	4	-1
$\begin{smallmatrix}  11\rangle \\  3 \end{smallmatrix}$	-1	4

**Q•Q eigenvalues**

**3** **3** **0**  $(j=2)$

**0** **5**  $(j=1)$

# 4.16.18 class 23: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

## (S<sub>n</sub>)\*(U(m)) shell model of electrostatic quadrupole-quadrupole-e interactions

Complete set of E<sub>jk</sub> matrix elements for the doublet (spin-1/2) p<sup>3</sup> orbits

Detailed sample applications of “Jawbone” formulae

Number operators

1-jump E<sub>i-1,i</sub> operators

2-jump E<sub>i-2,i</sub> operators

Angular momentum operators (for later application)

Multipole expansions and Coulomb (e-e)-electrostatic interaction

Linear multipoles; P<sub>1</sub>-dipole, P<sub>2</sub>-quadrupole, P<sub>3</sub>-octupole,...

Moving off-axis: On-z-axis linear multipole P<sub>ℓ</sub> (cosθ) wave expansion:

**Multipole Addition Theorem (should be called Group Multiplication Theorem)**

Coulomb (e-e)-electrostatic interaction and its Hamiltonian Matrix, Slater integrals

2-particle elementary e<sub>jk</sub> operator expressions for (e-e)-interaction matrix

Tensor tables are (2ℓ+1)-by-(2ℓ+1) arrays (p<sup>k</sup><sub>q</sub>) giving V<sub>q</sub><sup>k</sup> in terms of E<sub>p,q</sub>.

Relating V<sub>q</sub><sup>k</sup> to E<sub>m',m</sub> by (m'<sup>k</sup><sub>m</sub>) arrays

Atomic p-shell ee-interaction in elementary operator form

[2,1] tableau basis (from p.29) and matrices of v<sup>1</sup> dipole and v<sup>1</sup>•v<sup>1</sup>=L•L

[2,1] tableau basis (from p.29) and matrices of v<sup>2</sup> and v<sup>2</sup>•v<sup>2</sup> quadrupole

4S, 2P, and 2D energy calculation of quartet and doublet (spin-1/2) p<sup>3</sup> orbits

Corrected level diagrams Nitrogen p<sup>3</sup>



$\begin{smallmatrix} \square & \square \\ \square & \end{smallmatrix} = [2,1]$  tableau matrices of  $v^2$  quadrupole:  $^4S, ^2P$ , and  $^2D$  energy calculation

	$M=2$	$M=1$	$M=0$	$M=-1$	$M=-2$	
	$\begin{smallmatrix}  11\rangle \\  2 \end{smallmatrix}$	$\begin{smallmatrix}  12\rangle \\  2 \end{smallmatrix}$ $\begin{smallmatrix}  11\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  12\rangle \\  3 \end{smallmatrix}$ $\begin{smallmatrix}  13\rangle \\  2 \end{smallmatrix}$	$\begin{smallmatrix}  13\rangle \\  3 \end{smallmatrix}$ $\begin{smallmatrix}  22\rangle \\  3 \end{smallmatrix}$	$\begin{smallmatrix}  23\rangle \\  3 \end{smallmatrix}$	
$E_{jk} = \langle \begin{smallmatrix} 11 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (11) & (22) \\ 2 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (12) & (23) \\ 1 & 1 \end{smallmatrix}$	$\begin{smallmatrix} (13) & (13) \\ -\sqrt{\frac{1}{2}} & \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} \cdot & \cdot \\ \cdot & \cdot \end{smallmatrix}$	$\begin{smallmatrix} \cdot \\ \cdot \end{smallmatrix}$	
$\langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (21) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (11) & (22) \\ 1 & +2 \end{smallmatrix}$	$\begin{smallmatrix} (23) & (23) \\ \sqrt{\frac{1}{2}} & \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} \cdot & (13) \\ \cdot & -1 \end{smallmatrix}$	$\begin{smallmatrix} \cdot \\ \cdot \end{smallmatrix}$	
$\langle \begin{smallmatrix} 11 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} (32) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} \cdot & (11) & (33) \\ \cdot & 2 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (12) \\ \sqrt{2} \end{smallmatrix}$	$\begin{smallmatrix} (13) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} \cdot \\ \cdot \end{smallmatrix}$	
$\langle \begin{smallmatrix} 12 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} (31) \\ -\sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (21) \\ \sqrt{2} \end{smallmatrix}$	$\begin{smallmatrix} (11) & (22) & (33) \\ 1 & +1 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (23) & (12) \\ \sqrt{\frac{1}{2}} & \sqrt{2} \end{smallmatrix}$	$\begin{smallmatrix} (13) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$
$\langle \begin{smallmatrix} 13 \\ 2 \end{smallmatrix}  $	$\begin{smallmatrix} (31) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} \cdot & (11) & (22) & (33) \\ \cdot & 1 & +1 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (13) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	
$\langle \begin{smallmatrix} 13 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} \cdot \\ \cdot \end{smallmatrix}$	$\begin{smallmatrix} (31) \\ 1 \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (32) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (11) & (33) \\ 1 & +2 \end{smallmatrix}$	$\begin{smallmatrix} (12) \\ 1 \end{smallmatrix}$
$\langle \begin{smallmatrix} 22 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} \cdot \\ \cdot \end{smallmatrix}$	$\begin{smallmatrix} (31) \\ -1 \end{smallmatrix}$	$\begin{smallmatrix} (21) \\ \sqrt{2} \end{smallmatrix}$	$\begin{smallmatrix} \cdot & (22) & (33) \\ \cdot & 2 & +1 \end{smallmatrix}$	$\begin{smallmatrix} (23) \\ 1 \end{smallmatrix}$	
$\langle \begin{smallmatrix} 23 \\ 3 \end{smallmatrix}  $	$\begin{smallmatrix} \cdot \\ \cdot \end{smallmatrix}$	$\begin{smallmatrix} \cdot \\ \cdot \end{smallmatrix}$	$\begin{smallmatrix} (31) \\ \sqrt{\frac{1}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (31) \\ \sqrt{\frac{3}{2}} \end{smallmatrix}$	$\begin{smallmatrix} (21) & (32) \\ 1 & 1 \end{smallmatrix}$	$\begin{smallmatrix} (22) & (33) \\ 1 & +2 \end{smallmatrix}$

$$\langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} \begin{smallmatrix} (2) \\ (11) \end{smallmatrix} & \begin{smallmatrix} (2) \\ (12) \end{smallmatrix} & \begin{smallmatrix} (2) \\ (13) \end{smallmatrix} \\ \begin{smallmatrix} (2) \\ (21) \end{smallmatrix} & \begin{smallmatrix} (2) \\ (22) \end{smallmatrix} & \begin{smallmatrix} (2) \\ (23) \end{smallmatrix} \\ \begin{smallmatrix} (2) \\ (31) \end{smallmatrix} & \begin{smallmatrix} (2) \\ (32) \end{smallmatrix} & \begin{smallmatrix} (2) \\ (33) \end{smallmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^2 \rangle = \begin{pmatrix} 1 & -1 & 1 \\ 1 & -2 & 1 \\ 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{pmatrix}$$

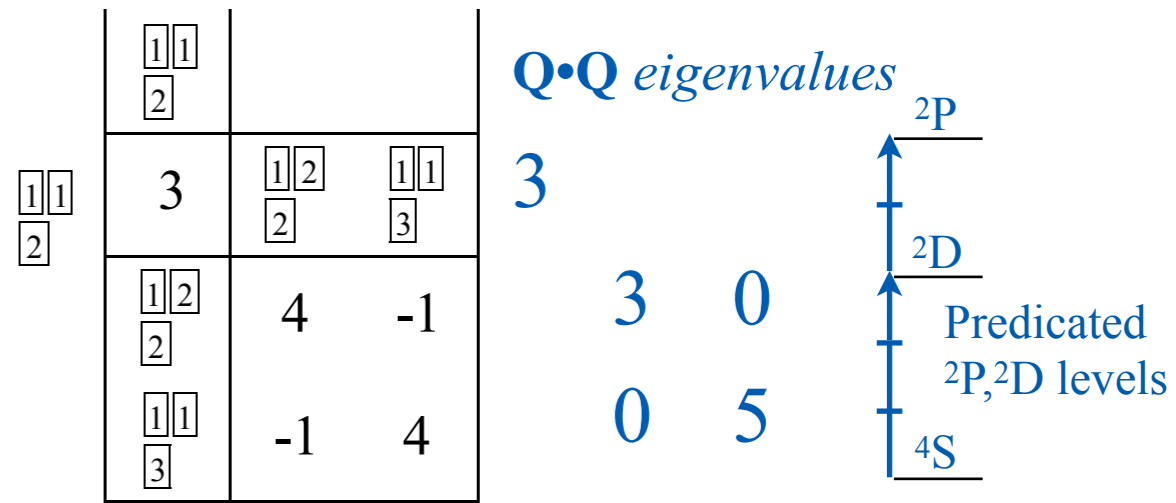
$$\langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} \begin{smallmatrix} (1) \\ (11) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (12) \end{smallmatrix} & \cdot \\ \begin{smallmatrix} (1) \\ (21) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (22) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (23) \end{smallmatrix} \\ \cdot & \begin{smallmatrix} (1) \\ (32) \end{smallmatrix} & \begin{smallmatrix} (1) \\ (33) \end{smallmatrix} \end{pmatrix} \quad \langle \mathbf{v}_q^1 \rangle = \begin{pmatrix} 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} \begin{smallmatrix} (0) \\ (11) \end{smallmatrix} \\ \cdot \\ \cdot \end{pmatrix} \quad \langle \mathbf{v}_0^0 \rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$$

$$\begin{aligned} \langle \begin{smallmatrix} 11 \\ 2 \end{smallmatrix} | V^2 \cdot V^2 | \begin{smallmatrix} 11 \\ 2 \end{smallmatrix} \rangle &= \left( 2 \binom{2}{11} + \binom{2}{22} \right)^2 + \binom{2}{21} \binom{2}{12} + \binom{2}{32} \binom{2}{23} + 2 \binom{2}{31} \binom{2}{13} \\ &= \frac{1}{6} (2 \cdot 1 - 2)^2 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 2 \cdot 1 \cdot 1 = 3 \end{aligned}$$

$$\begin{aligned} \langle \begin{smallmatrix} 12 \\ 2 \end{smallmatrix} | V^2 \cdot V^2 | \begin{smallmatrix} 12 \\ 2 \end{smallmatrix} \rangle &= \left( \binom{2}{11} + 2 \binom{2}{22} \right)^2 + \binom{2}{21} \binom{2}{12} + 2 \binom{2}{32} \binom{2}{23} + \binom{2}{31} \binom{2}{13} \\ &= \frac{1}{6} (1 \cdot 1 - 2 \cdot 2)^2 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 2 \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 1 \cdot 1 \\ &= \frac{3}{2} + \frac{1}{2} + 1 + 1 = 4 \end{aligned}$$

$$\begin{aligned} \langle \begin{smallmatrix} 11 \\ 3 \end{smallmatrix} | V^2 \cdot V^2 | \begin{smallmatrix} 11 \\ 3 \end{smallmatrix} \rangle &= \left( 2 \binom{2}{11} + \binom{2}{33} \right)^2 + \binom{2}{21} \binom{2}{12} + 2 \binom{2}{32} \binom{2}{23} + \binom{2}{31} \binom{2}{13} \\ &= \frac{1}{6} (2 \cdot 1 + 1 \cdot 1)^2 + 2 \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} + 1 \cdot 1 \\ &= \frac{3}{2} + 1 + \frac{1}{2} + 1 = 4 \end{aligned}$$



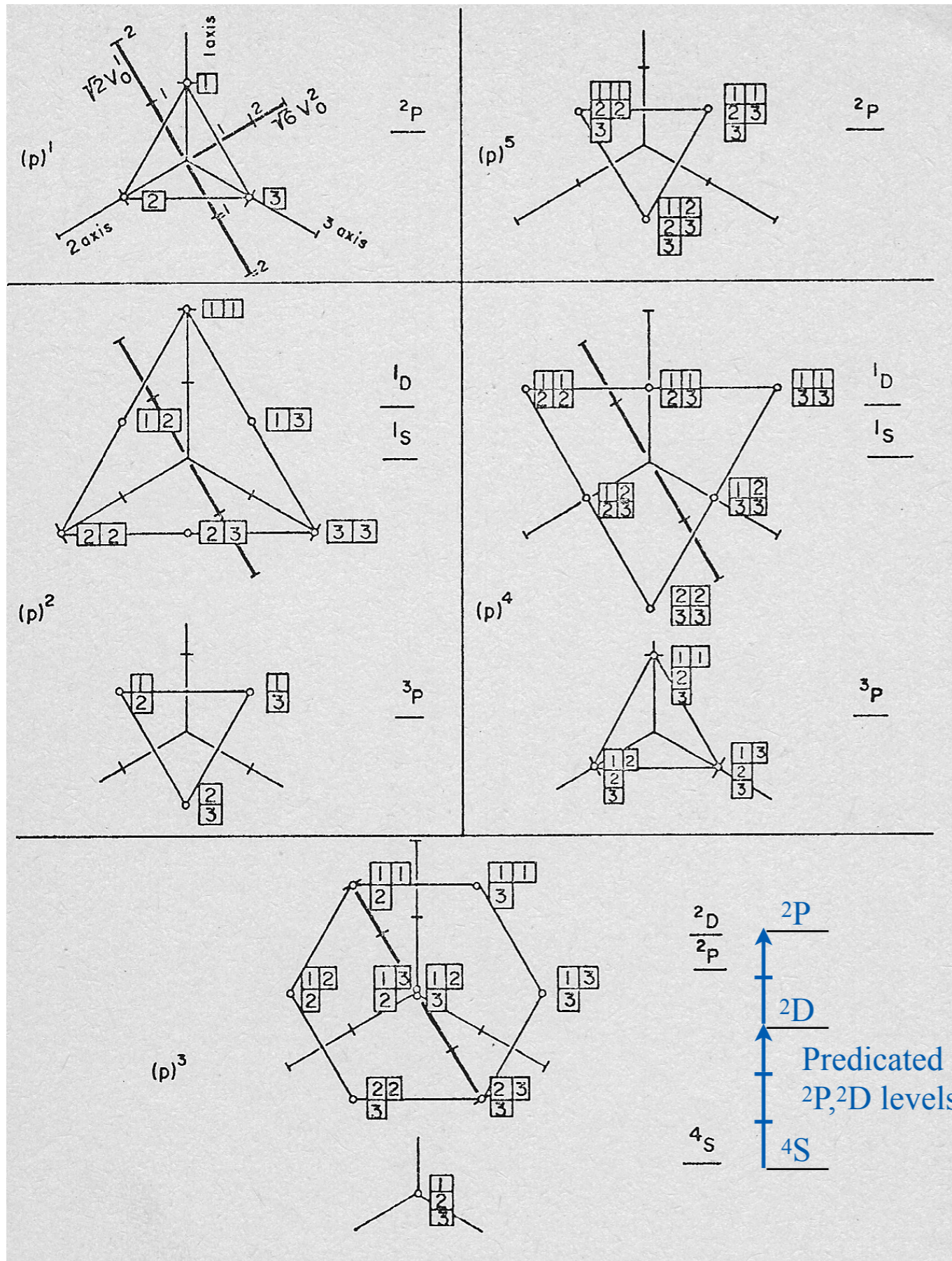


Fig.8 Weight or Moment Diagrams of Atomic  $(p)^n$  States  
 Each tableau is located at point  $(x_1 \ x_2 \ x_3)$  in a cartesian co-ordinate system for which  $x_n$  is the number of n's in the tableau. An alternative co-ordinate system is  $(v_0^2, v_0^1, v_0^0)$  defined by Eq.16 which gives the  $zz$ -quadrupole moment,  $z$ -magnetic dipole moment, and number of particles, respectively. The last axis ( $v_0^0$ ) would be pointing straight out of the figure, and each family of states lies in a plane perpendicular to it.

*A Unitary Calculus for Electronic Orbitals*  
 William G. Harter and Christopher W. Patterson  
 Springer-Verlag Lectures in Physics 49 1976

*Alternative basis for the theory of complex spectra I*  
 William G. Harter  
 Physical Review A 8 3 p2819 (1973)

*Alternative basis for the theory of complex spectra II*  
 William G. Harter and Christopher W. Patterson  
 Physical Review A 13 3 p1076-1082 (1976)

*Alternative basis for the theory of complex spectra III*  
 William G. Harter and Christopher W. Patterson  
 Physical Review A ??

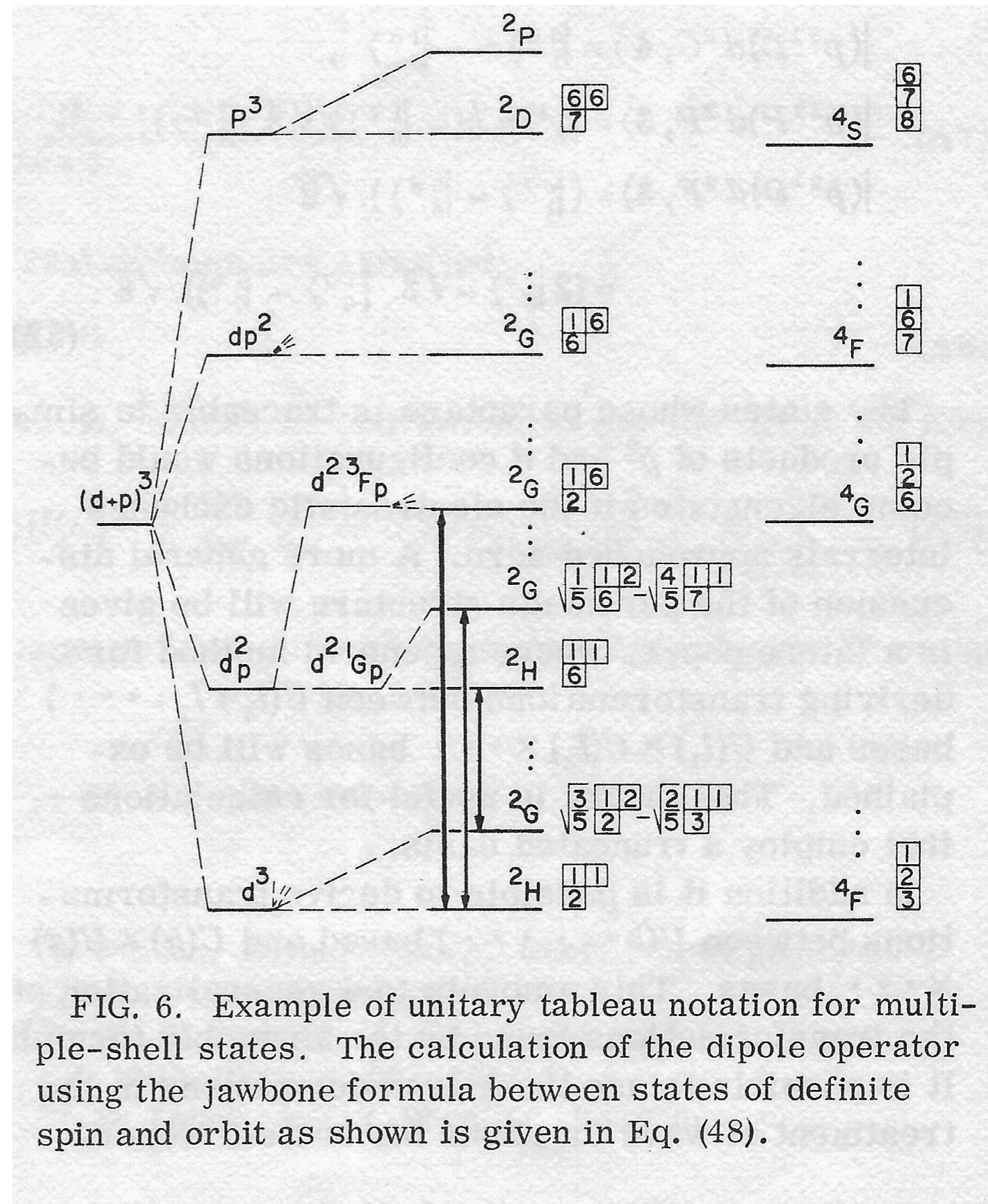
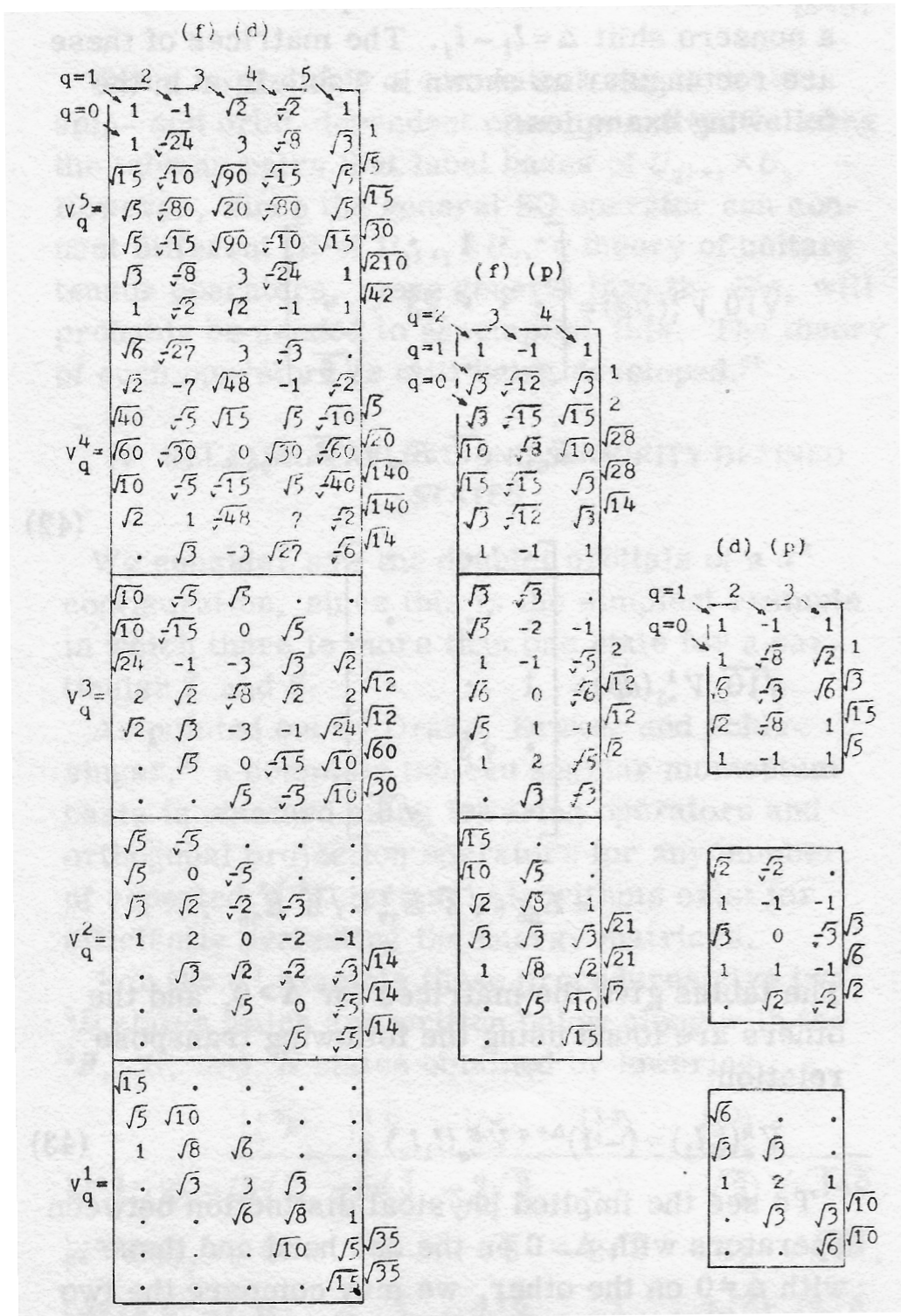


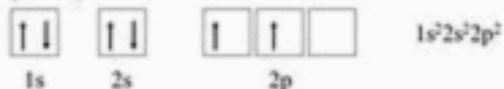
FIG. 6. Example of unitary tableau notation for multiple-shell states. The calculation of the dipole operator using the jawbone formula between states of definite spin and orbit as shown is given in Eq. (48).





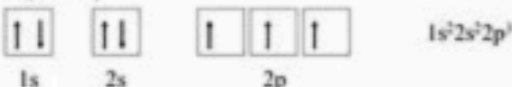
### The Aufbau Principal (cont.)

• Carbon (Z = 6)



**Hund's Rule:** Lowest energy configuration is the one in which the maximum number of unpaired electrons are distributed amongst a set of degenerate orbitals.

• Nitrogen (Z = 7)



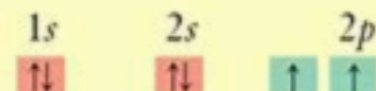
### Hund's Rule

- Within a sublevel, place one electron per orbital before pairing them.
- "Empty Bus Seat Rule"



### Hund's Rule and the Aufbau Principle

- **Aufbau principle** - when filling orbitals, start with the lowest energy and proceed to the next highest energy level.
- **Hund's rule** - within a subshell, electrons occupy the maximum number of orbitals possible.
- Electron configurations are sometimes depicted using boxes to represent orbitals. This depiction shows paired and unpaired electrons explicitly.



### Hund's rule of maximum multiplicity

- The three rules are:
- For a given electron configuration, the term with maximum multiplicity has the lowest energy. The multiplicity is equal to  $2S + 1$ , where  $S$  is the total spin angular momentum for all electrons.
- For a given multiplicity, the term with the largest value of the total orbital angular momentum quantum number has the lowest energy.

*Yay! (for the Googley internet)*

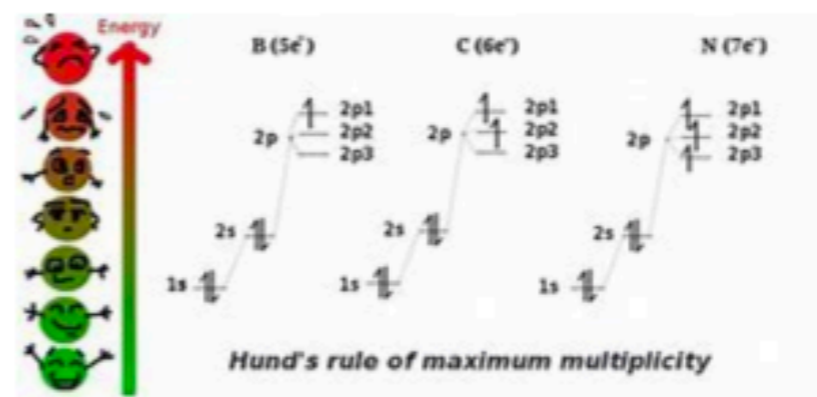
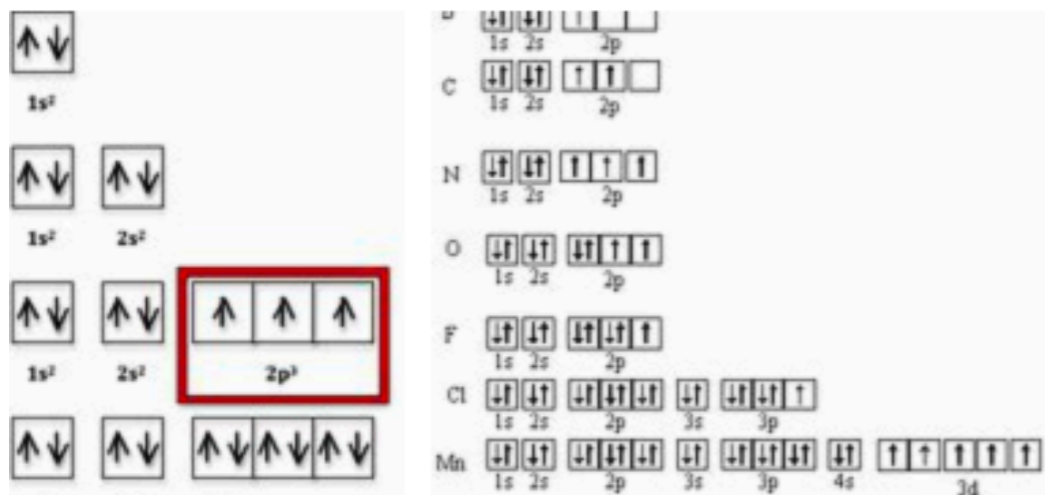
### Hund's Rule of maximum Multiplicity

- The above rules: not give idea abt filling the e- in to degenerate orbitals.
- For e.g., p-orbitals
- "when more than one orbitals of equal energies are available, then the e- will first occupy these orbitals separately with parallel spins. the pairing of e- will start only after all the orbitals of a given sub-level are singly occupied."
- Analogy: Students could fill each seat of a school bus, one person at a time, before doubling up.

### Hund's Rule

In a set of orbitals, the electrons will fill the orbitals in a way that would give the maximum number of parallel spins (maximum number of unpaired electrons)

Analogy: Students could fill each seat of a school bus, one person at a time, before doubling up.



# Complete set of $E_{jk}$ matrix elements for the doublet (spin- $1/2$ ) $p^3$ orbits

	$ \frac{1}{2}^1\rangle$ $M=2$	$ \frac{1}{2}^2\rangle$ $M=1$	$ \frac{1}{3}^1\rangle$ $M=0$	$ \frac{1}{3}^2\rangle$ $M=0$	$ \frac{1}{2}^3\rangle$ $M=-1$	$ \frac{1}{3}^3\rangle$ $M=-1$	$ \frac{2}{3}^2\rangle$ $M=-2$	$ \frac{2}{3}^3\rangle$ $M=-2$
$\langle \frac{1}{2}^1  $	$2^{(11)} + 1^{(22)}$	$1^{(12)}$	$1^{(23)}$	$-\sqrt{\frac{1}{2}}^{(13)}$	$\sqrt{\frac{3}{2}}^{(13)}$			
$\langle \frac{1}{2}^2  $		$1^{(11)} + 2^{(22)}$		$\sqrt{\frac{1}{2}}^{(23)}$	$\sqrt{\frac{3}{2}}^{(23)}$		$-1^{(13)}$	
$\langle \frac{1}{3}^1  $			$2^{(11)} + 1^{(33)}$	$\sqrt{2}^{(12)}$		$1^{(13)}$		
$\langle \frac{1}{3}^2  $			$1^{(11)} + 1^{(22)} + 1^{(33)}$		$\sqrt{\frac{1}{2}}^{(23)}$	$\sqrt{2}^{(12)}$	$\sqrt{\frac{1}{2}}^{(13)}$	$= \langle E_{ij} \rangle$
$\langle \frac{1}{2}^3  $				$1^{(11)} + 1^{(22)} + 1^{(33)}$	$\sqrt{\frac{3}{2}}^{(23)}$		$\sqrt{\frac{3}{2}}^{(13)}$	
$\langle \frac{1}{3}^3  $					$1^{(11)} + 2^{(33)}$		$1^{(12)}$	
$\langle \frac{2}{3}^2  $						$2^{(22)} + 1^{(33)}$	$1^{(23)}$	
$\langle \frac{2}{3}^3  $							$1^{(22)} + 2^{(33)}$	

notation:  
 $(jk)$  numbers tell  
 which  $E_{jk}$  gave that entry

## Diagonal examples in $n$ -particle notation:

$$\sqrt{3}\mathbf{V}_0^0 = E_{11} + E_{22} + E_{33}$$

$$\sqrt{2}\mathbf{V}_0^1 = E_{11} - E_{33} \equiv L_z$$

$$\sqrt{6}\mathbf{V}_0^2 = E_{11} - 2E_{22} + E_{33}$$

## Off-Diagonal examples in $n$ -particle notation:

$$\begin{aligned} \mathbf{V}_2^2 &= E_{13}, & -2\mathbf{V}_1^2 &= \sqrt{2}(E_{12} - E_{23}), & 2\mathbf{V}_{-1}^2 &= \sqrt{2}(E_{21} - E_{32}), & 2\mathbf{V}_{-2}^2 &= E_{31}, \\ -2\mathbf{V}_1^1 &= \sqrt{2}(E_{12} + E_{23}) \equiv L_+, & 2\mathbf{V}_{-1}^1 &= \sqrt{2}(E_{21} + E_{32}) \equiv L_-. \end{aligned}$$

# Tableau calculation of 3-electron $\ell=1$ orbital $p^3$ -states and their $V^k_q$ matrices

Start with highest angular momentum ( $L=2$ )  $p^3$  state:  $\left| {}^2D_{M=2}^{L=2} \right\rangle = \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 2 & \\ \hline \end{array}$  (Fermi spin-mate  $\begin{array}{|c|c|} \hline \uparrow & \uparrow \\ \hline \downarrow & \\ \hline \end{array}$ )

Then apply lowering operator  $L_- \equiv \sqrt{2}(E_{21} + E_{32})$   $\left| {}^2D_{M=1}^{L=2} \right\rangle = \frac{1}{2} L_- \left| {}^2D_{M=2}^{L=2} \right\rangle = \frac{1}{2} \sqrt{2} (E_{21} + E_{32}) \left| \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 2 & \\ \hline \end{array} \right\rangle$

Here this is done using Tableau "Jawbone" formula.  $= \frac{1}{\sqrt{2}} \left( \left| \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 2 & \\ \hline \end{array} \right\rangle + \left| \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 3 & \\ \hline \end{array} \right\rangle \right)$

Orthogonal to this is a  ${}^2P$  ( $M=1$ ) state

$$\left| {}^2P_{M=1}^{L=1} \right\rangle = \frac{1}{\sqrt{2}} \left( \left| \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 2 & \\ \hline \end{array} \right\rangle - \left| \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 3 & \\ \hline \end{array} \right\rangle \right)$$

Next we calculate  $2^n$ -pole moments the pair:

$$\begin{aligned} \left\langle {}^2P_{M=1}^{L=1} \left| V_0^k \right| {}^2D_{M=1}^{L=2} \right\rangle &= \\ \frac{1}{\sqrt{2}} \left( \left\langle \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 2 & \\ \hline \end{array} \right| + \left\langle \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 3 & \\ \hline \end{array} \right| \right) & \left[ \binom{k}{11} E_{11} + \binom{k}{22} E_{22} + \binom{k}{33} E_{33} \right] \left( \left| \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 2 & \\ \hline \end{array} \right\rangle - \left| \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 3 & \\ \hline \end{array} \right\rangle \right) \\ &= \frac{1}{2} \left[ -\binom{2}{11} E_{11} + 2\binom{2}{22} E_{22} - \binom{2}{33} \right] = -\sqrt{\frac{3}{2}} \quad \text{for : } k=2 \\ &= \frac{1}{2} \left[ -\binom{1}{11} E_{11} + 2\binom{1}{22} E_{22} - \binom{1}{33} \right] = 0 \quad \text{for : } k=1 \\ &= \frac{1}{2} \left[ -\binom{0}{11} E_{11} + 2\binom{0}{22} E_{22} - \binom{0}{33} \right] = 0 \quad \text{for : } k=0 \end{aligned}$$

(a)  $\langle T | E_{ii} | T \rangle = \delta_{T,T} (\text{number of } i\text{'s})$       (b)  $\langle T | E_{ij} | T \rangle = \langle T | E_{ji} | T \rangle$

(c)  $\left\langle \begin{array}{|c|c|} \hline i-1 \\ \hline i-1 \\ \hline \end{array} \right| E_{i-l,i} \left| \begin{array}{|c|c|} \hline i \\ \hline i-1 \\ \hline \end{array} \right\rangle = \sqrt{\frac{d+1}{d}} = \left\langle \begin{array}{|c|c|} \hline i-1 \\ \hline i-1 \\ \hline \end{array} \right| E_{i-l,i} \left| \begin{array}{|c|c|} \hline i \\ \hline i \\ \hline \end{array} \right\rangle$

(d)  $\left\langle \begin{array}{|c|c|} \hline i-1 \\ \hline i \\ \hline \end{array} \right| E_{i-l,i} \left| \begin{array}{|c|c|} \hline i \\ \hline i-1 \\ \hline \end{array} \right\rangle = \sqrt{\frac{d-1}{d}} = \left\langle \begin{array}{|c|c|} \hline i-1 \\ \hline i-1 \\ \hline \end{array} \right| E_{i-l,i} \left| \begin{array}{|c|c|} \hline i \\ \hline i \\ \hline \end{array} \right\rangle$

(e)  $E_{23} \begin{array}{|c|c|} \hline 1 & 3 \\ \hline 3 & \\ \hline \end{array} = \frac{1}{\sqrt{2}} \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \hline \end{array} + \frac{1}{\sqrt{2}} \begin{array}{|c|c|} \hline 1 & 3 \\ \hline 2 & \\ \hline \end{array}$

(f)  $E_{12} \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 1 & \\ \hline \end{array} = \sqrt{2} \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 1 & \\ \hline \end{array}$

(g)  $\left\langle \begin{array}{|c|c|} \hline i-1 \\ \hline i-1 \\ \hline \end{array} \right| E_{i-l,i} \left| \begin{array}{|c|c|} \hline i \\ \hline i \\ \hline \end{array} \right\rangle = 1 = \left\langle \begin{array}{|c|c|} \hline i-1 \\ \hline i-1 \\ \hline \end{array} \right| E_{i-l,i} \left| \begin{array}{|c|c|} \hline i \\ \hline i \\ \hline \end{array} \right\rangle$

(h)  $\left\langle \begin{array}{|c|c|} \hline i-1 \\ \hline i-1 \\ \hline \end{array} \right| E_{i-l,i} \left| \begin{array}{|c|c|} \hline i \\ \hline i-1 \\ \hline \end{array} \right\rangle = 1 = \left\langle \begin{array}{|c|c|} \hline i-1 \\ \hline i-1 \\ \hline \end{array} \right| E_{i-l,i} \left| \begin{array}{|c|c|} \hline i \\ \hline i \\ \hline \end{array} \right\rangle$

$$|1,2,3\rangle \equiv |1\rangle_{particle-a} |2\rangle_{particle-b} |3\rangle_{particle-c} \equiv |1\rangle_a |2\rangle_b |3\rangle_c$$

## Single particle $p^1$ -orbitals: $U(3)$ triplet $|p^1 \square\rangle$

$$e_{11} = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}, e_{12} = \begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}, e_{13} = \begin{pmatrix} \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}, e_{21} = \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}, \dots e_{33} = \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \end{pmatrix}.$$

$$\begin{aligned} e_{12}e_{21} &= e_{11} & |1\rangle\langle 2||2\rangle\langle 1| &= |1\rangle\langle 1| \\ e_{12}e_{22} &= e_{12} & |1\rangle\langle 2||2\rangle\langle 2| &= |1\rangle\langle 2| \\ & & \vdots & \\ e_{jk}e_{pq} &= \delta_{pk}e_{jq} & |j\rangle\langle k||p\rangle\langle q| &= \delta_{pk}|j\rangle\langle q| \end{aligned}$$

*Elementary matrix algebra*

General elementary operator commutation  $[E_{jk}, E_{pq}] = \delta_{kp}E_{jq} - \delta_{qj}E_{pk}$   
has same form as 1-particle commutation:  $[e_{jk}, e_{pq}] = \delta_{kp}e_{jq} - \delta_{qj}e_{pk}$

*Elementary-elementary  
operator commutation algebra*

This applies to all of multi-particle representations of  $E_{jk}$  and to momentum operators  $L_x$ ,  $L_y$ , and  $L_z$ .

Single particle  $p$ -orbit ( $\ell=1$ ) representation of  $L_x$ ,  $L_y$ , and  $L_z$

$$D_{mn}^1(L_x) = \frac{1}{\sqrt{2}} \begin{pmatrix} \cdot & 1 & \cdot \\ 1 & \cdot & 1 \\ \cdot & 1 & \cdot \end{pmatrix}, \quad D_{mn}^1(L_y) = \frac{-i}{\sqrt{2}} \begin{pmatrix} \cdot & 1 & \cdot \\ -1 & \cdot & 1 \\ \cdot & -1 & \cdot \end{pmatrix}, \quad D_{mn}^1(L_z) = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$$

Elementary operator form of  $L_x$ ,  $L_y$ , and  $L_z$

$$L_x = (E_{12} + E_{23} + E_{21} + E_{32}) / \sqrt{2}, \quad L_y = -i(E_{12} + E_{23} - E_{21} - E_{32}) / \sqrt{2}, \quad L_z = E_{11} - E_{33}$$

...and of raise-lower operators  $L_+$  and  $L_-$

$$L_+ = L_x + iL_y = \sqrt{2}(E_{12} + E_{23}), \quad L_- = L_x - iL_y = \sqrt{2}(E_{21} + E_{32}) = L_+^\dagger, \quad L_z = [L_+, L_-]$$