AMOP reference links on page 2

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-½) 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 $\mathbf{e}_{jk}$ operator expressions for *(e-e)*-interaction matrix
Tensor tables are $(2\ell+1)$-by-$(2\ell+1)$ arrays $\left({}_p{}^k{}_q\right)$ giving $\mathbf{V}_q^k$ in terms of $\mathbf{E}_{p,q}$.
Relating $\mathbf{V}_q^k$ to $\mathbf{E}_{m',m}$ by $\left({}_{m'}{}^k{}_m\right)$ arrays
Atomic p-shell *ee*-interaction in elementary operator form
[2,1] tableau basis (from p.29) and matrices of $\mathbf{v}^1$ dipole and $\mathbf{v}^1\bullet\mathbf{v}^1=\mathbf{L}\bullet\mathbf{L}$
[2,1] tableau basis (from p.29) and matrices of $\mathbf{v}^2$ and $\mathbf{v}^2\bullet\mathbf{v}^2$ quadrupole
^4S,^2P, and ^2D energy calculation of quartet and doublet (spin-½) p^3 orbits
Corrected level diagrams Nitrogen p^3

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

Web Resources - front page
UAF Physics UTube channel

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

2014 AMOP
2017 Group Theory for QM
2018 AMOP

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

Theory of hyperfine and superfine levels in symmetric polyatomic molecules.

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

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

Rotation–vibration spectra of icosahedral molecules.

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

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

RESONANCE AND REVIVALS

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

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

(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-½) 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
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- Linear multipoles; P_1-dipole, P_2-quadrupole, P_3-octupole,…
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- Relating $\mathbf{V}_q^k$ to $\mathbf{E}_{m',m}$ by $({}_{m'}{}^k{}_m)$ arrays
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[2,1] tableau basis (from p.29) and matrices of $\mathbf{v}^1$ dipole and $\mathbf{v}^1\bullet\mathbf{v}^1=\mathbf{L}\bullet\mathbf{L}$

[2,1] tableau basis (from p.29) and matrices of $\mathbf{v}^2$ and $\mathbf{v}^2\bullet\mathbf{v}^2$ quadrupole
- ${}^4S$, ${}^2P$, and ${}^2D$ energy calculation of quartet and doublet (spin-½) p^3 orbits

Corrected level diagrams Nitrogen p^3

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

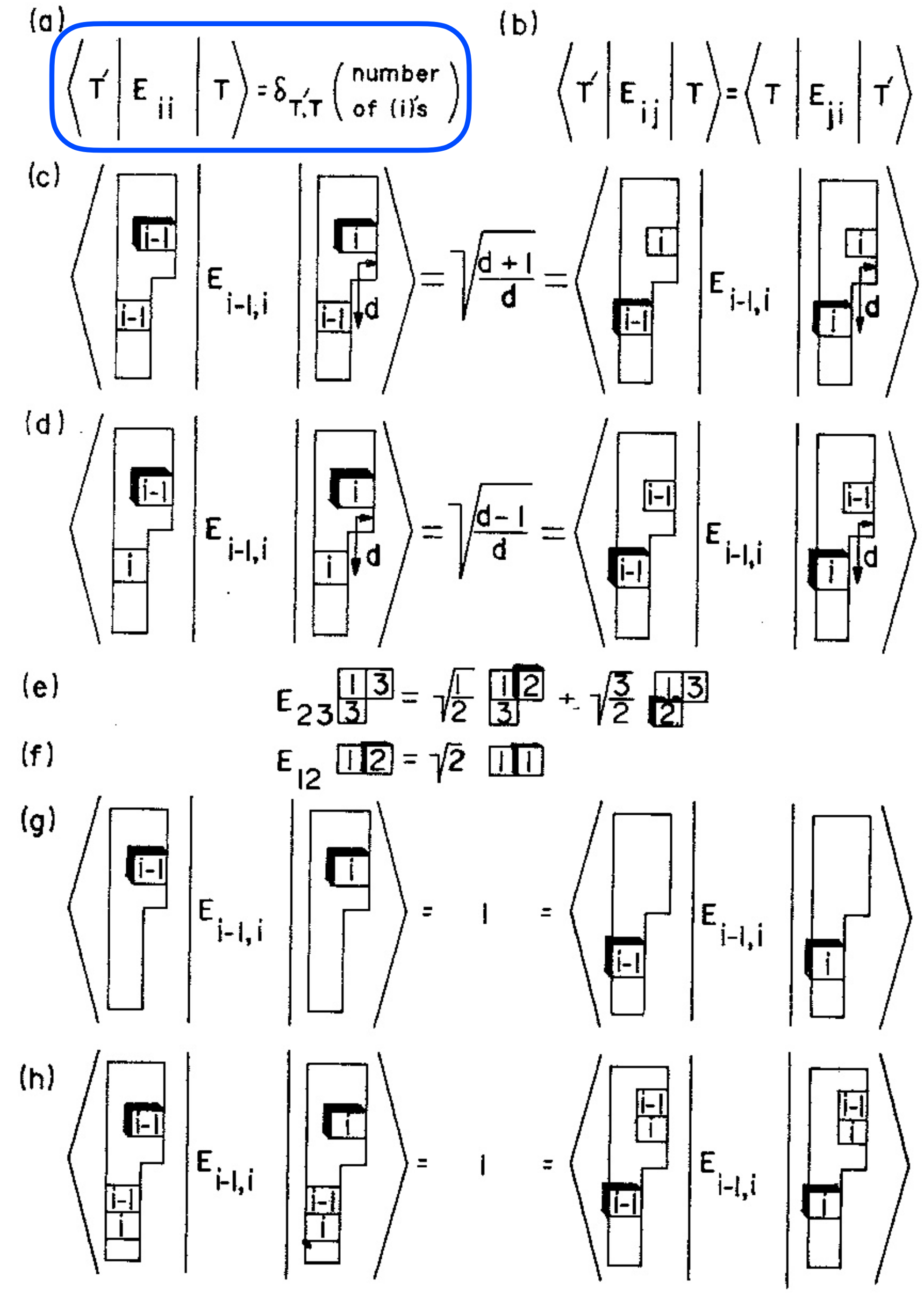
	M=2	*M=1*		*M=0*		*M=-1*		*M=-2*
	$\left\|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\|$	$\overset{(11)}{2} + \overset{(22)}{1}$	$\overset{(12)}{1}$	$\overset{(23)}{1}$	$\overset{(13)}{-\sqrt{\frac{1}{2}}}$	$\overset{(13)}{\sqrt{\frac{3}{2}}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\|$		$\overset{(11)}{1} + \overset{(22)}{2}$	·	$\overset{(23)}{\sqrt{\frac{1}{2}}}$	$\overset{(23)}{\sqrt{\frac{3}{2}}}$	·	$\overset{(13)}{-1}$	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\|$		·	$\overset{(11)}{2} + \overset{(33)}{1}$	$\overset{(12)}{\sqrt{2}}$	·	$\overset{(13)}{1}$	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\|$				$\overset{(11)}{1} + \overset{(22)}{1} + \overset{(33)}{1}$	·	$\overset{(23)}{\sqrt{\frac{1}{2}}}$	$\overset{(12)}{\sqrt{2}}$	$\overset{(13)}{\sqrt{\frac{1}{2}}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\|$				·	$\overset{(11)}{1} + \overset{(22)}{1} + \overset{(33)}{1}$	$\overset{(23)}{\sqrt{\frac{3}{2}}}$	·	$\overset{(13)}{\sqrt{\frac{3}{2}}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\|$						$\overset{(11)}{1} + \overset{(33)}{2}$	·	$\overset{(12)}{1}$
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\|$						·	$\overset{(22)}{2} + \overset{(33)}{1}$	$\overset{(23)}{1}$
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\|$								$\overset{(22)}{1} + \overset{(33)}{2}$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

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

$$\left\langle {11 \atop 2} \middle| E_{11} \middle| {11 \atop 2} \right\rangle = 2 \qquad \left\langle {11 \atop 2} \middle| E_{22} \middle| {11 \atop 2} \right\rangle = 1$$



Sample applications of "Jawbone" number operators

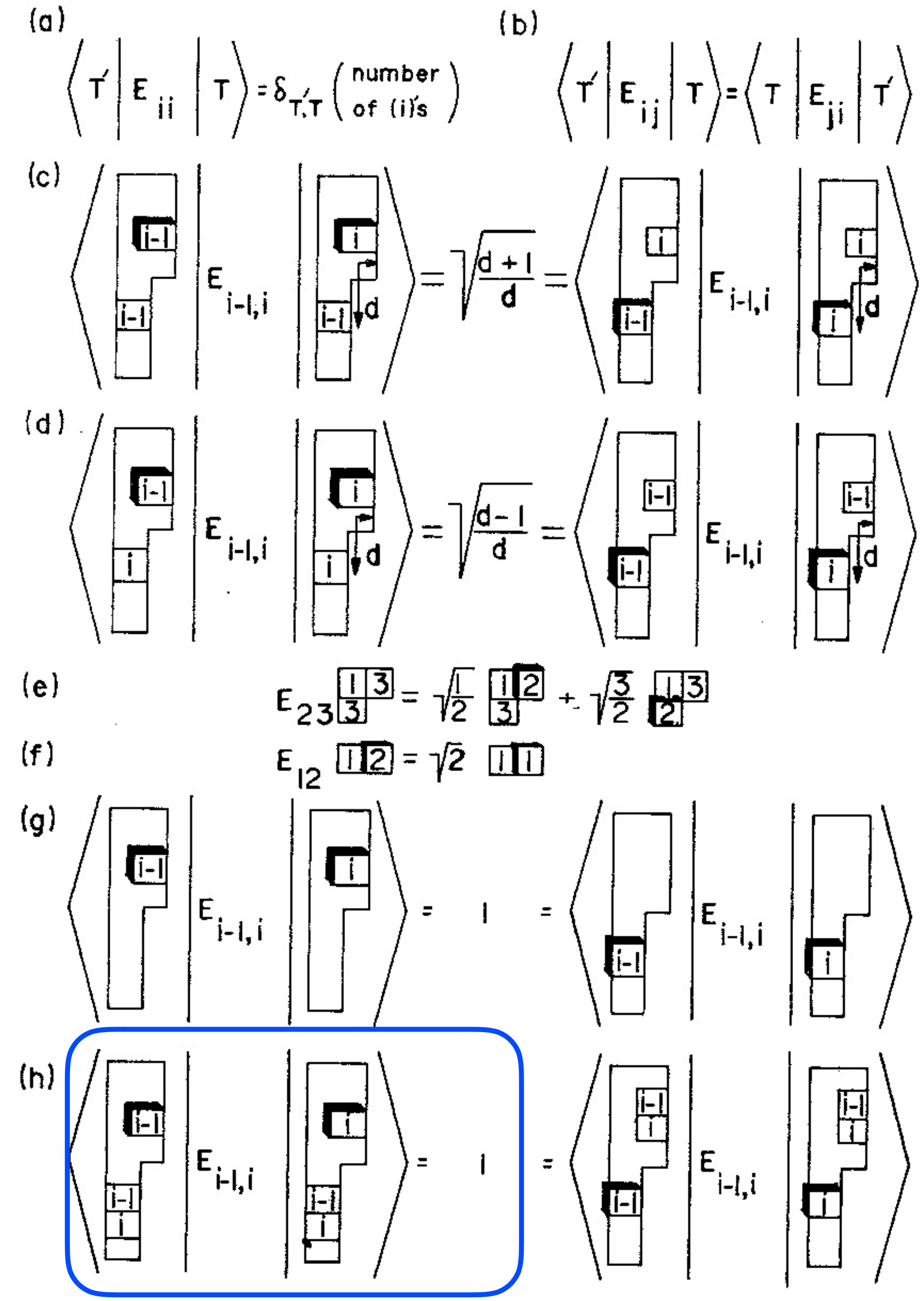
$$\left\langle {11 \atop 2} \middle| E_{11} \middle| {11 \atop 2} \right\rangle = 2 \qquad \left\langle {11 \atop 2} \middle| E_{22} \middle| {11 \atop 2} \right\rangle = 1$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left\lvert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\rvert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\rvert$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\rvert$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\rvert$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\rvert$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\rvert$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\rvert$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\rvert$								(22) (33) $1+2$

$$\left\langle\begin{matrix}11\\2\end{matrix}\middle| E_{11} \middle|\begin{matrix}11\\2\end{matrix}\right\rangle = 2 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\middle| E_{22} \middle|\begin{matrix}11\\2\end{matrix}\right\rangle = 1$$



Sample applications of "Jawbone" formulae

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

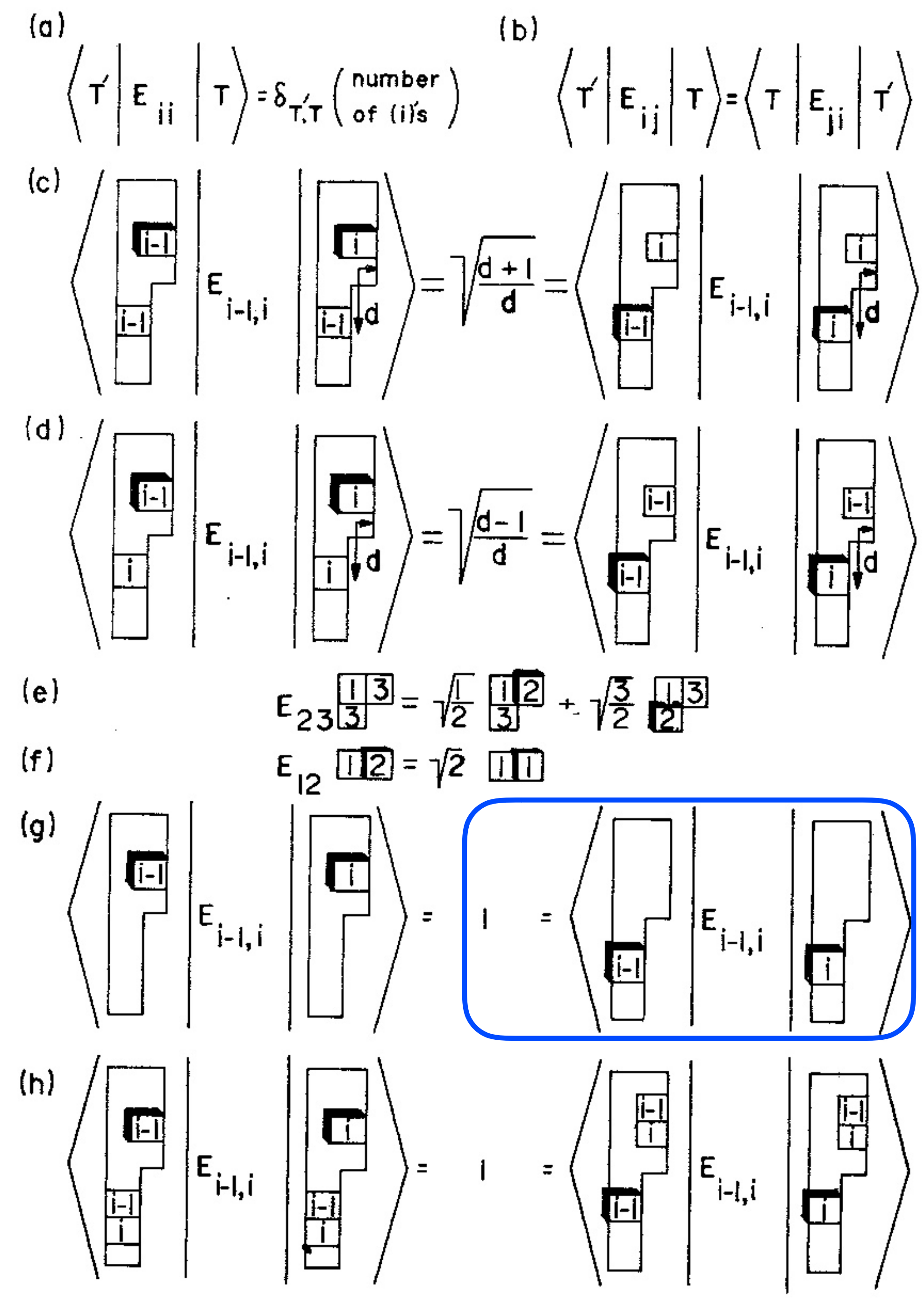
$$\left\langle\begin{matrix}11\\2\end{matrix}\middle| E_{12} \middle|\begin{matrix}12\\2\end{matrix}\right\rangle = 1 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\middle| E_{23} \middle|\begin{matrix}11\\3\end{matrix}\right\rangle = 1$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2 $\left\|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	*M=1* $\left\|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	*M=1* $\left\|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	*M=0* $\left\|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	*M=0* $\left\|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	*M=-1* $\left\|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	*M=-1* $\left\|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	*M=-2* $\left\|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\|$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\|$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\|$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\|$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\|$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\|$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\|$								(22) (33) $1+2$

$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|E_{11}\left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle=2 \qquad \left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|E_{22}\left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle=1$$



Sample applications of "Jawbone" formulae

$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|E_{12}\left|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle=1 \qquad \left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|E_{23}\left|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle=1$$

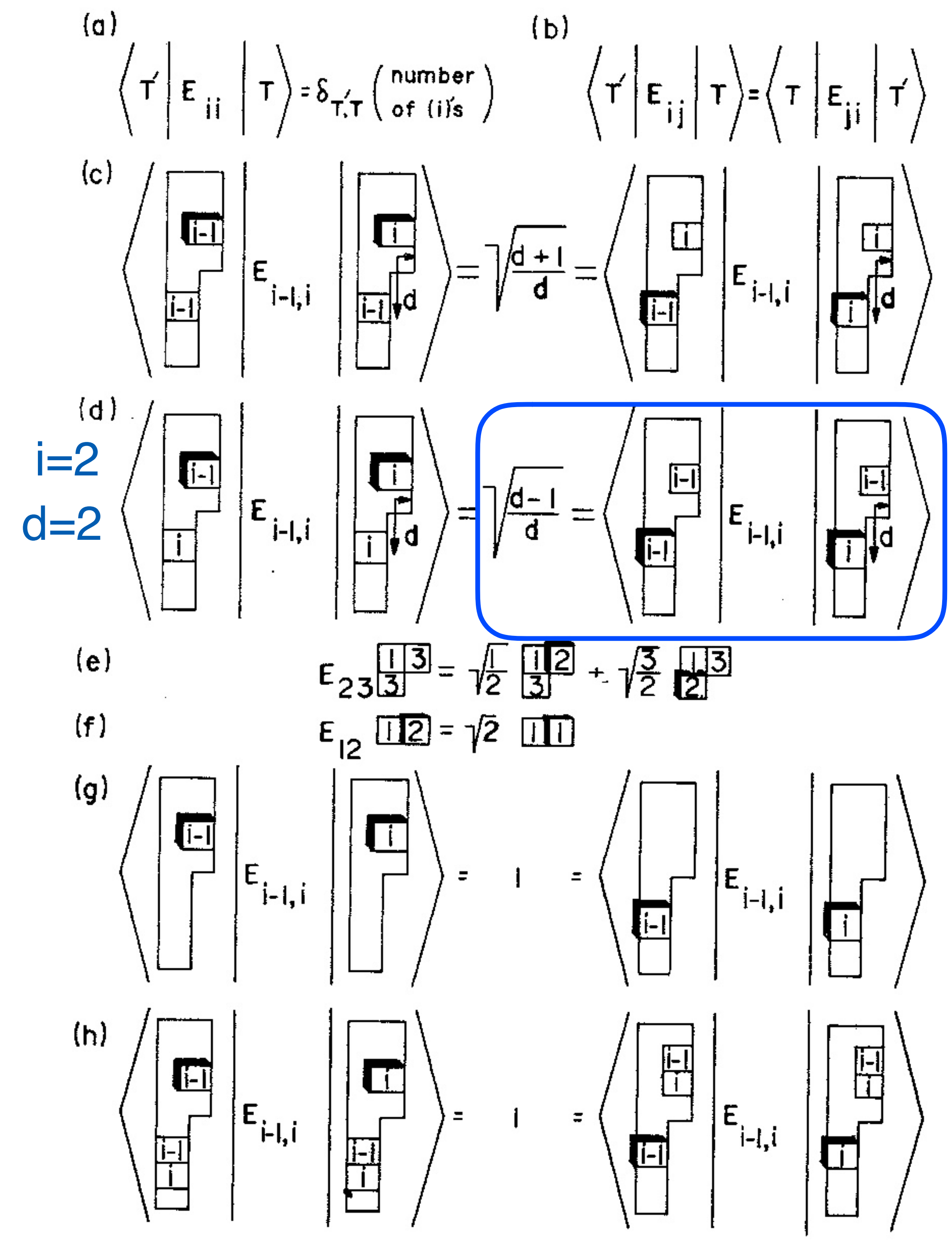
(1-jump $E_{i-1,i}$)

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\vert$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\vert$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\vert$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\vert$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\vert$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\vert$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\vert$								(22) (33) $1+2$

$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert E_{11}\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle = 2 \qquad \left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert E_{22}\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle = 1$$



Sample applications of "Jawbone" formulae

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

$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert E_{12}\left\vert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle = 1 \qquad \left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert E_{23}\left\vert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle = 1$$

$$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\vert E_{23}\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle = \sqrt{\frac{1}{2}}$$

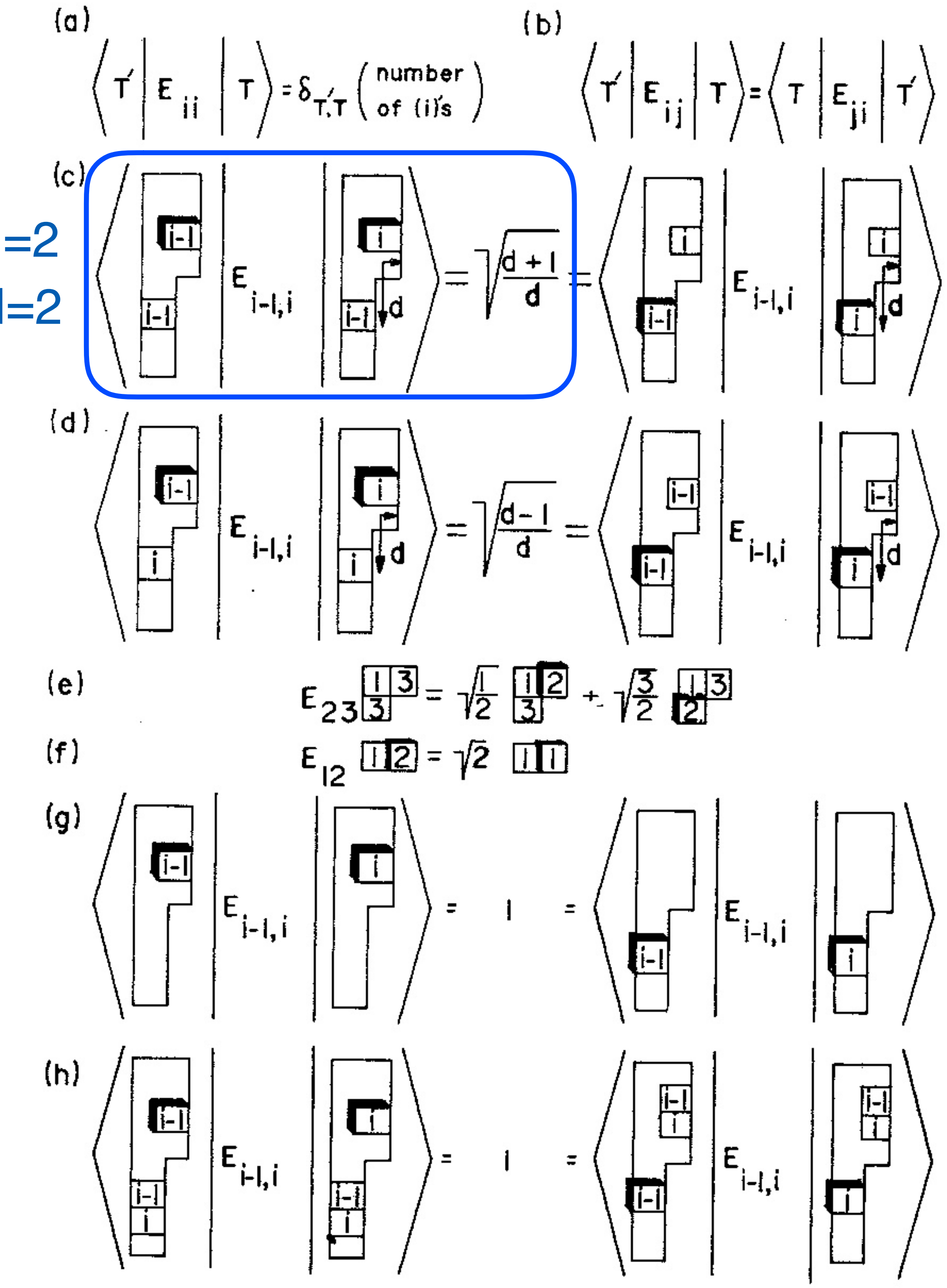
Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2 $\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	*M=1* $\left\vert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	*M=1* $\left\vert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	*M=0* $\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	*M=0* $\left\vert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	*M=-1* $\left\vert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	*M=-1* $\left\vert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	*M=-2* $\left\vert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\vert$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\vert$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\vert$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\vert$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\vert$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\vert$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\vert$								(22) (33) $1+2$

$$\left\langle \begin{matrix}11\\2\end{matrix} \middle| E_{11} \middle| \begin{matrix}11\\2\end{matrix} \right\rangle = 2 \qquad \left\langle \begin{matrix}11\\2\end{matrix} \middle| E_{22} \middle| \begin{matrix}11\\2\end{matrix} \right\rangle = 1$$

i=2
d=2



Sample applications of "Jawbone" formulae

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

$$\left\langle \begin{matrix}11\\2\end{matrix} \middle| E_{12} \middle| \begin{matrix}12\\2\end{matrix} \right\rangle = 1 \qquad \left\langle \begin{matrix}11\\2\end{matrix} \middle| E_{23} \middle| \begin{matrix}11\\3\end{matrix} \right\rangle = 1$$

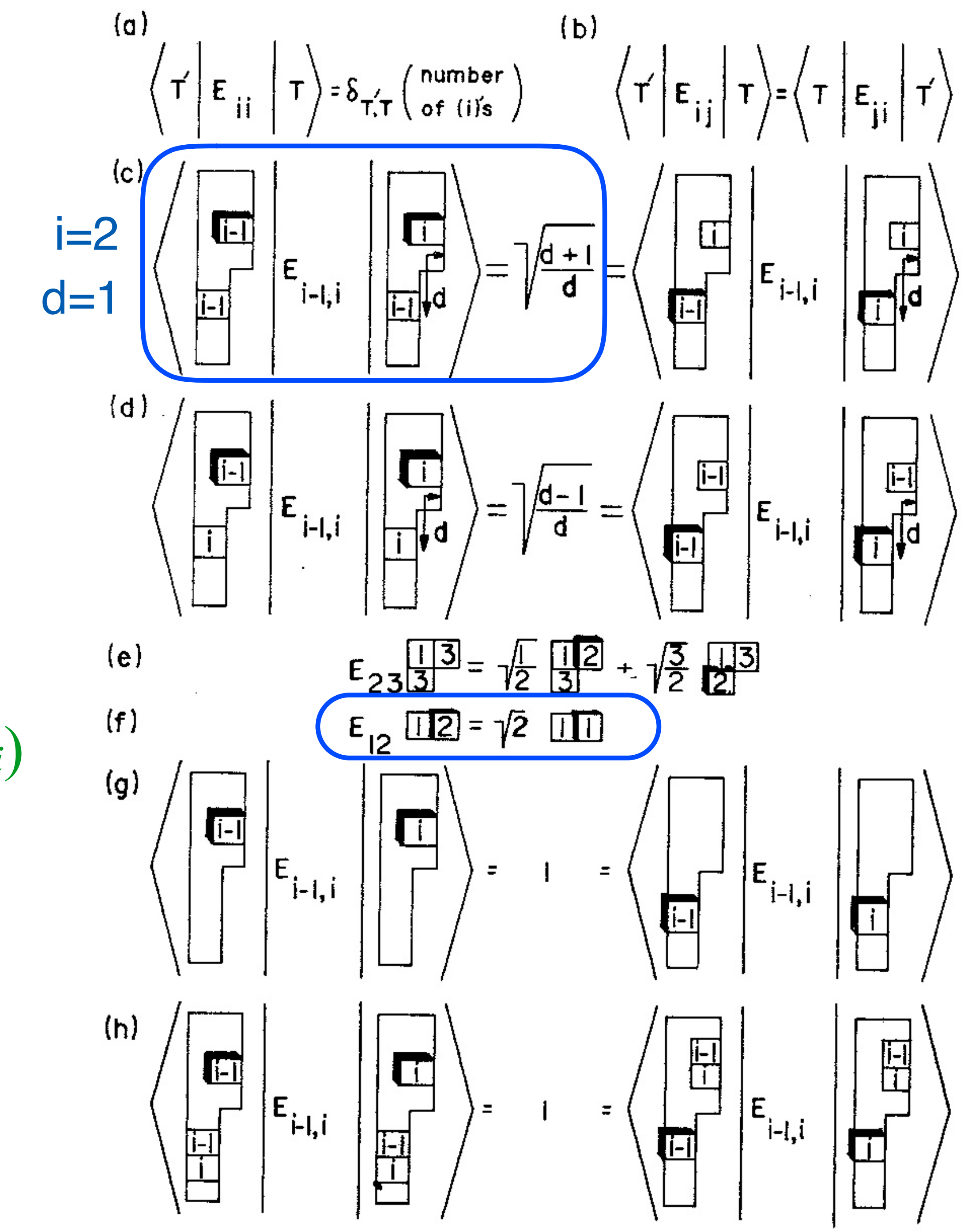
$$\left\langle \begin{matrix}12\\2\end{matrix} \middle| E_{23} \middle| \begin{matrix}13\\2\end{matrix} \right\rangle = \sqrt{\frac{3}{2}} \qquad \left\langle \begin{matrix}12\\2\end{matrix} \middle| E_{23} \middle| \begin{matrix}12\\3\end{matrix} \right\rangle = \sqrt{\frac{1}{2}}$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2: $\left\|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	M=1: $\left\|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	M=1: $\left\|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	M=0: $\left\|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	M=0: $\left\|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	M=-1: $\left\|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	M=-1: $\left\|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	M=-2: $\left\|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\|$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\|$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\|$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\|$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\|$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\|$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\|$								(22) (33) $1+2$

$$\left\langle\begin{matrix}11\\2\end{matrix}\middle|E_{11}\middle|\begin{matrix}11\\2\end{matrix}\right\rangle=2 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\middle|E_{22}\middle|\begin{matrix}11\\2\end{matrix}\right\rangle=1$$



Sample applications of "Jawbone" formulae

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

$$\left\langle\begin{matrix}11\\2\end{matrix}\middle|E_{12}\middle|\begin{matrix}12\\2\end{matrix}\right\rangle=1 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\middle|E_{23}\middle|\begin{matrix}11\\3\end{matrix}\right\rangle=1$$

$$\left\langle\begin{matrix}12\\2\end{matrix}\middle|E_{23}\middle|\begin{matrix}13\\2\end{matrix}\right\rangle=\sqrt{\frac{3}{2}} \qquad \left\langle\begin{matrix}12\\2\end{matrix}\middle|E_{23}\middle|\begin{matrix}12\\3\end{matrix}\right\rangle=\sqrt{\frac{1}{2}}$$

$$\left\langle\begin{matrix}11\\3\end{matrix}\middle|E_{12}\middle|\begin{matrix}12\\3\end{matrix}\right\rangle=\sqrt{2}$$

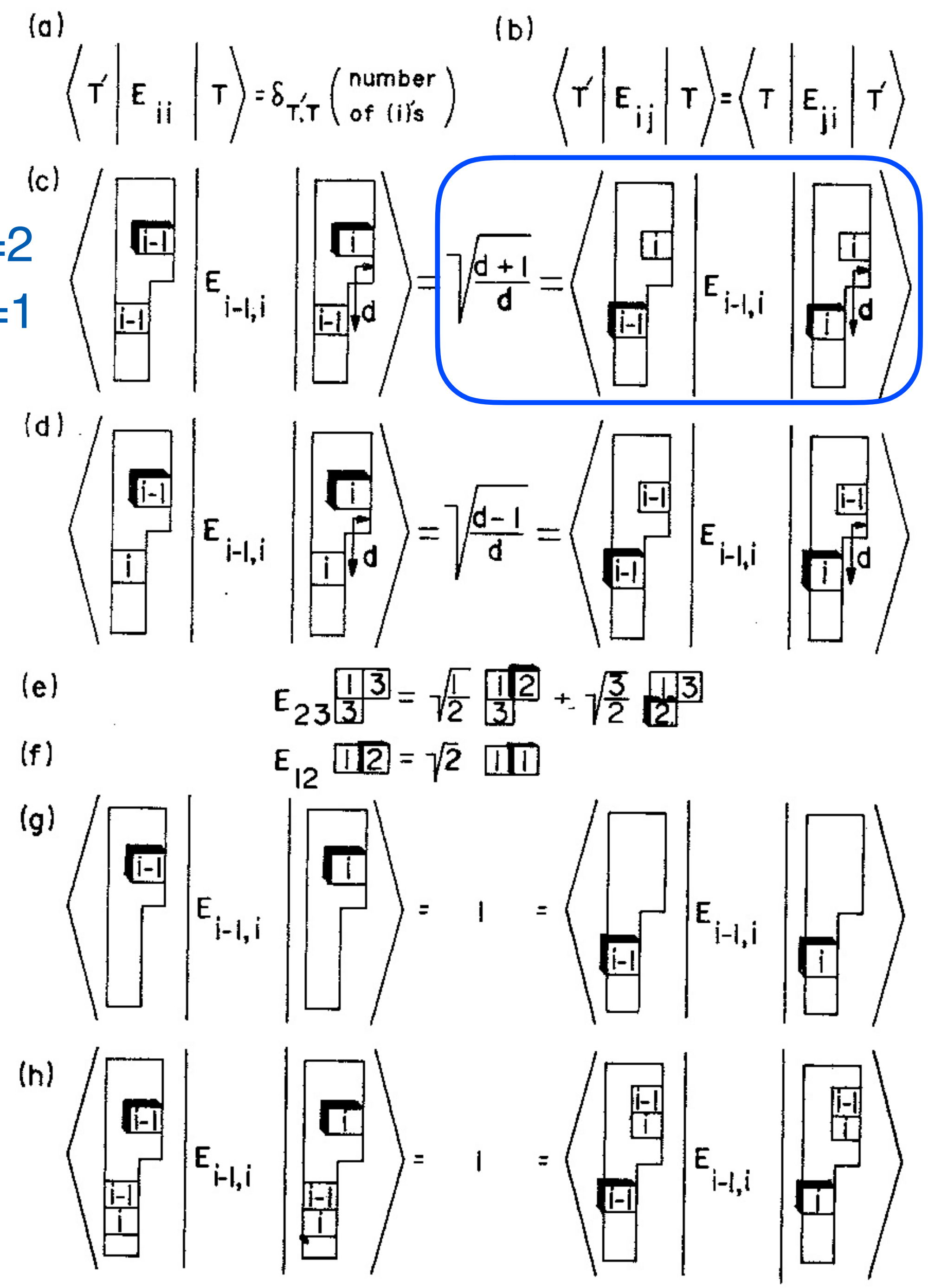
Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

E_{jk} =

	M=2	M=1		M=0		M=-1		M=-2
	$\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\vert$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\vert$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\vert$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\vert$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\vert$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\vert$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\vert$								(22) (33) $1+2$

$$\left\langle\begin{matrix}11\\2\end{matrix}\right\vert E_{11}\left\vert\begin{matrix}11\\2\end{matrix}\right\rangle = 2 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\right\vert E_{22}\left\vert\begin{matrix}11\\2\end{matrix}\right\rangle = 1$$

i=2
d=1



Sample applications of "Jawbone" formulae

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

$$\left\langle\begin{matrix}11\\2\end{matrix}\right\vert E_{12}\left\vert\begin{matrix}12\\2\end{matrix}\right\rangle = 1 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\right\vert E_{23}\left\vert\begin{matrix}11\\3\end{matrix}\right\rangle = 1$$

$$\left\langle\begin{matrix}12\\2\end{matrix}\right\vert E_{23}\left\vert\begin{matrix}13\\2\end{matrix}\right\rangle = \sqrt{\frac{3}{2}} \qquad \left\langle\begin{matrix}12\\2\end{matrix}\right\vert E_{23}\left\vert\begin{matrix}12\\3\end{matrix}\right\rangle = \sqrt{\frac{1}{2}}$$

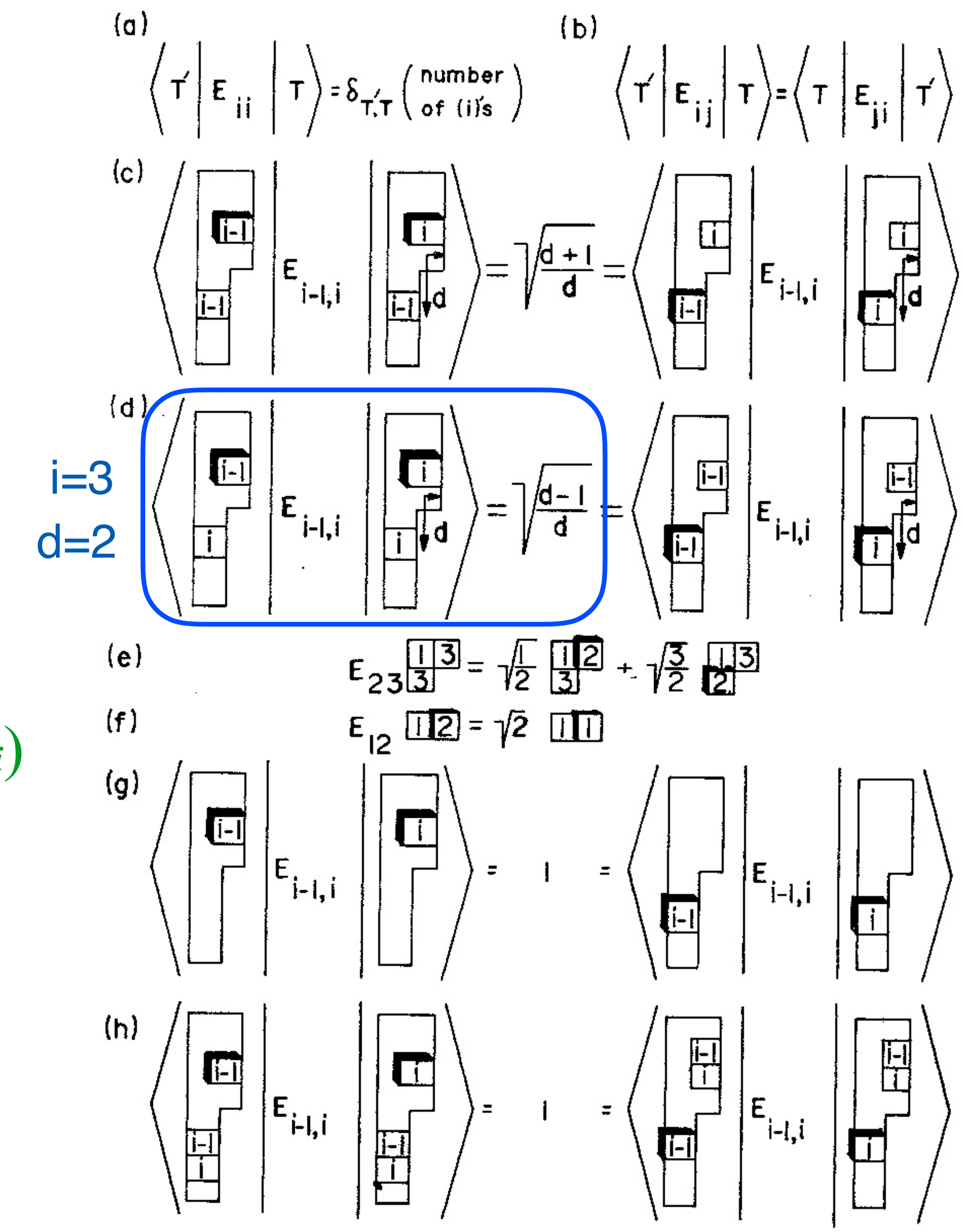
$$\left\langle\begin{matrix}12\\3\end{matrix}\right\vert E_{12}\left\vert\begin{matrix}22\\3\end{matrix}\right\rangle = \sqrt{2} \qquad \left\langle\begin{matrix}12\\3\end{matrix}\right\vert E_{12}\left\vert\begin{matrix}22\\3\end{matrix}\right\rangle = \sqrt{2}$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2: $\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	M=1: $\left\vert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	M=1: $\left\vert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	M=0: $\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	M=0: $\left\vert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	M=-1: $\left\vert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	M=-1: $\left\vert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	M=-2: $\left\vert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\vert$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\vert$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\vert$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\vert$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\vert$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\vert$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\vert$								(22) (33) $1+2$

$$\left\langle\begin{matrix}11\\2\end{matrix}\middle\vert E_{11}\middle\vert\begin{matrix}11\\2\end{matrix}\right\rangle = 2 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\middle\vert E_{22}\middle\vert\begin{matrix}11\\2\end{matrix}\right\rangle = 1$$



Sample applications of "Jawbone" formulae

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

$$\left\langle\begin{matrix}11\\2\end{matrix}\middle\vert E_{12}\middle\vert\begin{matrix}12\\2\end{matrix}\right\rangle = 1 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\middle\vert E_{23}\middle\vert\begin{matrix}11\\3\end{matrix}\right\rangle = 1$$

$$\left\langle\begin{matrix}12\\2\end{matrix}\middle\vert E_{23}\middle\vert\begin{matrix}13\\2\end{matrix}\right\rangle = \sqrt{\frac{3}{2}} \qquad \left\langle\begin{matrix}12\\2\end{matrix}\middle\vert E_{23}\middle\vert\begin{matrix}12\\3\end{matrix}\right\rangle = \sqrt{\frac{1}{2}}$$

$$\left\langle\begin{matrix}12\\3\end{matrix}\middle\vert E_{12}\middle\vert\begin{matrix}22\\3\end{matrix}\right\rangle = \sqrt{2} \qquad \left\langle\begin{matrix}12\\3\end{matrix}\middle\vert E_{12}\middle\vert\begin{matrix}22\\3\end{matrix}\right\rangle = \sqrt{2}$$

$$\left\langle\begin{matrix}12\\3\end{matrix}\middle\vert E_{23}\middle\vert\begin{matrix}13\\3\end{matrix}\right\rangle = \sqrt{\frac{1}{2}}$$

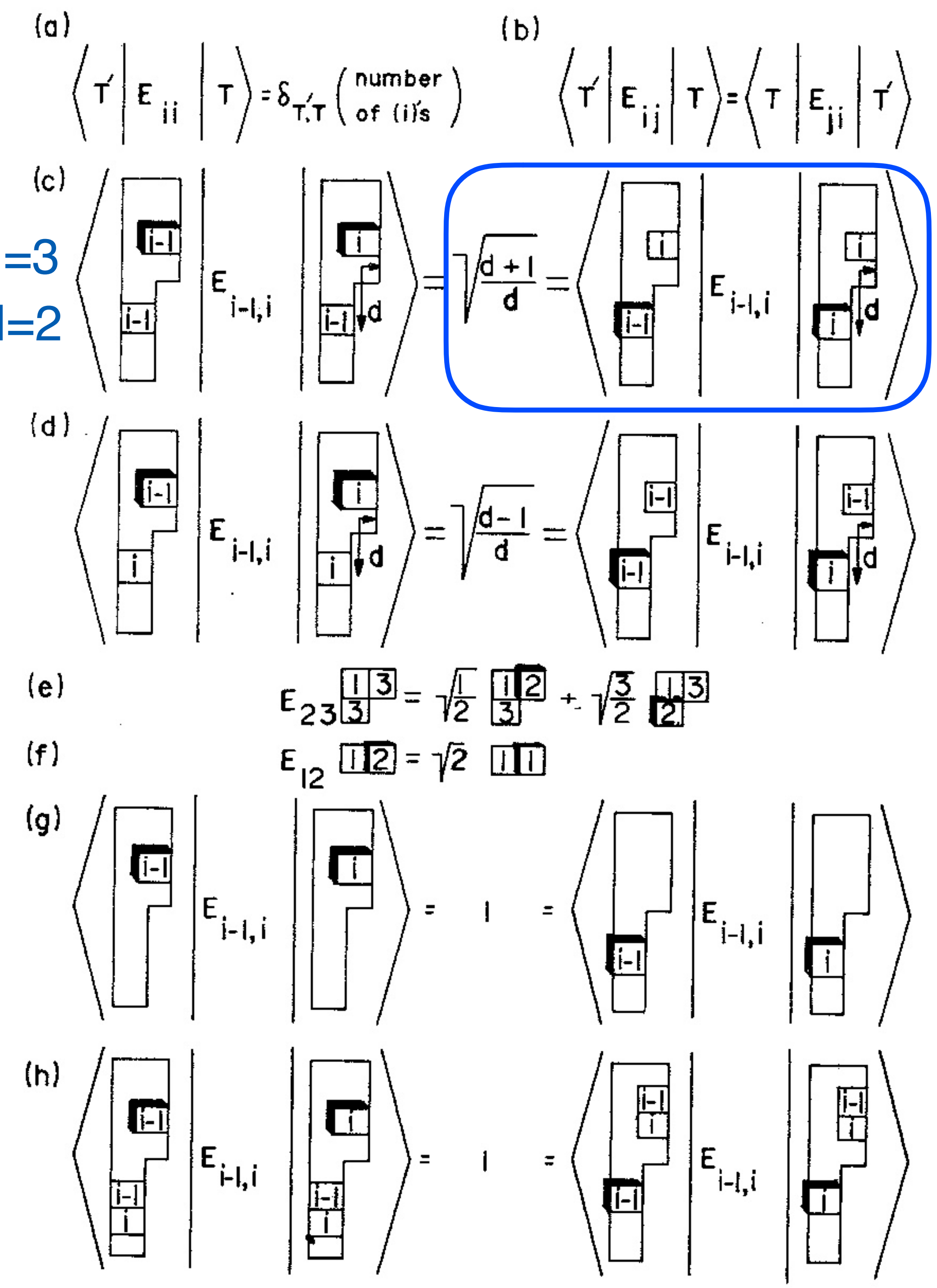
Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left\|\begin{matrix}11\\2\end{matrix}\right\rangle$	$\left\|\begin{matrix}12\\2\end{matrix}\right\rangle$	$\left\|\begin{matrix}11\\3\end{matrix}\right\rangle$	$\left\|\begin{matrix}12\\3\end{matrix}\right\rangle$	$\left\|\begin{matrix}13\\2\end{matrix}\right\rangle$	$\left\|\begin{matrix}13\\3\end{matrix}\right\rangle$	$\left\|\begin{matrix}22\\3\end{matrix}\right\rangle$	$\left\|\begin{matrix}23\\3\end{matrix}\right\rangle$
$\left\langle\begin{matrix}11\\2\end{matrix}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{matrix}12\\2\end{matrix}\right\|$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{matrix}11\\3\end{matrix}\right\|$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{matrix}12\\3\end{matrix}\right\|$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{matrix}13\\2\end{matrix}\right\|$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{matrix}13\\3\end{matrix}\right\|$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{matrix}22\\3\end{matrix}\right\|$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{matrix}23\\3\end{matrix}\right\|$								(22) (33) $1+2$

$$\left\langle\begin{matrix}11\\2\end{matrix}\right|E_{11}\left|\begin{matrix}11\\2\end{matrix}\right\rangle=2 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\right|E_{22}\left|\begin{matrix}11\\2\end{matrix}\right\rangle=1$$

i=3
d=2



Sample applications of "Jawbone" formulae

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

$$\left\langle\begin{matrix}11\\2\end{matrix}\right|E_{12}\left|\begin{matrix}12\\2\end{matrix}\right\rangle=1 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\right|E_{23}\left|\begin{matrix}11\\3\end{matrix}\right\rangle=1$$

$$\left\langle\begin{matrix}12\\2\end{matrix}\right|E_{23}\left|\begin{matrix}13\\2\end{matrix}\right\rangle=\sqrt{\frac{3}{2}} \qquad \left\langle\begin{matrix}12\\2\end{matrix}\right|E_{23}\left|\begin{matrix}12\\3\end{matrix}\right\rangle=\sqrt{\frac{1}{2}}$$

$$\left\langle\begin{matrix}12\\3\end{matrix}\right|E_{12}\left|\begin{matrix}22\\3\end{matrix}\right\rangle=\sqrt{2} \qquad \left\langle\begin{matrix}12\\3\end{matrix}\right|E_{12}\left|\begin{matrix}22\\3\end{matrix}\right\rangle=\sqrt{2}$$

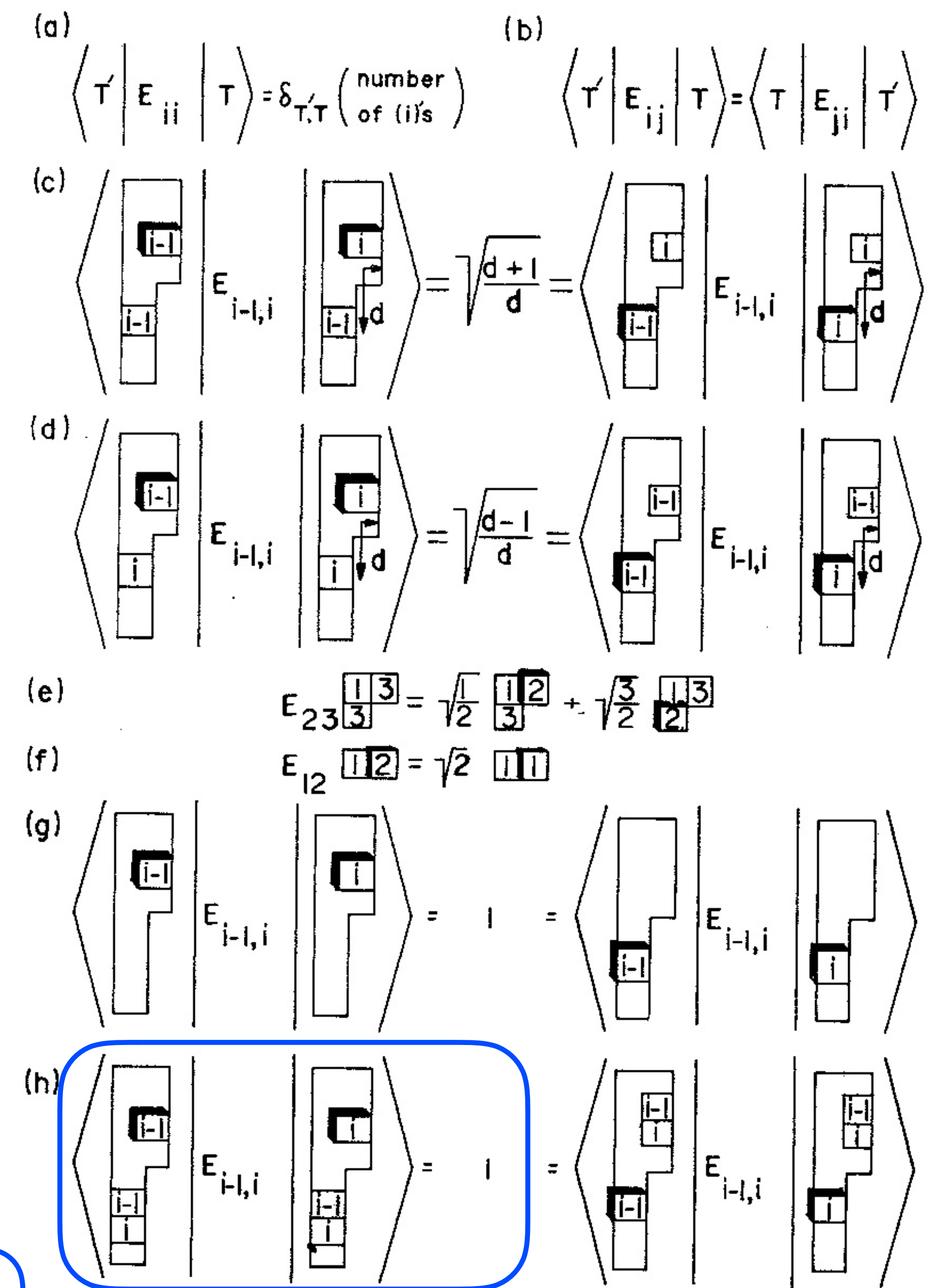
$$\left\langle\begin{matrix}12\\3\end{matrix}\right|E_{23}\left|\begin{matrix}13\\3\end{matrix}\right\rangle=\sqrt{\frac{1}{2}} \qquad \left\langle\begin{matrix}13\\2\end{matrix}\right|E_{23}\left|\begin{matrix}13\\3\end{matrix}\right\rangle=\sqrt{\frac{3}{2}}$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left\|{11 \atop 2}\right\rangle$	$\left\|{12 \atop 2}\right\rangle$	$\left\|{11 \atop 3}\right\rangle$	$\left\|{12 \atop 3}\right\rangle$	$\left\|{13 \atop 2}\right\rangle$	$\left\|{13 \atop 3}\right\rangle$	$\left\|{22 \atop 3}\right\rangle$	$\left\|{23 \atop 3}\right\rangle$
$\left\langle{11 \atop 2}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle{12 \atop 2}\right\|$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle{11 \atop 3}\right\|$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle{12 \atop 3}\right\|$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle{13 \atop 2}\right\|$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle{13 \atop 3}\right\|$						(11) (33) $1+2$	.	(12) 1
$\left\langle{22 \atop 3}\right\|$						.	(22) (33) $2+1$	(23) 1
$\left\langle{23 \atop 3}\right\|$								(22) (33) $1+2$

$$\left\langle{11 \atop 2}\middle|E_{11}\middle|{11 \atop 2}\right\rangle = 2 \qquad \left\langle{11 \atop 2}\middle|E_{22}\middle|{11 \atop 2}\right\rangle = 1$$



Sample applications of "Jawbone" formulae

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

$$\left\langle{11 \atop 2}\middle|E_{12}\middle|{12 \atop 2}\right\rangle = 1 \qquad \left\langle{11 \atop 2}\middle|E_{23}\middle|{11 \atop 3}\right\rangle = 1$$

$$\left\langle{12 \atop 2}\middle|E_{23}\middle|{13 \atop 2}\right\rangle = \sqrt{\frac{3}{2}} \qquad \left\langle{12 \atop 2}\middle|E_{23}\middle|{12 \atop 3}\right\rangle = \sqrt{\frac{1}{2}}$$

$$\left\langle{12 \atop 3}\middle|E_{12}\middle|{22 \atop 3}\right\rangle = \sqrt{2} \qquad \left\langle{12 \atop 3}\middle|E_{12}\middle|{22 \atop 3}\right\rangle = \sqrt{2}$$

$$\left\langle{12 \atop 3}\middle|E_{23}\middle|{13 \atop 3}\right\rangle = \sqrt{\frac{1}{2}} \qquad \left\langle{13 \atop 2}\middle|E_{23}\middle|{13 \atop 3}\right\rangle = \sqrt{\frac{3}{2}} \qquad \left\langle{22 \atop 3}\middle|E_{23}\middle|{23 \atop 3}\right\rangle = 1$$

AMOP reference links on page 2

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-½) 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 $\mathbf{e}_{jk}$ operator expressions for *(e-e)*-interaction matrix

Tensor tables are $(2\ell+1)$-by-$(2\ell+1)$ arrays $\left({}_p{}^k{}_q\right)$ giving $\mathbf{V}_q^k$ in terms of $\mathbf{E}_{p,q}$.
- Relating $\mathbf{V}_q^k$ to $\mathbf{E}_{m',m}$ by $\left({}_{m'}{}^k{}_m\right)$ arrays
- Atomic p-shell *ee*-interaction in elementary operator form

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

[2,1] tableau basis (from p.29) and matrices of $\mathbf{v}^2$ and $\mathbf{v}^2\bullet\mathbf{v}^2$ quadrupole
- ^4S, ^2P, and ^2D energy calculation of quartet and doublet (spin-½) p^3 orbits

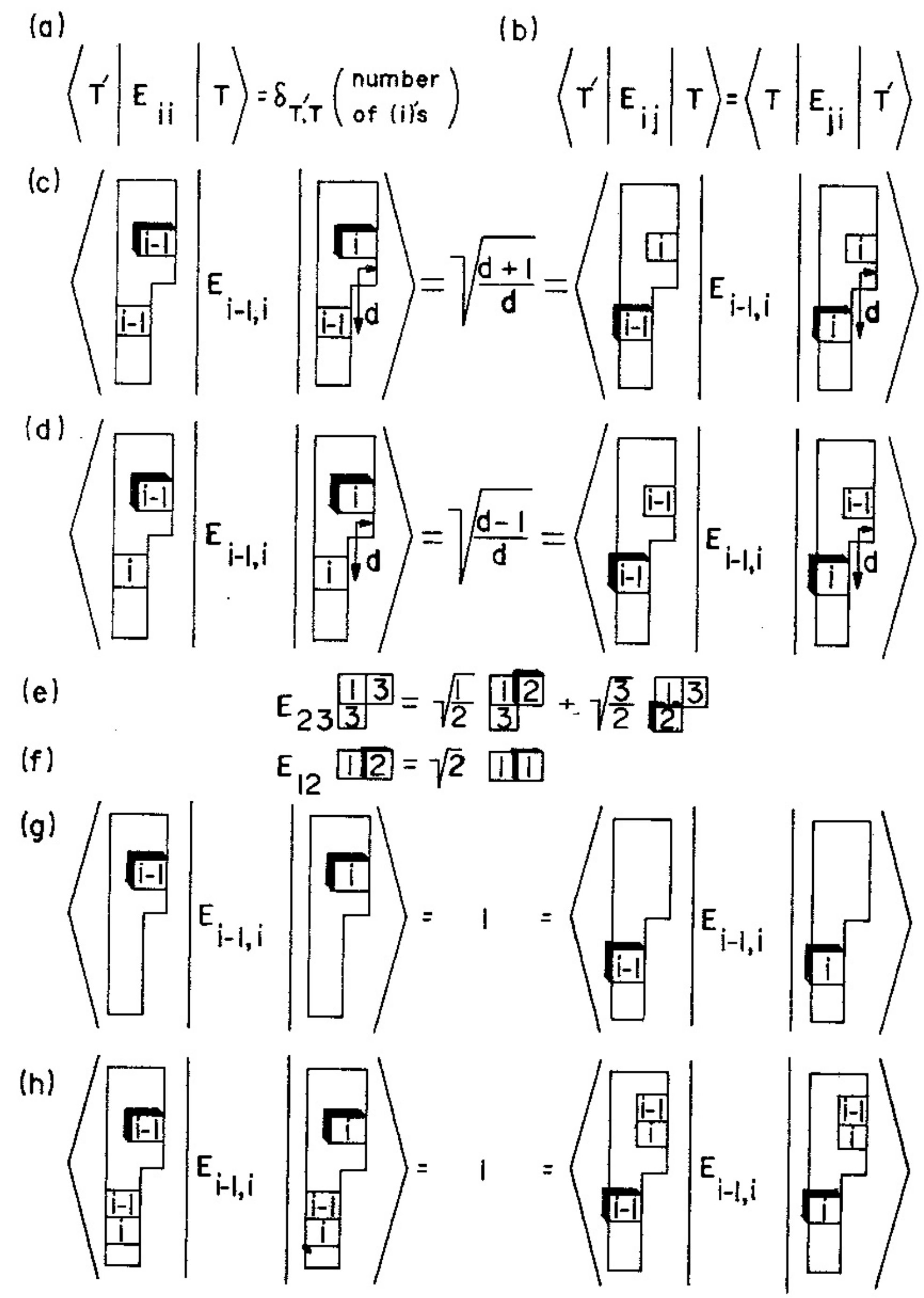
Corrected level diagrams Nitrogen p^3

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2 $\left\|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	*M=1* $\left\|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	*M=0* $\left\|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	*M=-1* $\left\|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	*M=-2* $\left\|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\|$		(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\|$		·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\|$				(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\|$				·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\|$						(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\|$						·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\|$								(22) (33) $1+2$

$$\left\langle\begin{matrix}11\\2\end{matrix}\middle|E_{11}\middle|\begin{matrix}11\\2\end{matrix}\right\rangle=2 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\middle|E_{22}\middle|\begin{matrix}11\\2\end{matrix}\right\rangle=1$$



Sample applications of "Jawbone" formulae

$$E_{13}=[E_{12},E_{23}]=E_{12}E_{23} \quad -E_{23}E_{12}$$

(2-jump $E_{i-2,i}$)

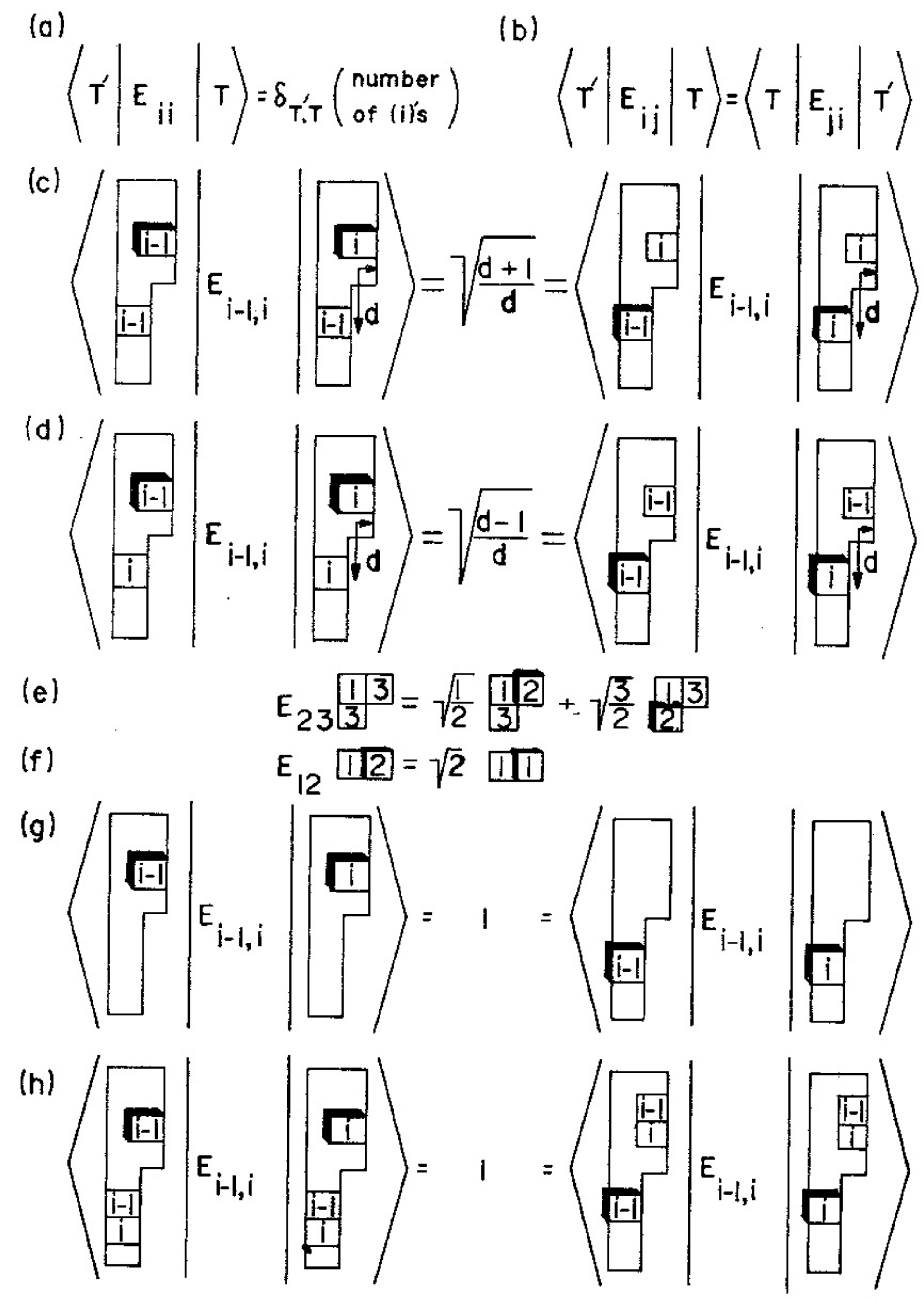
$$\left\langle\begin{matrix}11\\2\end{matrix}\middle|E_{13}\middle|\begin{matrix}12\\3\end{matrix}\right\rangle=??$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left\|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\|$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\|$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\|$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\|$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\|$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\|$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\|$								(22) (33) $1+2$

$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|E_{11}\left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle = 2 \qquad \left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|E_{22}\left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle = 1$$



Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

$$E_{13}=[E_{12},E_{23}]=E_{12}E_{23} \quad -E_{23}E_{12}$$

$$E_{13}\left|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle = E_{12}E_{23}\left|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle - E_{23}E_{12}\left|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$$

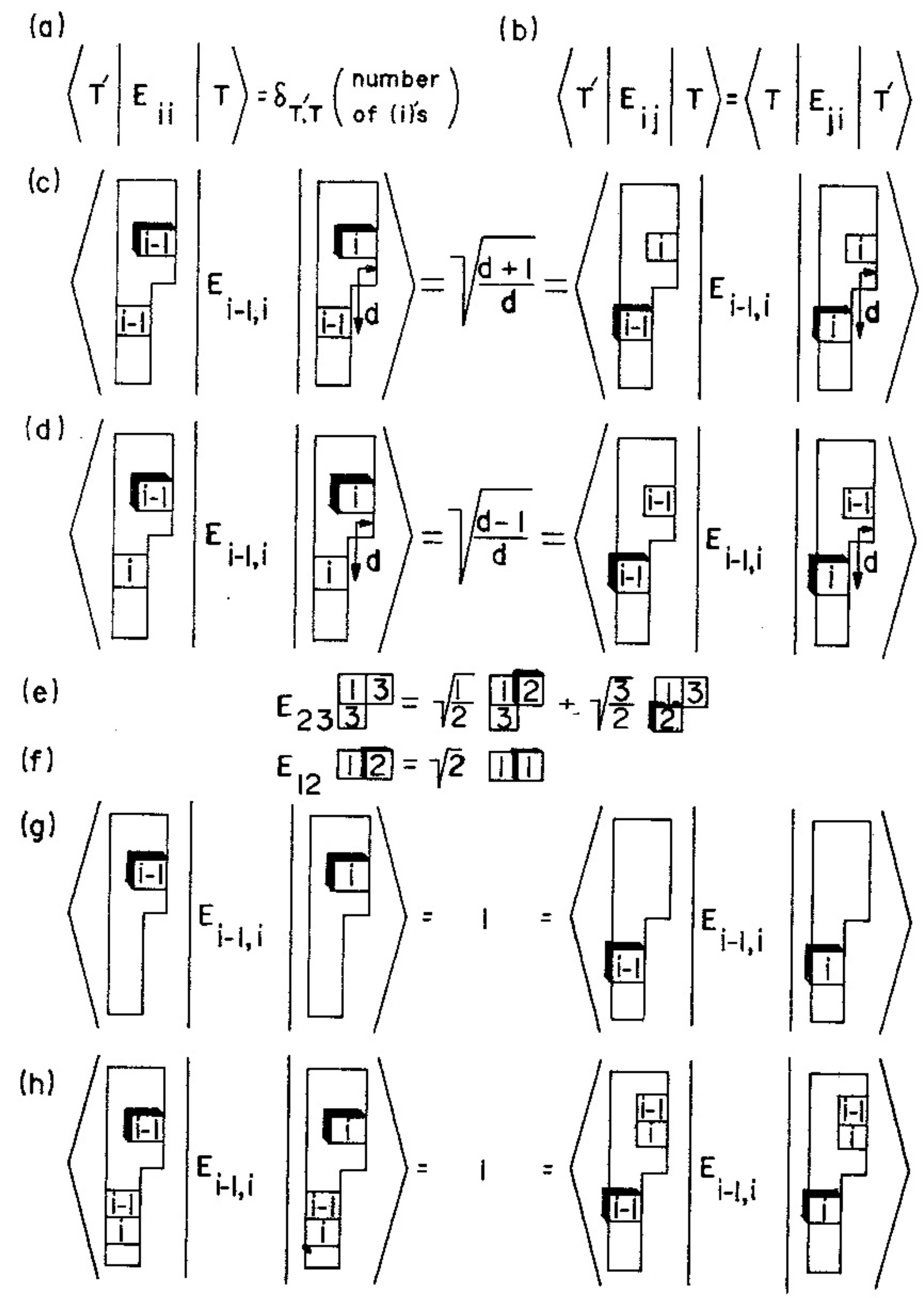
$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|E_{13}\left|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle = ??$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	$M=2$: $\left\|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$M=1$: $\left\|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$M=1$: $\left\|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$M=0$: $\left\|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$M=0$: $\left\|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$M=-1$: $\left\|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$M=-1$: $\left\|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$M=-2$: $\left\|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\|$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\|$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\|$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\|$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\|$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\|$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\|$								(22) (33) $1+2$

$$\left\langle\begin{matrix}11\\2\end{matrix}\right|E_{11}\left|\begin{matrix}11\\2\end{matrix}\right\rangle=2 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\right|E_{22}\left|\begin{matrix}11\\2\end{matrix}\right\rangle=1$$



Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

$$E_{13}=[E_{12},E_{23}]=E_{12}E_{23} \quad -E_{23}E_{12}$$

$$E_{13}\left|\begin{matrix}12\\3\end{matrix}\right\rangle = E_{12}E_{23}\left|\begin{matrix}12\\3\end{matrix}\right\rangle - E_{23}E_{12}\left|\begin{matrix}12\\3\end{matrix}\right\rangle$$

$$= E_{12}\sqrt{\frac{1}{2}}\left|\begin{matrix}12\\2\end{matrix}\right\rangle - E_{23}\sqrt{2}\left|\begin{matrix}11\\3\end{matrix}\right\rangle$$

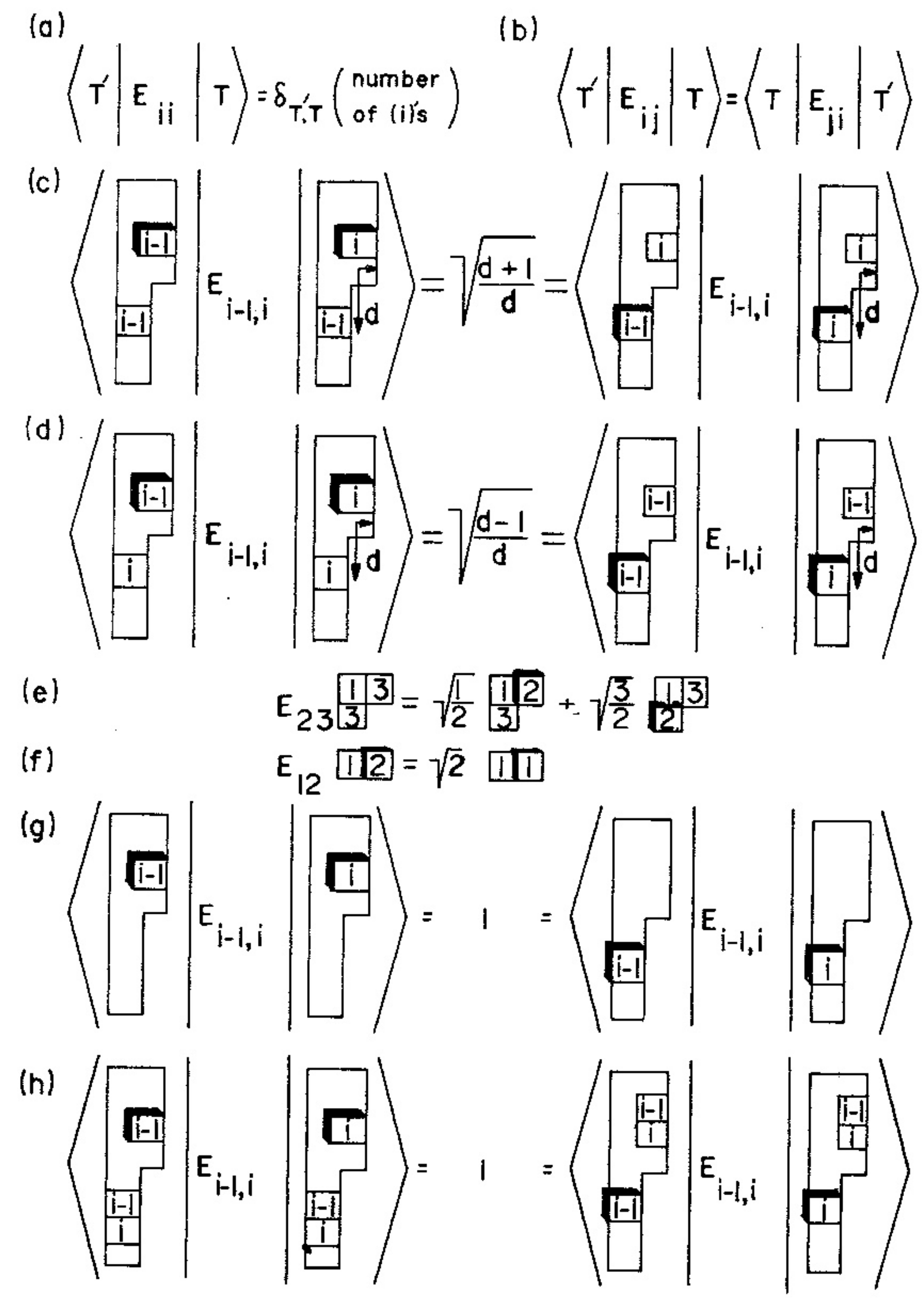
$$\left\langle\begin{matrix}11\\2\end{matrix}\right|E_{13}\left|\begin{matrix}12\\3\end{matrix}\right\rangle = ??$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2: $\left|{}^{11}_{2}\right\rangle$	M=1: $\left|{}^{12}_{2}\right\rangle$	M=1: $\left|{}^{11}_{3}\right\rangle$	M=0: $\left|{}^{12}_{3}\right\rangle$	M=0: $\left|{}^{13}_{2}\right\rangle$	M=-1: $\left|{}^{13}_{3}\right\rangle$	M=-1: $\left|{}^{22}_{3}\right\rangle$	M=-2: $\left|{}^{23}_{3}\right\rangle$
$\left\langle{}^{11}_{2}\right|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle{}^{12}_{2}\right|$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle{}^{11}_{3}\right|$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle{}^{12}_{3}\right|$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle{}^{13}_{2}\right|$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle{}^{13}_{3}\right|$						(11) (33) $1+2$	.	(12) 1
$\left\langle{}^{22}_{3}\right|$						.	(22) (33) $2+1$	(23) 1
$\left\langle{}^{23}_{3}\right|$								(22) (33) $1+2$

$$\left\langle{}^{11}_{2}\right|E_{11}\left|{}^{11}_{2}\right\rangle = 2 \qquad \left\langle{}^{11}_{2}\right|E_{22}\left|{}^{11}_{2}\right\rangle = 1$$



Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} \quad - E_{23}E_{12}$$

$$E_{13}\left|{}^{12}_{3}\right\rangle = E_{12}E_{23}\left|{}^{12}_{3}\right\rangle - E_{23}E_{12}\left|{}^{12}_{3}\right\rangle$$

$$= E_{12}\sqrt{\frac{1}{2}}\left|{}^{12}_{2}\right\rangle - E_{23}\sqrt{2}\left|{}^{11}_{3}\right\rangle$$

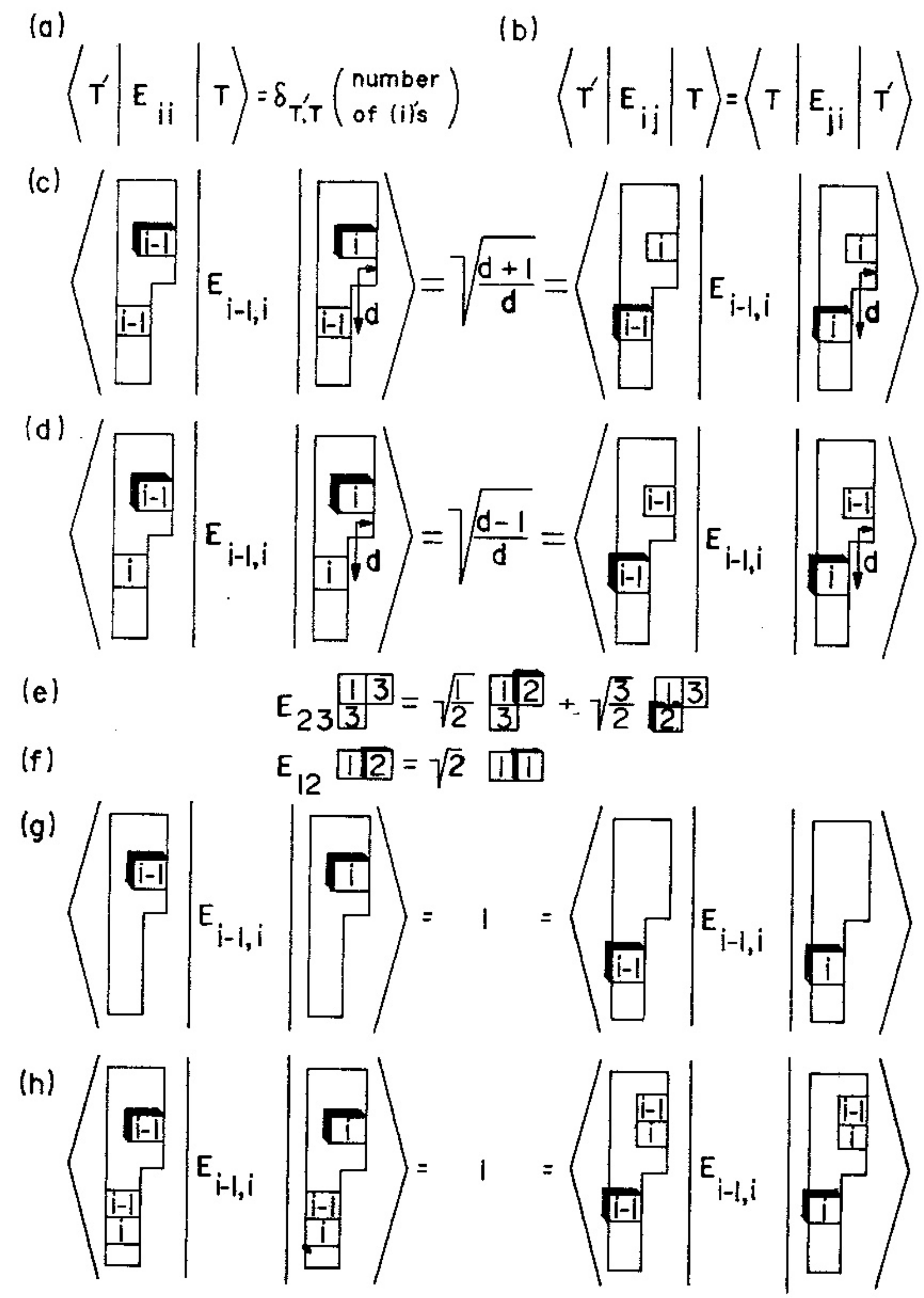
$$\left\langle{}^{11}_{2}\right|E_{13}\left|{}^{12}_{3}\right\rangle = ??$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

E_{jk} =

	M=2	M=1		M=0		M=-1		M=-2
	$\left\|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\|$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\|$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\|$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\|$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\|$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\|$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\|$								(22) (33) $1+2$

$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|E_{11}\left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle=2 \qquad \left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|E_{22}\left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle=1$$



Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

$$E_{13}=[E_{12},E_{23}]=E_{12}E_{23}\quad -E_{23}E_{12}$$

$$E_{13}\left|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle = E_{12}E_{23}\left|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle - E_{23}E_{12}\left|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$$

$$= E_{12}\sqrt{\frac{1}{2}}\left|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle - E_{23}\sqrt{2}\left|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$$

$$= 1\sqrt{\frac{1}{2}}\left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle - 1\sqrt{2}\left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$$

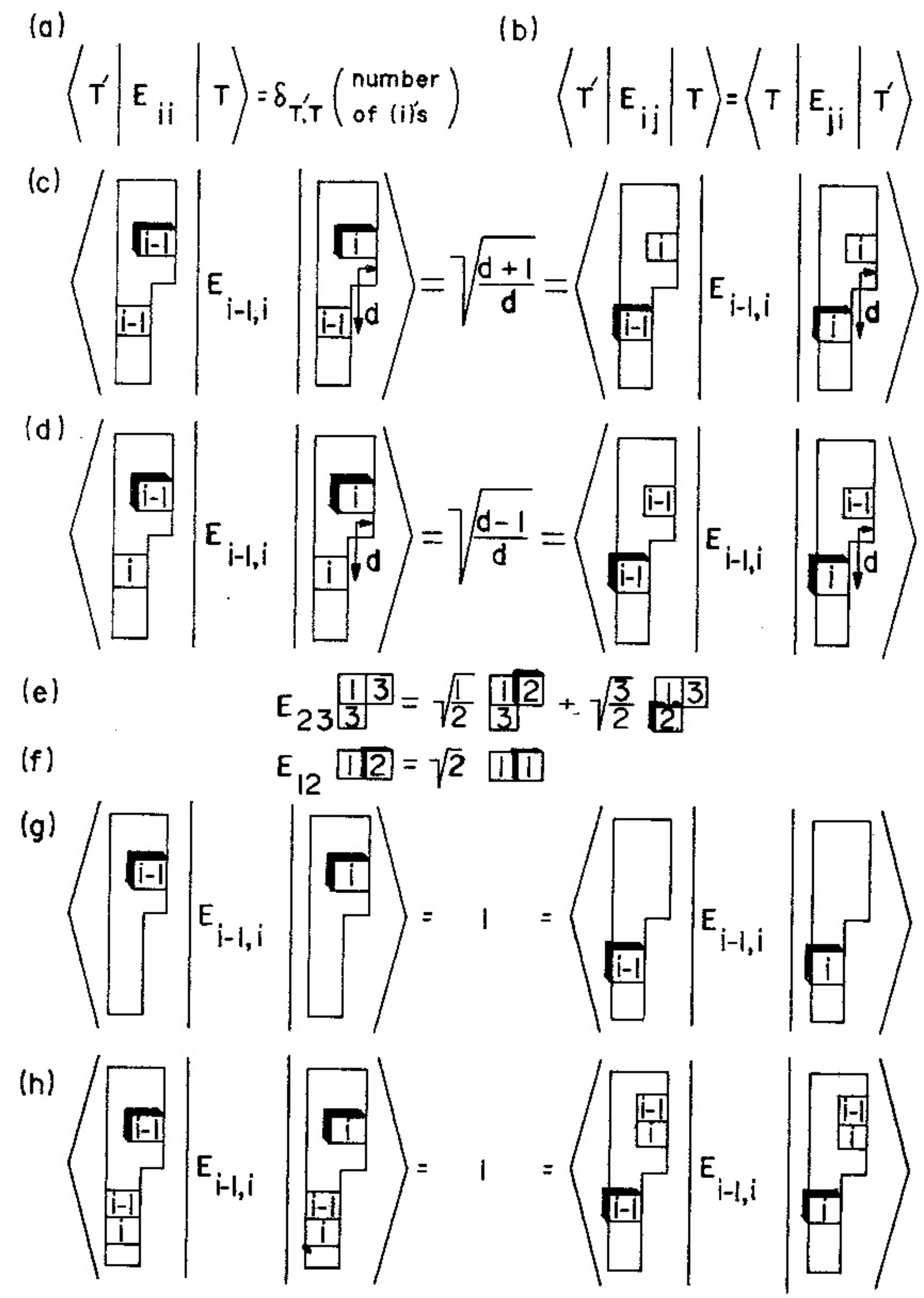
$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|E_{13}\left|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle = ??$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\vert$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\vert$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\vert$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\vert$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\vert$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\vert$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\vert$								(22) (33) $1+2$

$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert E_{11}\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle = 2 \qquad \left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert E_{22}\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle = 1$$



Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} \quad - E_{23}E_{12}$$

$$E_{13}\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle = E_{12}E_{23}\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle - E_{23}E_{12}\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$$

$$= E_{12}\sqrt{\frac{1}{2}}\left\vert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle - E_{23}\sqrt{2}\left\vert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$$

$$= 1\sqrt{\frac{1}{2}}\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle - 1\sqrt{2}\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$$

$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert E_{13}\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle = ??$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left\|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\|$		(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\|$		·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\|$				(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\|$				·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\|$						(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\|$						·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\|$								(22) (33) $1+2$

$$\left\langle\begin{matrix}11\\2\end{matrix}\middle|E_{11}\middle|\begin{matrix}11\\2\end{matrix}\right\rangle = 2 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\middle|E_{22}\middle|\begin{matrix}11\\2\end{matrix}\right\rangle = 1$$

Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

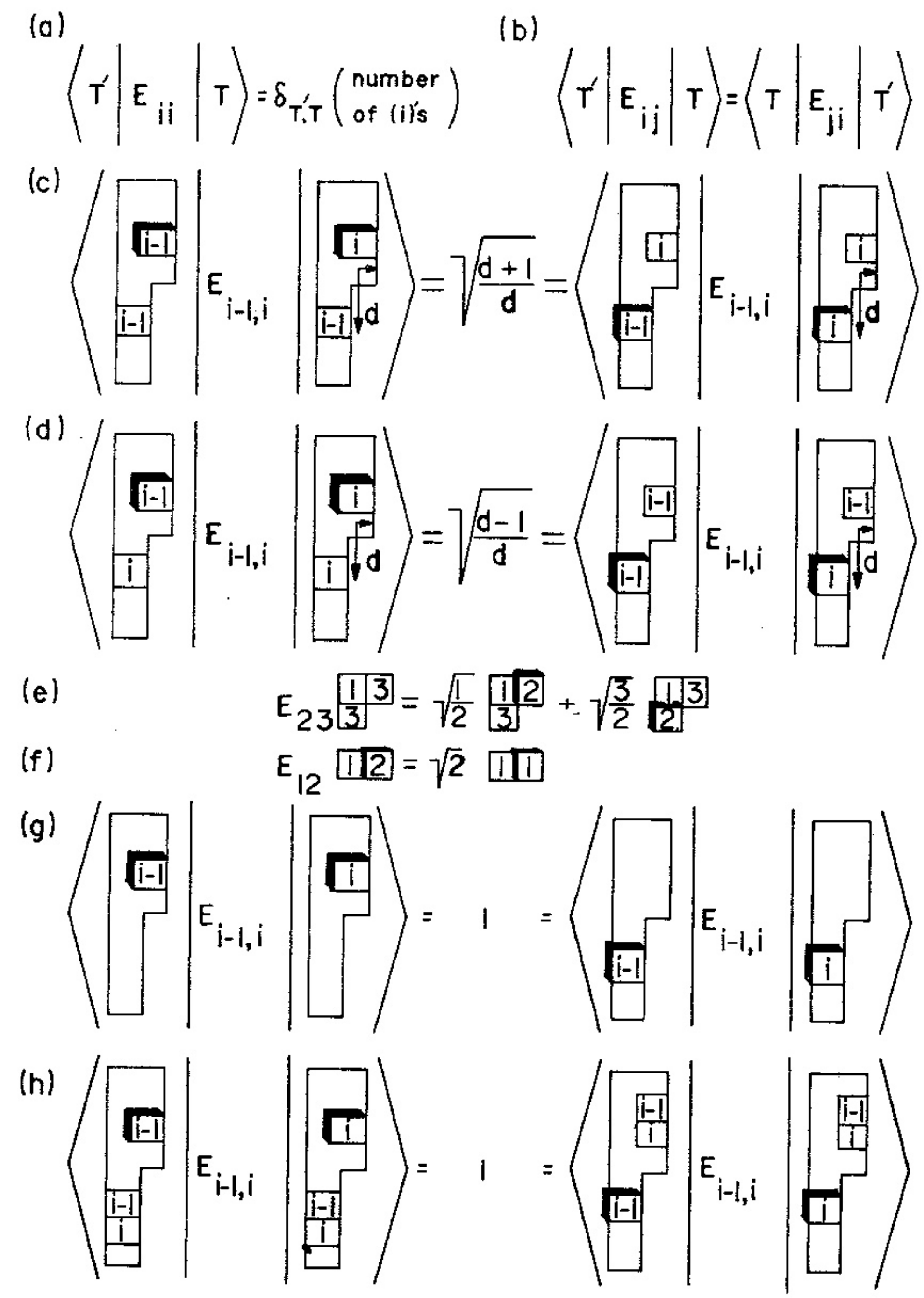
$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} \quad - E_{23}E_{12}$$

$$E_{13}\left|\begin{matrix}12\\3\end{matrix}\right\rangle = E_{12}E_{23}\left|\begin{matrix}12\\3\end{matrix}\right\rangle - E_{23}E_{12}\left|\begin{matrix}12\\3\end{matrix}\right\rangle$$

$$= E_{12}\sqrt{\frac{1}{2}}\left|\begin{matrix}12\\2\end{matrix}\right\rangle - E_{23}\sqrt{2}\left|\begin{matrix}11\\3\end{matrix}\right\rangle$$

$$= 1\sqrt{\frac{1}{2}}\left|\begin{matrix}11\\2\end{matrix}\right\rangle - 1\sqrt{2}\left|\begin{matrix}11\\2\end{matrix}\right\rangle$$

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

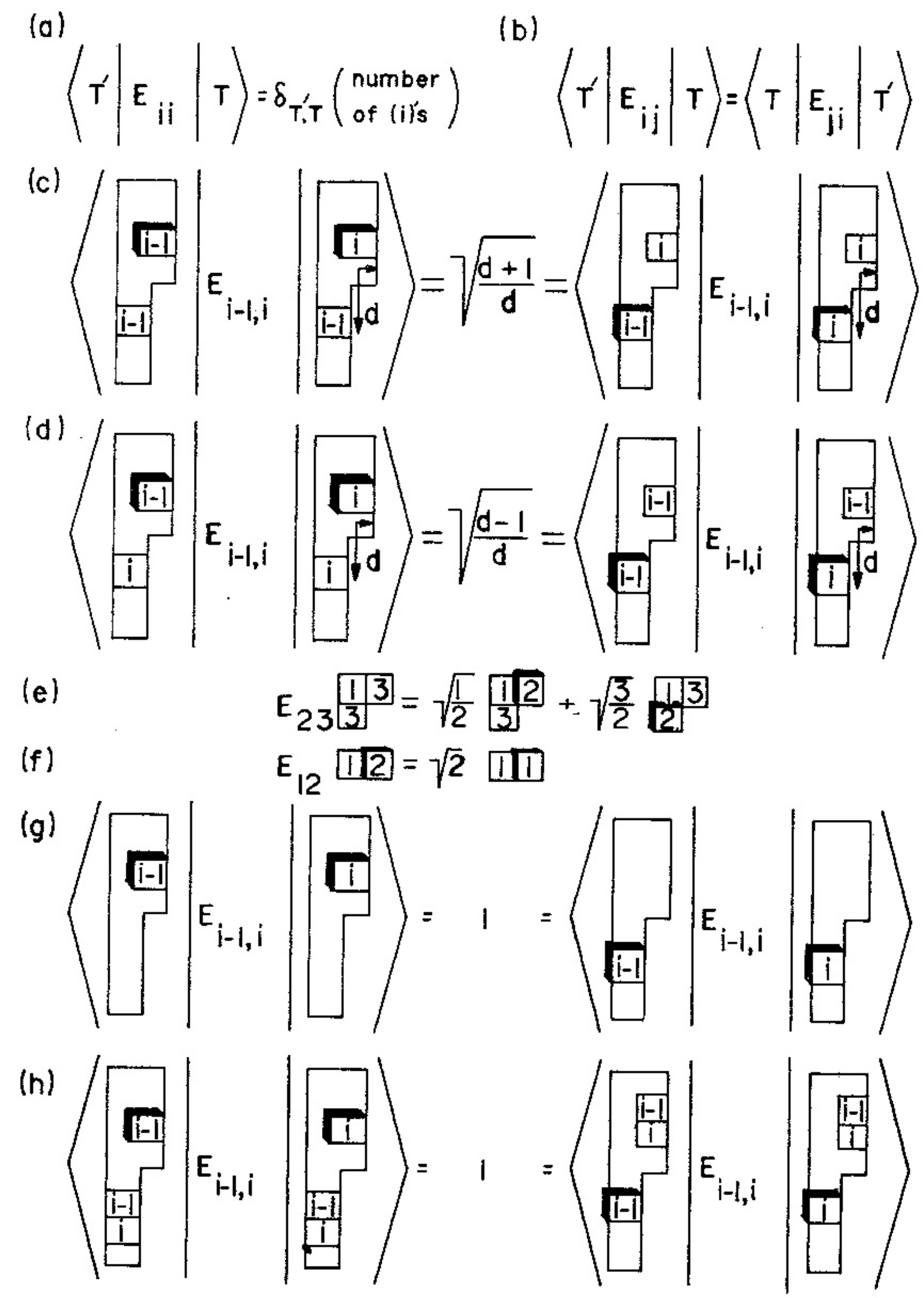


Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	*M=1*		*M=0*		*M=-1*		*M=-2*
	$\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\vert$		(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\vert$		·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\vert$				(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\vert$				·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\vert$						(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\vert$						·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\vert$								(22) (33) $1+2$

$$\left\langle\begin{matrix}11\\2\end{matrix}\right| E_{11} \left|\begin{matrix}11\\2\end{matrix}\right\rangle = 2 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\right| E_{22} \left|\begin{matrix}11\\2\end{matrix}\right\rangle = 1$$



Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} \quad -E_{23}E_{12}$$

$$E_{13}\left|\begin{matrix}13\\2\end{matrix}\right\rangle \quad = E_{12}E_{23}\left|\begin{matrix}13\\2\end{matrix}\right\rangle - E_{23}E_{12}\left|\begin{matrix}13\\2\end{matrix}\right\rangle$$

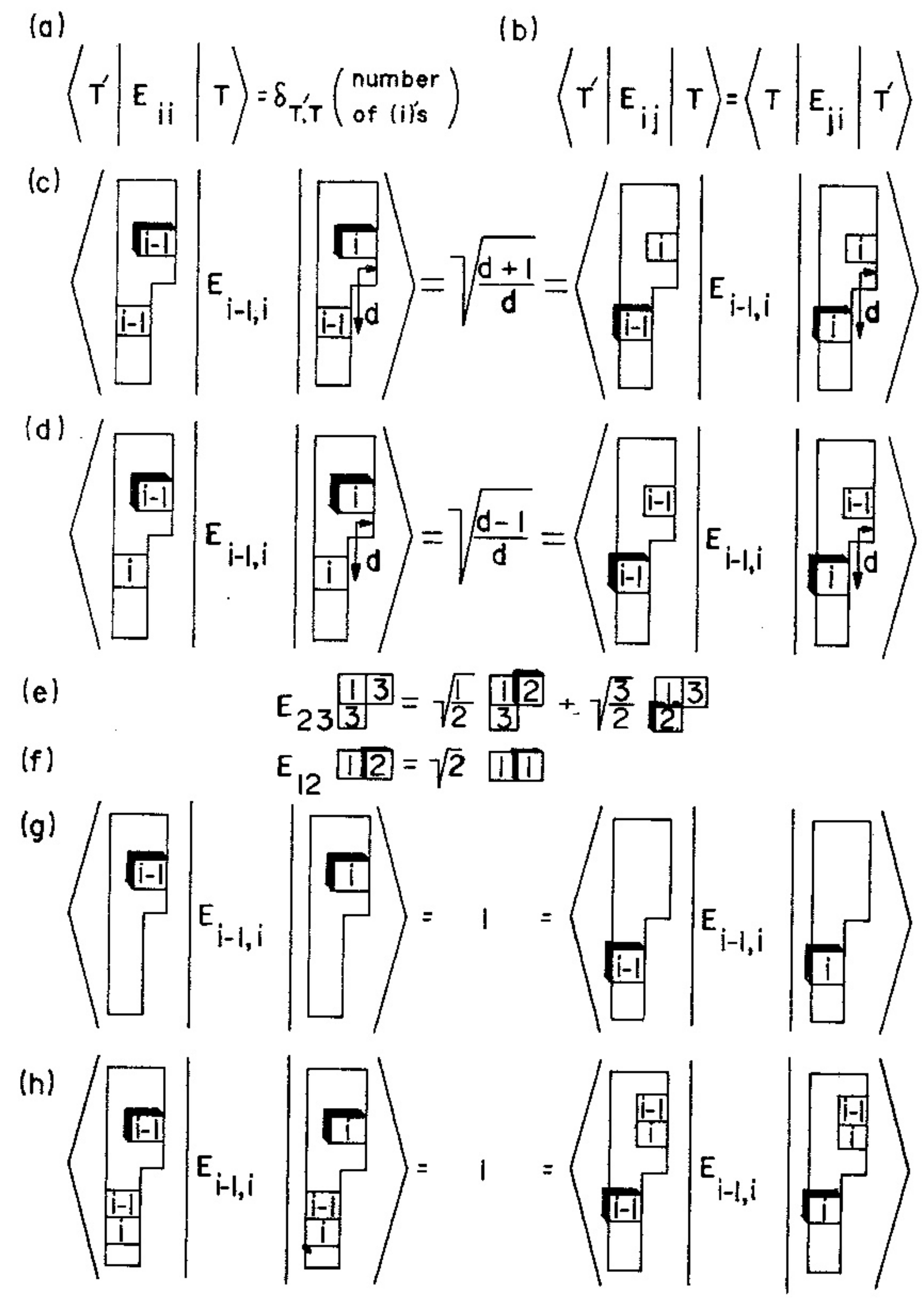
$$\left\langle\begin{matrix}11\\2\end{matrix}\right| E_{13} \left|\begin{matrix}13\\2\end{matrix}\right\rangle = ??$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left\|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\|$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\|$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\|$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\|$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\|$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\|$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\|$								(22) (33) $1+2$

$$\left\langle\begin{matrix}11\\2\end{matrix}\right|E_{11}\left|\begin{matrix}11\\2\end{matrix}\right\rangle=2 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\right|E_{22}\left|\begin{matrix}11\\2\end{matrix}\right\rangle=1$$



Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

$$E_{13}=[E_{12},E_{23}]=E_{12}E_{23}\quad -E_{23}E_{12}$$

$$E_{13}\left|\begin{matrix}13\\2\end{matrix}\right\rangle = E_{12}E_{23}\left|\begin{matrix}13\\2\end{matrix}\right\rangle - E_{23}E_{12}\left|\begin{matrix}13\\2\end{matrix}\right\rangle$$

$$= E_{12}\sqrt{\frac{3}{2}}\left|\begin{matrix}12\\2\end{matrix}\right\rangle - E_{23}0\left|\begin{matrix}13\\1\end{matrix}\right\rangle$$

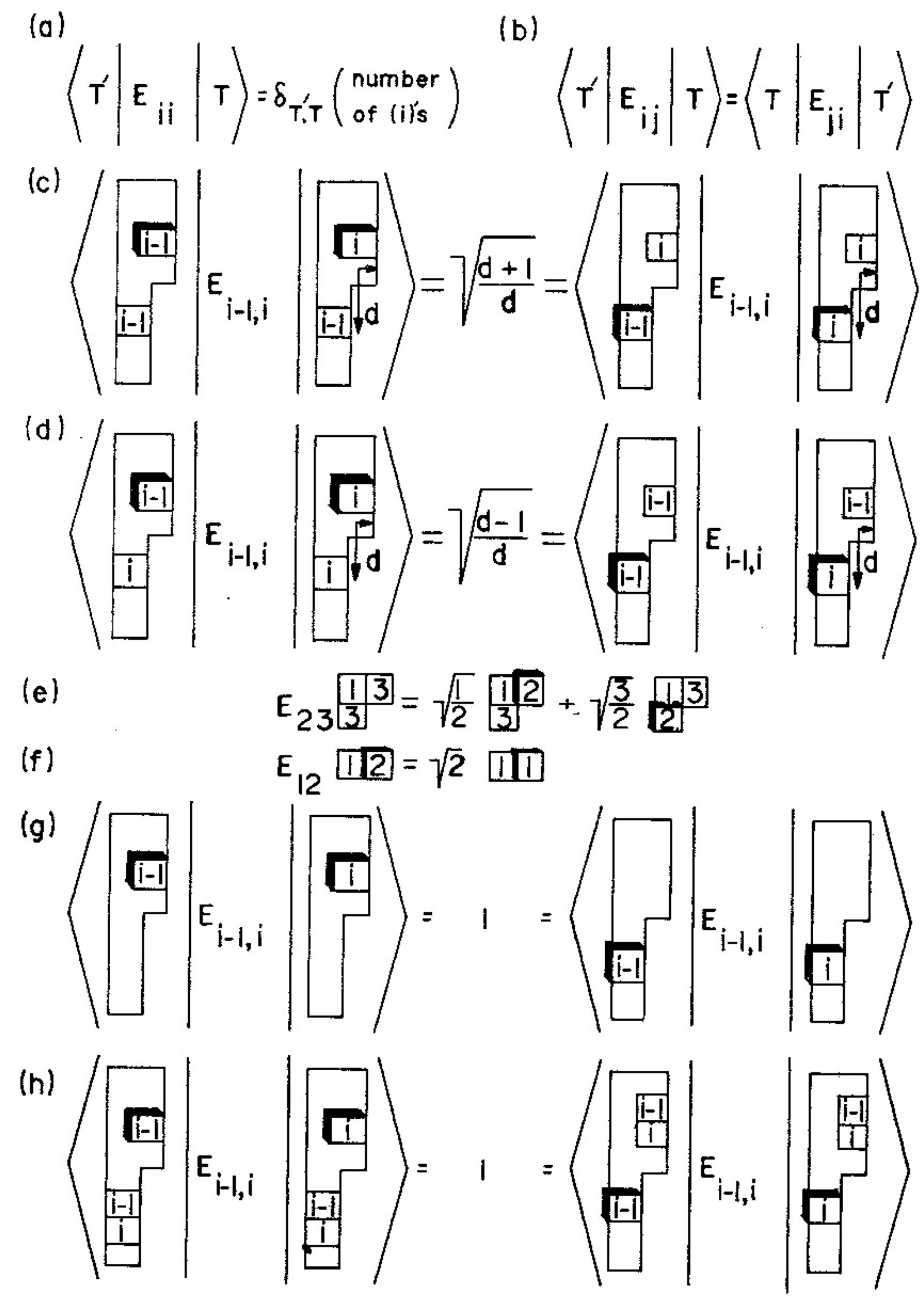
$$\left\langle\begin{matrix}11\\2\end{matrix}\right|E_{13}\left|\begin{matrix}13\\2\end{matrix}\right\rangle = ??$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2: $\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	M=1: $\left\vert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	M=1: $\left\vert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	M=0: $\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	M=0: $\left\vert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	M=-1: $\left\vert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	M=-1: $\left\vert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	M=-2: $\left\vert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\vert$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\vert$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\vert$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\vert$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\vert$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\vert$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\vert$								(22) (33) $1+2$

$$\left\langle\begin{matrix}11\\2\end{matrix}\right\vert E_{11}\left\vert\begin{matrix}11\\2\end{matrix}\right\rangle = 2 \qquad \left\langle\begin{matrix}11\\2\end{matrix}\right\vert E_{22}\left\vert\begin{matrix}11\\2\end{matrix}\right\rangle = 1$$



Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} \quad -E_{23}E_{12}$$

$$E_{13}\left\vert\begin{matrix}13\\2\end{matrix}\right\rangle = E_{12}E_{23}\left\vert\begin{matrix}13\\2\end{matrix}\right\rangle - E_{23}E_{12}\left\vert\begin{matrix}13\\2\end{matrix}\right\rangle$$

$$= E_{12}\sqrt{\frac{3}{2}}\left\vert\begin{matrix}12\\2\end{matrix}\right\rangle - E_{23}0\left\vert\begin{matrix}13\\1\end{matrix}\right\rangle$$

$$= 1 \sqrt{\frac{3}{2}}\left\vert\begin{matrix}11\\2\end{matrix}\right\rangle - \quad 0$$

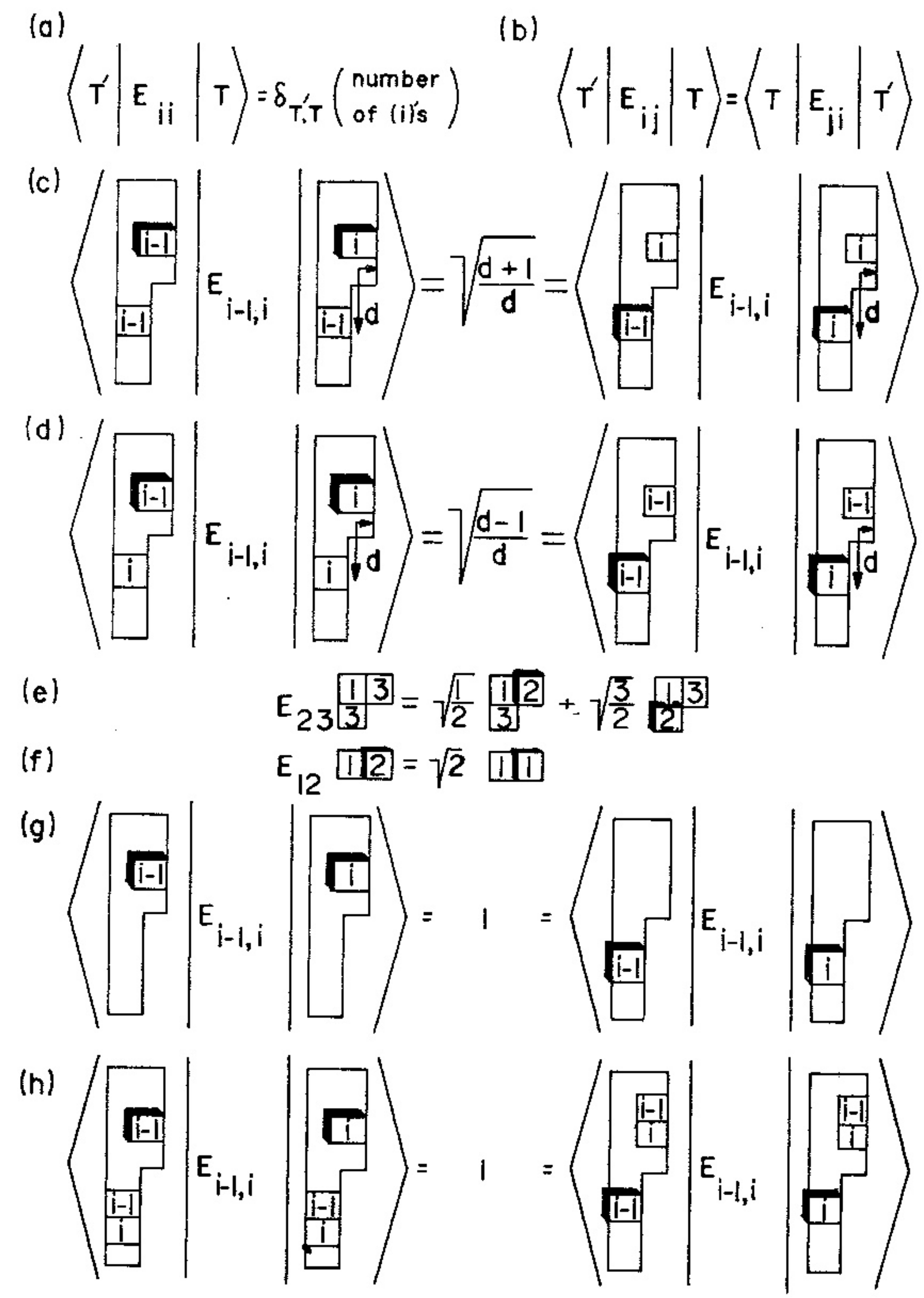
$$\left\langle\begin{matrix}11\\2\end{matrix}\right\vert E_{13}\left\vert\begin{matrix}13\\2\end{matrix}\right\rangle = ??$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left\|{11 \atop 2}\right\rangle$	$\left\|{12 \atop 2}\right\rangle$	$\left\|{11 \atop 3}\right\rangle$	$\left\|{12 \atop 3}\right\rangle$	$\left\|{13 \atop 2}\right\rangle$	$\left\|{13 \atop 3}\right\rangle$	$\left\|{22 \atop 3}\right\rangle$	$\left\|{23 \atop 3}\right\rangle$
$\left\langle{11 \atop 2}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle{12 \atop 2}\right\|$		(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle{11 \atop 3}\right\|$		·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle{12 \atop 3}\right\|$				(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle{13 \atop 2}\right\|$				·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle{13 \atop 3}\right\|$						(11) (33) $1+2$	·	(12) 1
$\left\langle{22 \atop 3}\right\|$						·	(22) (33) $2+1$	(23) 1
$\left\langle{23 \atop 3}\right\|$								(22) (33) $1+2$

$$\left\langle{11 \atop 2}\right| E_{11} \left|{11 \atop 2}\right\rangle = 2 \qquad \left\langle{11 \atop 2}\right| E_{22} \left|{11 \atop 2}\right\rangle = 1$$



Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} \quad - E_{23}E_{12}$$

$$E_{13}\left|{13 \atop 2}\right\rangle = E_{12}E_{23}\left|{13 \atop 2}\right\rangle - E_{23}E_{12}\left|{13 \atop 2}\right\rangle$$

$$= E_{12}\sqrt{\frac{3}{2}}\left|{12 \atop 2}\right\rangle - E_{23}0\left|{13 \atop 1}\right\rangle$$

$$= 1 \sqrt{\frac{3}{2}}\left|{11 \atop 2}\right\rangle - 0$$

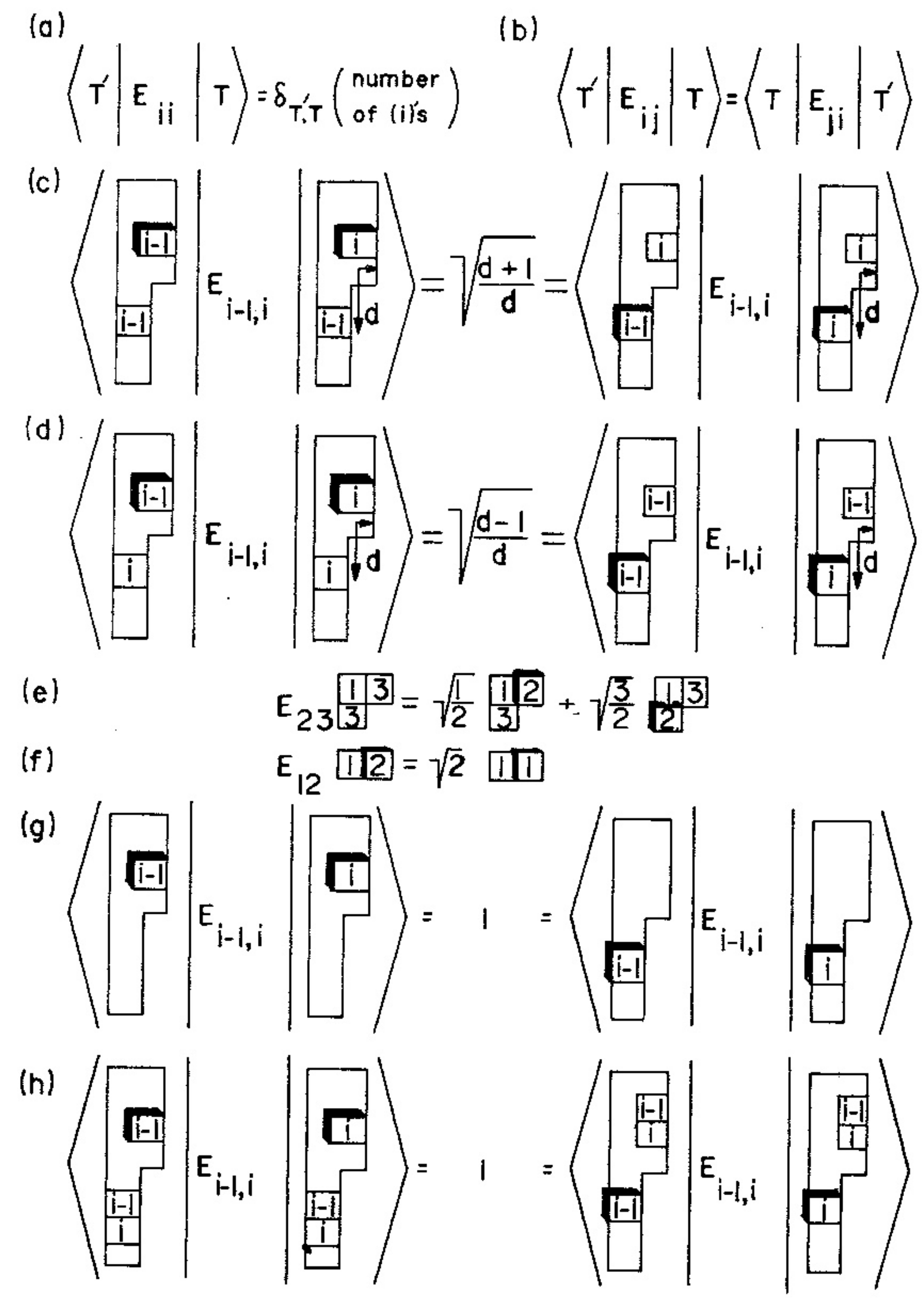
$$\left\langle{11 \atop 2}\right| E_{13} \left|{13 \atop 2}\right\rangle = \sqrt{\frac{3}{2}}$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	*M=1*		*M=0*		*M=-1*		*M=-2*
	$\vert\begin{smallmatrix}11\\2\end{smallmatrix}\rangle$	$\vert\begin{smallmatrix}12\\2\end{smallmatrix}\rangle$	$\vert\begin{smallmatrix}11\\3\end{smallmatrix}\rangle$	$\vert\begin{smallmatrix}12\\3\end{smallmatrix}\rangle$	$\vert\begin{smallmatrix}13\\2\end{smallmatrix}\rangle$	$\vert\begin{smallmatrix}13\\3\end{smallmatrix}\rangle$	$\vert\begin{smallmatrix}22\\3\end{smallmatrix}\rangle$	$\vert\begin{smallmatrix}23\\3\end{smallmatrix}\rangle$
$\langle\begin{smallmatrix}11\\2\end{smallmatrix}\vert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\langle\begin{smallmatrix}12\\2\end{smallmatrix}\vert$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\langle\begin{smallmatrix}11\\3\end{smallmatrix}\vert$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\langle\begin{smallmatrix}12\\3\end{smallmatrix}\vert$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\langle\begin{smallmatrix}13\\2\end{smallmatrix}\vert$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\langle\begin{smallmatrix}13\\3\end{smallmatrix}\vert$						(11) (33) $1+2$	.	(12) 1
$\langle\begin{smallmatrix}22\\3\end{smallmatrix}\vert$						.	(22) (33) $2+1$	(23) 1
$\langle\begin{smallmatrix}23\\3\end{smallmatrix}\vert$								(22) (33) $1+2$

$$\left\langle \begin{smallmatrix}11\\2\end{smallmatrix} \middle| E_{11} \middle| \begin{smallmatrix}11\\2\end{smallmatrix} \right\rangle = 2 \qquad \left\langle \begin{smallmatrix}11\\2\end{smallmatrix} \middle| E_{22} \middle| \begin{smallmatrix}11\\2\end{smallmatrix} \right\rangle = 1$$



Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} \quad -E_{23}E_{12}$$

$$E_{13}\left|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle = E_{12}E_{23}\left|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle - E_{23}E_{12}\left|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$$

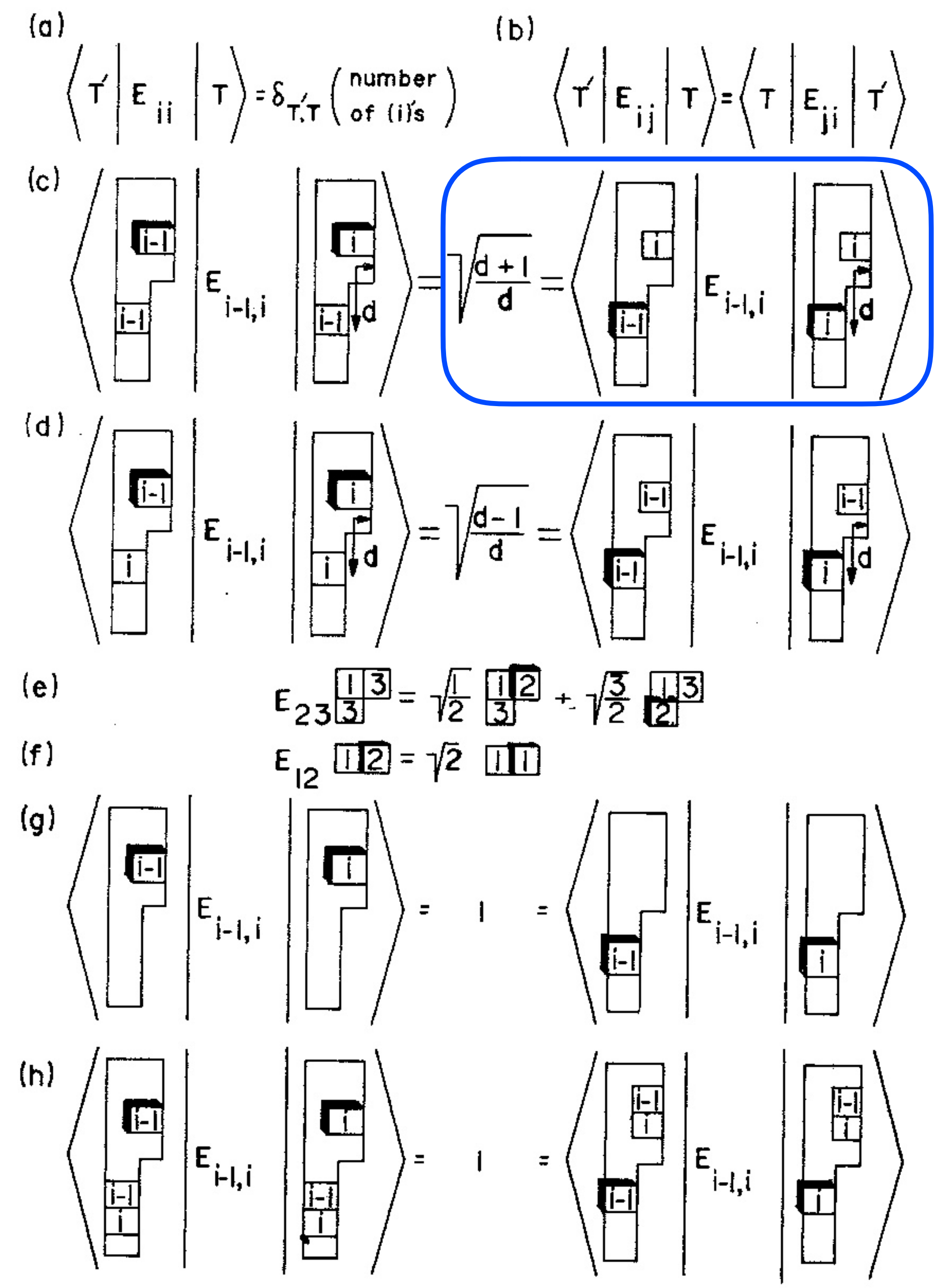
$$\left\langle \begin{smallmatrix}12\\2\end{smallmatrix} \middle| E_{13} \middle| \begin{smallmatrix}22\\3\end{smallmatrix} \right\rangle = ??$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left\lvert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\rvert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\rvert$		(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\rvert$		.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\rvert$				(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\rvert$				.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\rvert$						(11) (33) $1+2$	.	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\rvert$						.	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\rvert$								(22) (33) $1+2$

$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\rvert E_{11}\left\lvert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle = 2 \qquad \left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\rvert E_{22}\left\lvert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle = 1$$



Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} \quad - E_{23}E_{12}$$

$$E_{13}\left\lvert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle = E_{12}E_{23}\left\lvert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle - E_{23}E_{12}\left\lvert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$$

$$E_{13}\left\lvert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle = 0 \quad - E_{23}\sqrt{2}\left\lvert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$$

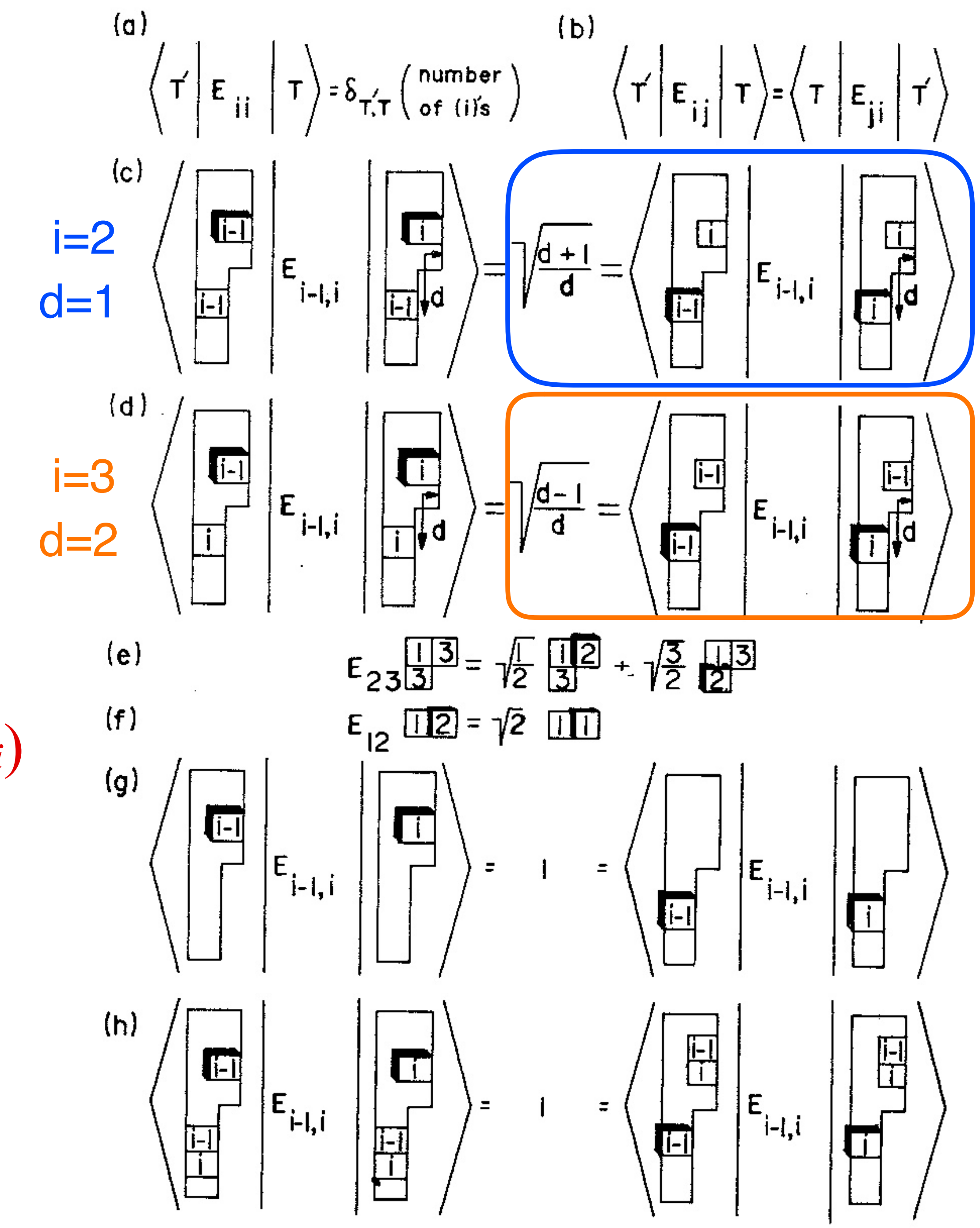
$$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\rvert E_{13}\left\lvert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle = ??$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left\lvert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\rvert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\rvert$		(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\rvert$		·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\rvert$				(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\rvert$				·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\rvert$						(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\rvert$						·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\rvert$								(22) (33) $1+2$

$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right| E_{11} \left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle = 2 \qquad \left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right| E_{22} \left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle = 1$$



Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

$$E_{13} = [E_{12}, E_{23}] = E_{12}E_{23} - E_{23}E_{12}$$

$$E_{13}\left|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle = E_{12}E_{23}\left|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle - E_{23}E_{12}\left|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$$

$$E_{13}\left|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle = 0 - E_{23}\sqrt{2}\left|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$$

$$E_{13}\left|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle = 0 - \frac{1}{\sqrt{2}}\sqrt{2}\left|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$$

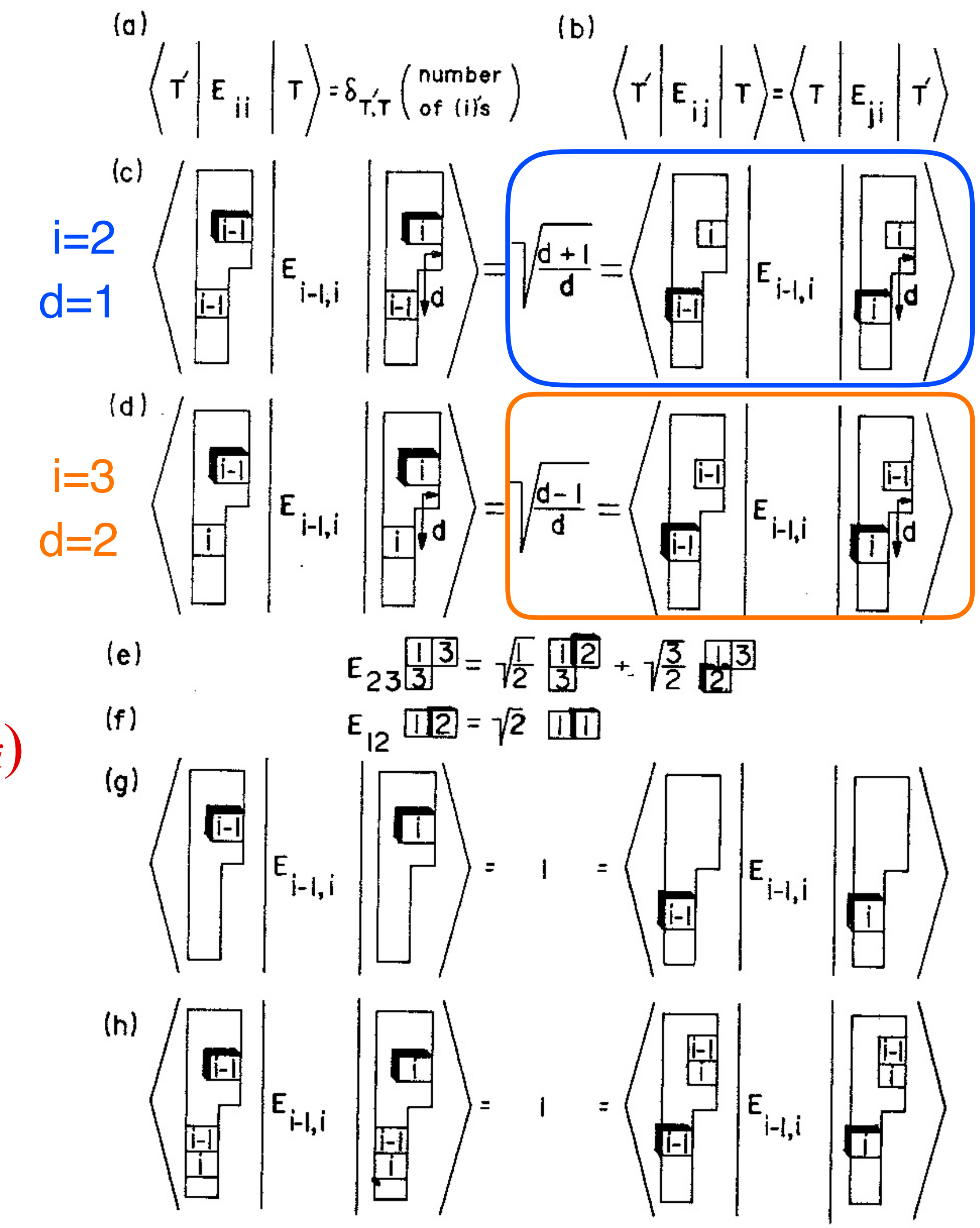
$$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right| E_{13} \left|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle = ??$$

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$E_{jk} =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right|$		(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right|$		·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right|$				(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right|$				·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right|$						(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right|$						·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right|$								(22) (33) $1+2$

$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|E_{11}\left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle=2 \qquad \left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|E_{22}\left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle=1$$



Sample applications of "Jawbone" formulae

(2-jump $E_{i-2,i}$)

$$E_{13}=[E_{12},E_{23}]=E_{12}E_{23}-E_{23}E_{12}$$

$$E_{13}\left|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle = E_{12}E_{23}\left|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle - E_{23}E_{12}\left|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$$

$$E_{13}\left|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle = 0 - E_{23}\sqrt{2}\left|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$$

$$E_{13}\left|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle = 0 - \frac{1}{\sqrt{2}}\sqrt{2}\left|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$$

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

AMOP reference links on page 2

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-½) 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 $\mathbf{e}_{jk}$ operator expressions for *(e-e)*-interaction matrix

Tensor tables are $(2\ell+1)$-by-$(2\ell+1)$ arrays $\left({}_p{}^k{}_q\right)$ giving $\mathbf{V}_q^k$ in terms of $\mathbf{E}_{p,q}$.
- Relating $\mathbf{V}_q^k$ to $\mathbf{E}_{m',m}$ by $\left({}_{m'}{}^k{}_m\right)$ arrays
- Atomic p-shell *ee*-interaction in elementary operator form

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

[2,1] tableau basis (from p.29) and matrices of $\mathbf{v}^2$ and $\mathbf{v}^2\bullet\mathbf{v}^2$ quadrupole
- ${}^4S, {}^2P$, and ${}^2D$ energy calculation of quartet and doublet (spin-½) p^3 orbits

Corrected level diagrams Nitrogen p^3

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

$\langle L_- \diagdown E_{jk} \rangle =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left\lvert \begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\lvert \begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\lvert \begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\lvert \begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\lvert \begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\lvert \begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\lvert \begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\lvert \begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle \begin{smallmatrix}11\\2\end{smallmatrix}\right\rvert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle \begin{smallmatrix}12\\2\end{smallmatrix}\right\rvert$		(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle \begin{smallmatrix}11\\3\end{smallmatrix}\right\rvert$		·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle \begin{smallmatrix}12\\3\end{smallmatrix}\right\rvert$				(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle \begin{smallmatrix}13\\2\end{smallmatrix}\right\rvert$				·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle \begin{smallmatrix}13\\3\end{smallmatrix}\right\rvert$						(11) (33) $1+2$	·	(12) 1
$\left\langle \begin{smallmatrix}22\\3\end{smallmatrix}\right\rvert$						·	(22) (33) $2+1$	(23) 1
$\left\langle \begin{smallmatrix}23\\3\end{smallmatrix}\right\rvert$								(22) (33) $1+2$

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

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

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

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

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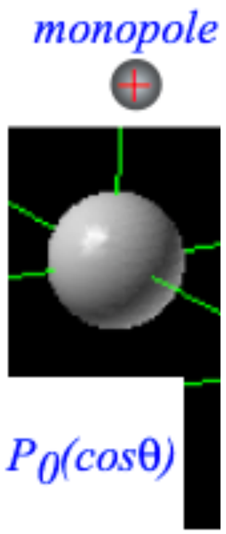

QTCA Unit 8 *Wavefunctions* begins on p. 24

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

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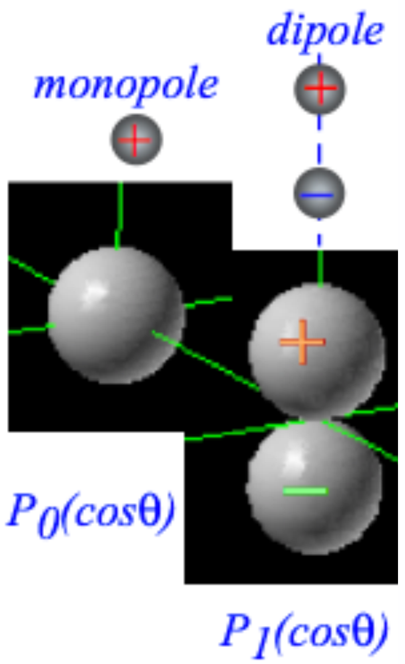

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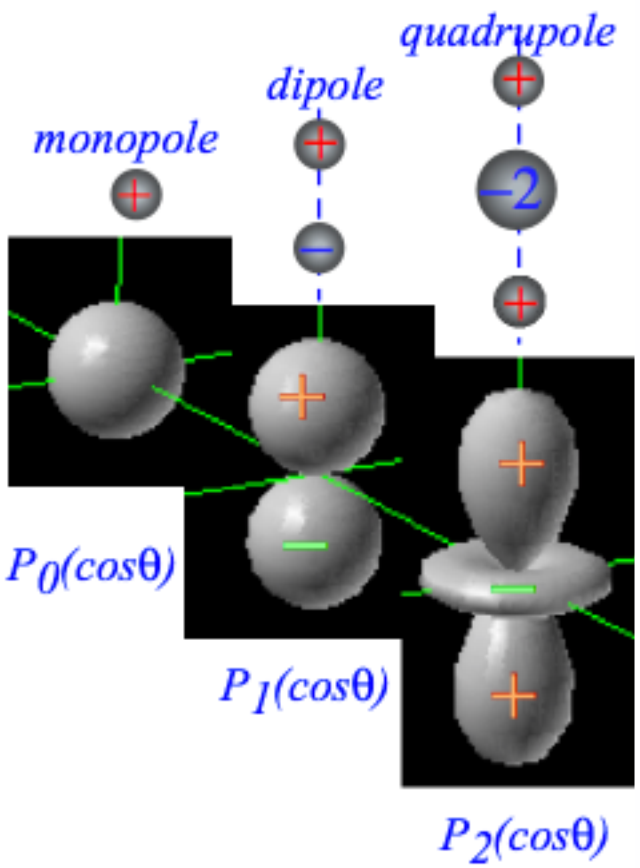

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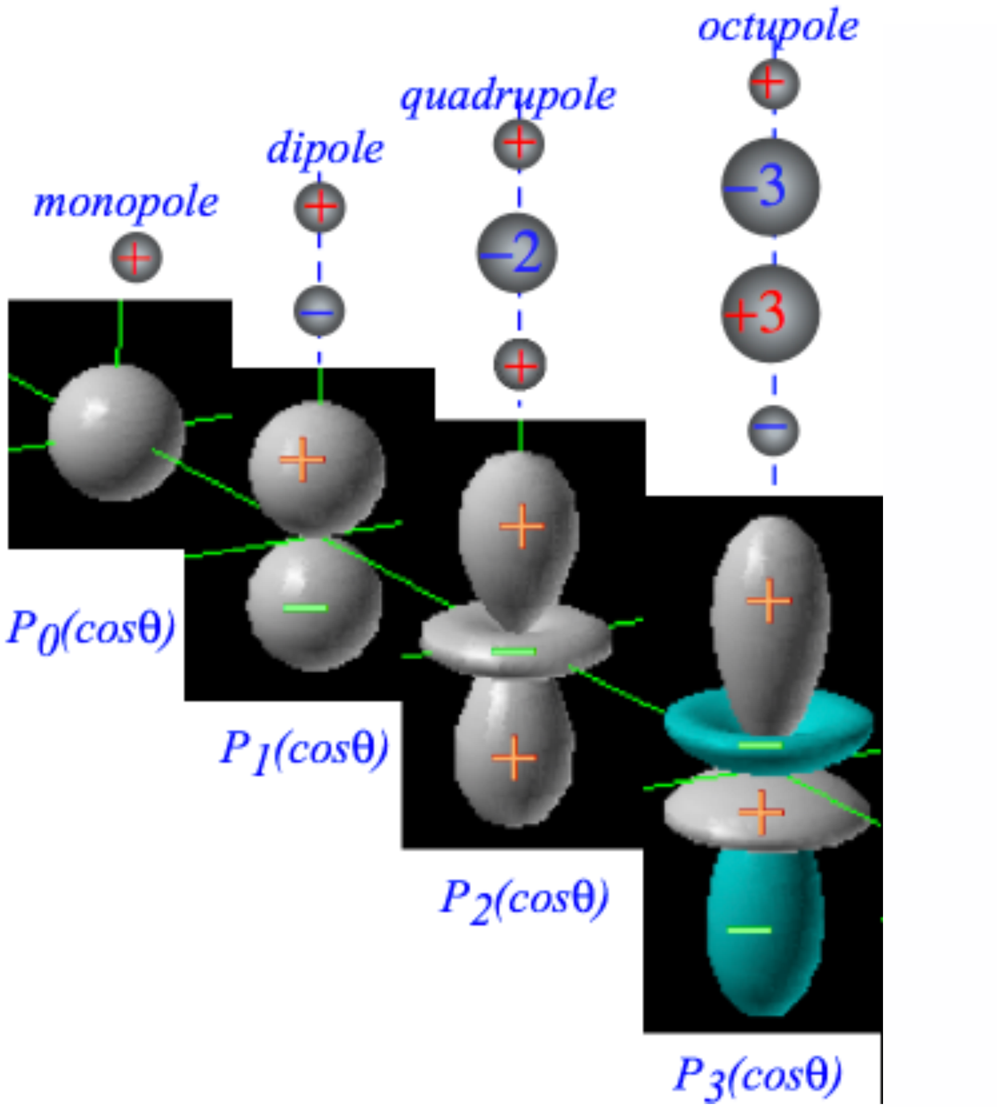

QTCA Unit 8 *Wavefunctions* *begins on p. 24*

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

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

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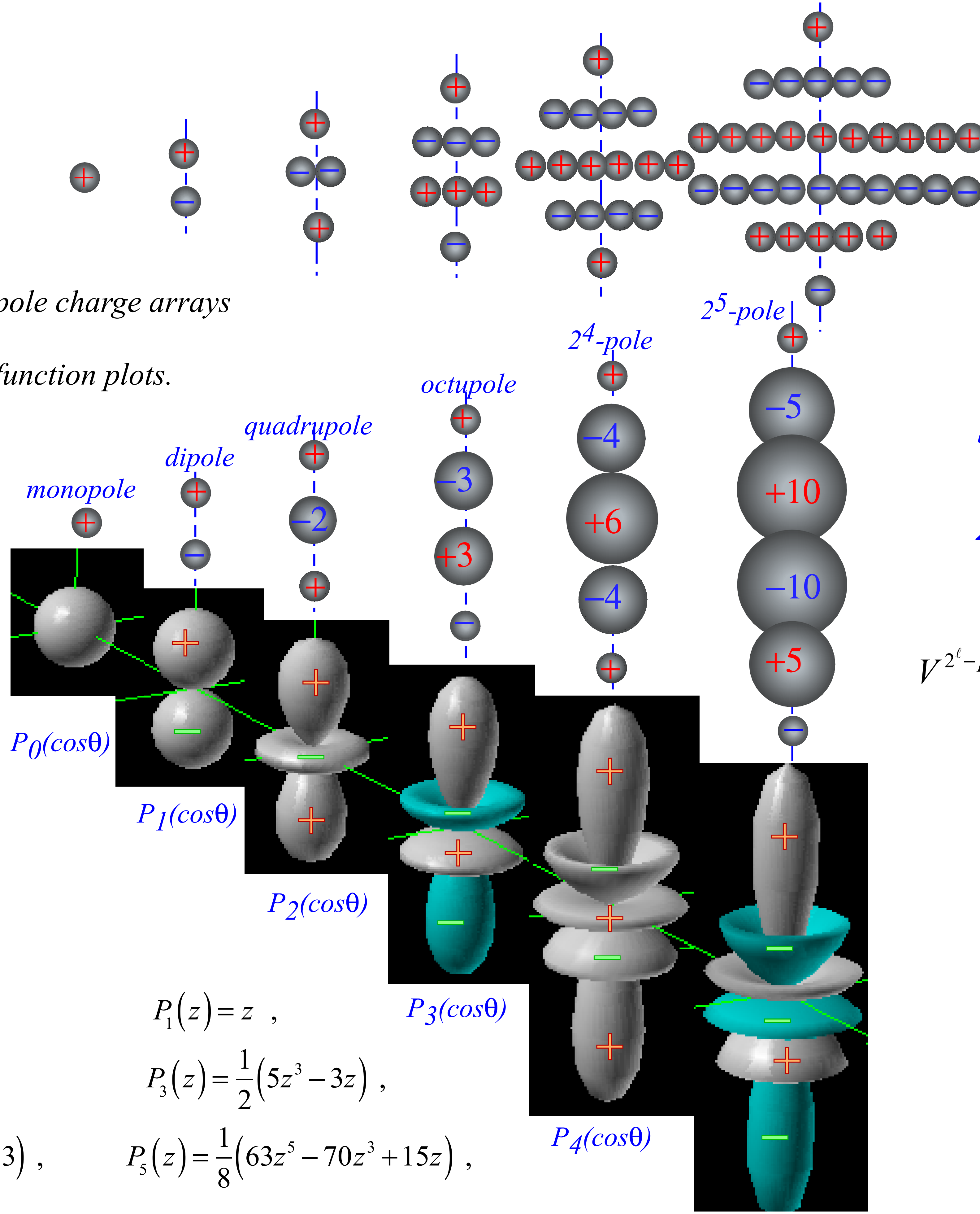

Fig. 23.3.4 Linear 2^k-pole charge arrays and potential or wave function plots.

linear multi-pole
or
2^ℓ-pole potential

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

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

$P_0(z) = 1$, $\quad P_1(z) = z$,

$P_2(z) = \frac{1}{2}(3z^2 - 1)$, $\quad P_3(z) = \frac{1}{2}(5z^3 - 3z)$,

$P_4(z) = \frac{1}{8}(35z^4 - 30z^2 + 3)$, $\quad P_5(z) = \frac{1}{8}(63z^5 - 70z^3 + 15z)$,

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Moving off-axis: On-z-axis linear multipole *Pℓ (cos*θ*)* wave expansion:

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

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

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

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

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

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

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

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

$$=\sum_{m=-\ell}^{\ell}\left|\begin{matrix}\ell\\m,0\end{matrix}\right\rangle D^\ell_{m,0}(\alpha,\beta,0)=\sum_{m=-\ell}^{\ell}\left|\begin{matrix}\ell\\m,0\end{matrix}\right\rangle Y^{\ell *}_m(\alpha,\beta)\sqrt{\frac{4\pi}{2\ell+1}}$$

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

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

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

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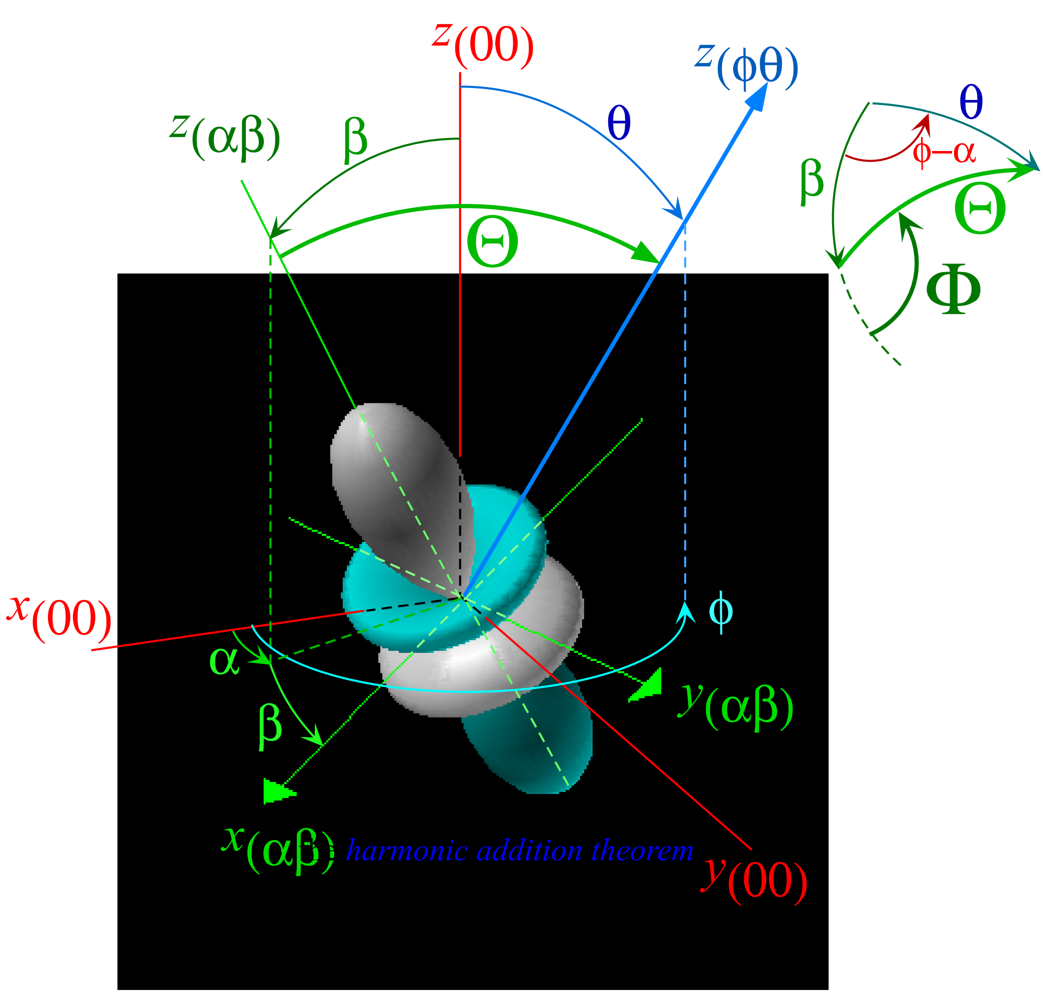
Off-z-axis $P_\ell(\cos\theta)$ wave by Euler rotation: $\left|{\ell \atop 0}\right\rangle_{(\alpha,\beta)}=\mathbf{R}(\alpha,\beta,0)\left|{\ell \atop 0,0}\right\rangle$

$$=\sum_{m=-\ell}^{\ell}\left|{\ell \atop m,0}\right\rangle D^\ell_{m,0}(\alpha,\beta,0)=\sum_{m=-\ell}^{\ell}\left|{\ell \atop m,0}\right\rangle Y^{\ell *}_m(\alpha,\beta)\sqrt{\frac{4\pi}{2\ell+1}}$$

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

$$=\sum_{m=-\ell}^{\ell}\left\langle\phi,\theta\middle|{\ell \atop m,0}\right\rangle Y^{\ell *}_m(\alpha,\beta)\sqrt{\frac{4\pi}{2\ell+1}}$$

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



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

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

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

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:

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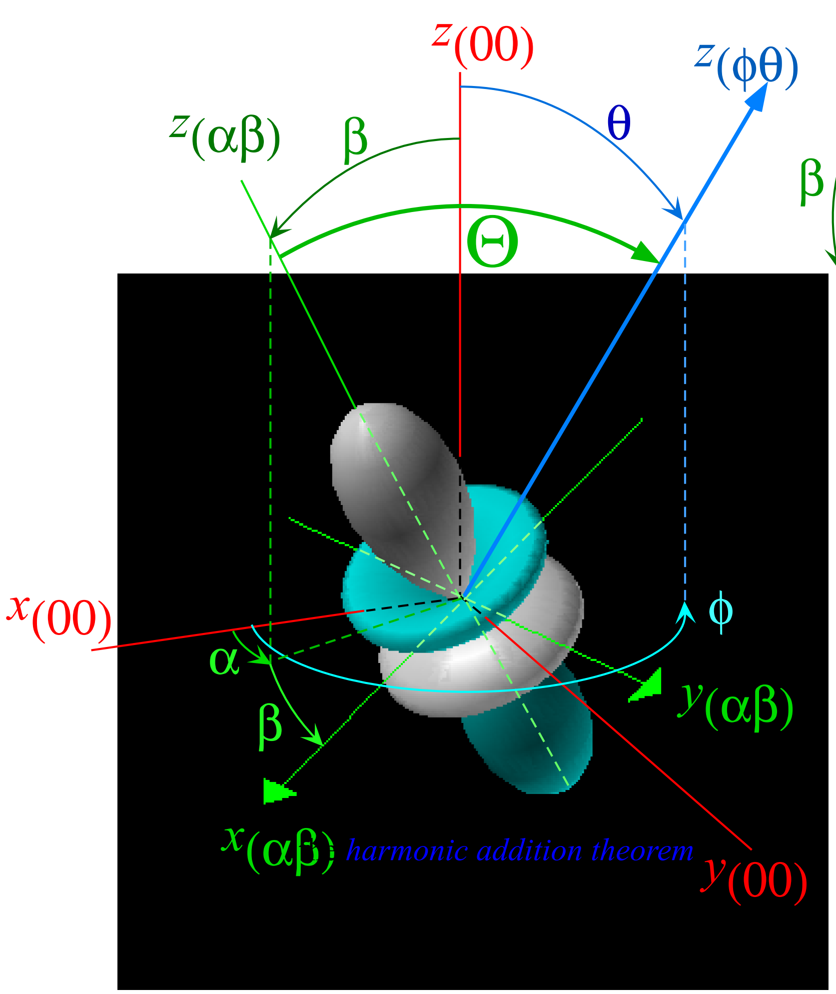

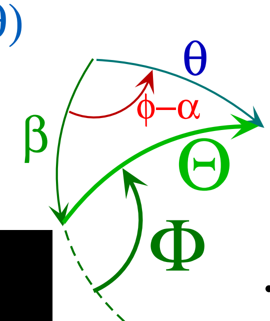

…representing a group product $\mathbf{R}^\dagger(\alpha,\beta,0)\mathbf{R}(\phi,\theta,0)=\mathbf{R}(\Phi,\Theta,0)$.

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

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

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

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

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

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

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:

$$\left|\begin{smallmatrix}\ell\\0\end{smallmatrix}\right\rangle_{(\alpha,\beta)}=\mathbf{R}(\alpha,\beta,0)\left|\begin{smallmatrix}\ell\\0,0\end{smallmatrix}\right\rangle$$

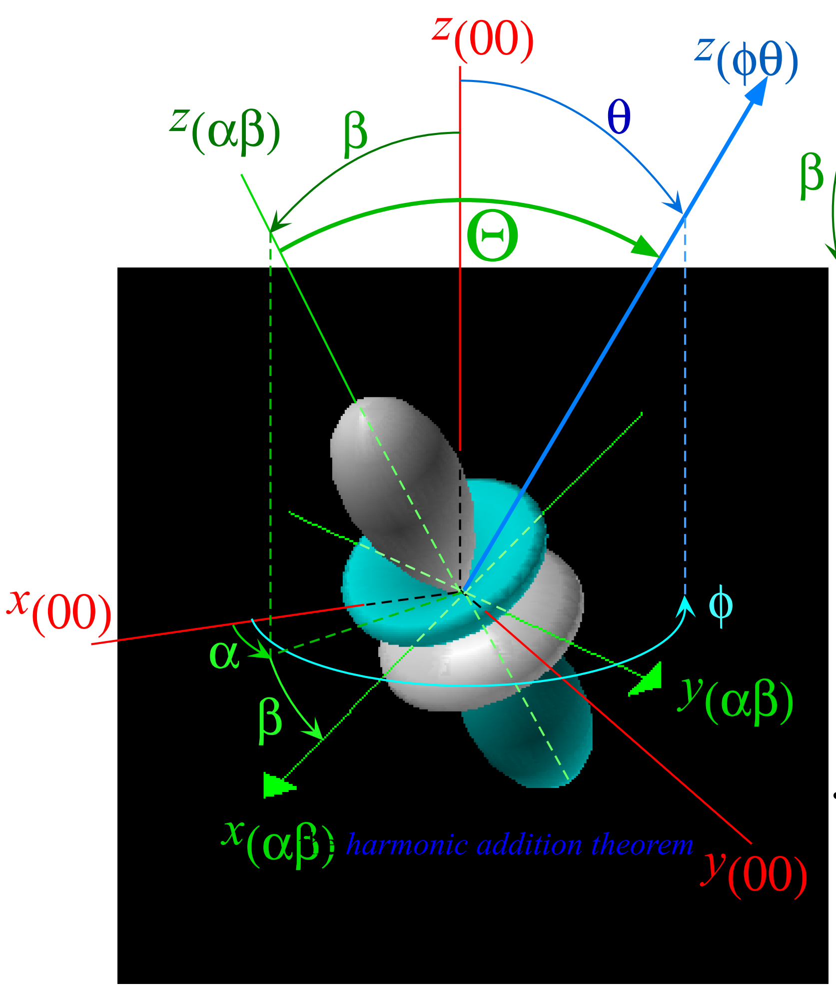
$$=\sum_{m=-\ell}^{\ell}\left|\begin{smallmatrix}\ell\\m,0\end{smallmatrix}\right\rangle D^\ell_{m,0}(\alpha,\beta,0)=\sum_{m=-\ell}^{\ell}\left|\begin{smallmatrix}\ell\\m,0\end{smallmatrix}\right\rangle Y^{\ell*}_m(\alpha,\beta)\sqrt{\frac{4\pi}{2\ell+1}}$$

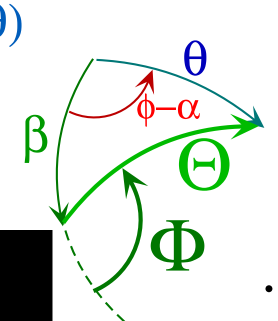
Amplitude at polar position $|\phi,\theta,0\rangle$ of rotated P-wave:

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

$$=\sum_{m=-\ell}^{\ell}\left\langle\phi,\theta\middle|\begin{smallmatrix}\ell\\m,0\end{smallmatrix}\right\rangle Y^{\ell*}_m(\alpha,\beta)\sqrt{\frac{4\pi}{2\ell+1}}$$

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





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

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

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

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

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

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

AMOP reference links on page 2

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-½) p^3 orbits
- Detailed sample applications of "Jawbone" formulae
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- 1-jump $E_{i-1,i}$ operators
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- 2-particle elementary $\mathbf{e}_{jk}$ operator expressions for *(e-e)*-interaction matrix

Tensor tables are $(2\ell+1)$-by-$(2\ell+1)$ arrays $\left({}_p{}^k{}_q\right)$ giving $\mathbf{V}_q^k$ in terms of $\mathbf{E}_{p,q}$.
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[2,1] tableau basis (from p.29) and matrices of $\mathbf{v}^2$ and $\mathbf{v}^2\bullet\mathbf{v}^2$ quadrupole
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Corrected level diagrams Nitrogen p^3

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

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

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

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

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

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

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Shorthand Tensor form of (e-e)-interaction

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

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(e-e)-interaction matrix (multi-ℓ-shell)

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

Given in terms of Slater radial integral(s):

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

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

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

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

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

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

Shorthand Tensor form of (e-e)-interaction

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

(e-e)-interaction matrix (multi-ℓ-shell)

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

Given in terms of Slater radial integral(s):

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

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

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

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

AMOP reference links on page 2

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(Repeating from preceding page) *(e-e)-interaction matrix (multi-ℓ-shell)*

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

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

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:

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

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

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

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

with tensor factors: $\binom{k}{1'1} = C^{k\,\ell_1\,\ell'_1}_{-q\,m_1\,m_1-q} \sqrt{\frac{2k+1}{2\ell'_1+1}}$ and $\binom{k}{2'2} = C^{k\,\ell_2\,\ell'_2}_{-q\,m_2\,m_2-q} \sqrt{\frac{2k+1}{2\ell'_2+1}}$

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-ℓ-shell)*

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

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

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:

$$1' \to \begin{smallmatrix} \ell'_1 \\ m'_1 \end{smallmatrix}, \quad 1 \to \begin{smallmatrix} \ell_1 \\ m_1 \end{smallmatrix}$$

$$2' \to \begin{smallmatrix} \ell'_2 \\ m'_2 \end{smallmatrix}, \quad 2 \to \begin{smallmatrix} \ell_2 \\ m_2 \end{smallmatrix}$$

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

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

with tensor factors: $\left(\begin{smallmatrix} k \\ 1'1 \end{smallmatrix} \right) = C^{k\,\ell_1\,\ell'_1}_{-q\, m_1\, m_1 - q} \sqrt{\frac{2k+1}{2\ell'_1+1}}$ and $\left(\begin{smallmatrix} k \\ 2'2 \end{smallmatrix} \right) = C^{k\,\ell_2\,\ell'_2}_{-q\, m_2\, m_2 - q} \sqrt{\frac{2k+1}{2\ell'_2+1}}$

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 $\mathbf{E}_{jk} = \Sigma_\alpha \mathbf{e}_{jk}(\alpha)$ *summed* operator expressions (Using $\mathbf{e}_{ij}(\alpha)\mathbf{e}_{km}(\alpha) = \delta_{jk}\mathbf{e}_{im}(\alpha)$)

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

(Repeating from preceding page) *(e-e)-interaction matrix (multi-ℓ-shell)*

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

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

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:

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

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

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

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

with tensor factors: $\binom{k}{1'1} = C^{k\,\ell_1\,\ell'_1}_{-q\,m_1\,m_1-q} \sqrt{\frac{2k+1}{2\ell'_1+1}}$ and $\binom{k}{2'2} = C^{k\,\ell_2\,\ell'_2}_{-q\,m_2\,m_2-q} \sqrt{\frac{2k+1}{2\ell'_2+1}}$

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 $\mathbf{E}_{jk} = \Sigma_\alpha \mathbf{e}_{jk}(\alpha)$ *summed* operator expressions (Using $\mathbf{e}_{ij}(\alpha)\mathbf{e}_{km}(\alpha) = \delta_{jk}\mathbf{e}_{im}(\alpha)$)

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

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

AMOP reference links on page 2

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

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

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits
- Detailed sample applications of "Jawbone" formulae
- Number operators
- 1-jump $E_{i-1,i}$ operators
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  - 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,…
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➡ Tensor tables are $(2\ell+1)$-by-$(2\ell+1)$ arrays $\left({}_p{}^k{}_q\right)$ giving $\mathbf{V}_q^k$ in terms of $\mathbf{E}_{p,q}$.
- Relating $\mathbf{V}_q^k$ to $\mathbf{E}_{m',m}$ by $\left({}_{m'}{}^k{}_m\right)$ arrays
- Atomic p-shell *ee*-interaction in elementary operator form

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

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Norms for $-q$ same as for $+q$.

QTCA Unit 8 Ch.25 *Tensor tables begins on p. 9*

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

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

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

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

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

$$\langle\mathbf{v}^0_{0}\rangle=\begin{pmatrix}\binom{0}{11}&\cdot&\cdot\\\cdot&\binom{0}{22}&\cdot\\\cdot&\cdot&\binom{0}{33}\end{pmatrix}\qquad \langle\mathbf{v}^0_{0}\rangle=\begin{pmatrix}1&\cdot&\cdot\\\cdot&1&\cdot\\\cdot&\cdot&1\end{pmatrix}\tfrac{1}{\sqrt{3}}$$

† Lines drawn for $q\geq 0$ only

Norms for $-q$ same as for $+q$.

$({}_p{}^k{}_q)$ arrays are phased Clebsch-Gordan coefficients

$$\left({}_{m'}{}^{k}{}_{m}\right)=(-1)^{\ell-m'}\sqrt{2k+1}\begin{pmatrix}\ell&k&\ell\\-m'&q&m\end{pmatrix}=(-1)^k\sqrt{\frac{2k+1}{2\ell+1}}C^{k\ \ell\ \ell}_{q\ m\ m'=m+q}$$

QTCA Unit 8 Ch.25 *Tensor tables begins on p. 9*

Single-ℓ atomic shells p^n, d^n, f^n,...

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

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

$$=\left(\mathbf{V}^k_0\right)^2+\sum_{q=-k}^{k}\left(\tilde{\mathbf{V}}^k_q\mathbf{V}^k_q+\mathbf{V}^k_q\tilde{\mathbf{V}}^k_q\right)$$

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

$\ell=1$ p=shell example:

A compact format helps display.

$$\left\langle\mathbf{v}^2_{-2}\right\rangle=\begin{pmatrix}\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot\\1&\cdot&\cdot\end{pmatrix}\quad \left\langle\mathbf{v}^2_{-1}\right\rangle=\begin{pmatrix}\cdot&\cdot&\cdot\\1&\cdot&\cdot\\\cdot&-1&\cdot\end{pmatrix}\tfrac{1}{\sqrt{2}}\quad \left\langle\mathbf{v}^2_{0}\right\rangle=\begin{pmatrix}1&\cdot&\cdot\\\cdot&-2&\cdot\\\cdot&\cdot&1\end{pmatrix}\tfrac{1}{\sqrt{6}}\quad \left\langle\mathbf{v}^2_{+1}\right\rangle=\begin{pmatrix}\cdot&-1&\cdot\\\cdot&\cdot&1\\\cdot&\cdot&\cdot\end{pmatrix}\tfrac{1}{\sqrt{2}}\quad \left\langle\mathbf{v}^2_{+2}\right\rangle=\begin{pmatrix}\cdot&\cdot&1\\\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot\end{pmatrix}$$

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

$$\left\langle\mathbf{v}^0_{0}\right\rangle=\begin{pmatrix}1&\cdot&\cdot\\\cdot&1&\cdot\\\cdot&\cdot&1\end{pmatrix}\tfrac{1}{\sqrt{3}}$$

$$\left\langle\mathbf{v}^2_q\right\rangle=\begin{pmatrix}\binom{2}{11}&\binom{2}{12}&\binom{2}{13}\\\binom{2}{21}&\binom{2}{22}&\binom{2}{23}\\\binom{2}{31}&\binom{2}{32}&\binom{2}{33}\end{pmatrix}\quad \left\langle\mathbf{v}^1_q\right\rangle=\begin{pmatrix}\binom{1}{11}&\binom{1}{12}&\cdot\\\binom{1}{21}&\binom{1}{22}&\binom{1}{23}\\\cdot&\binom{1}{32}&\binom{1}{33}\end{pmatrix}\quad \left\langle\mathbf{v}^0_0\right\rangle=\begin{pmatrix}\binom{0}{11}&\cdot&\cdot\\\cdot&\binom{0}{22}&\cdot\\\cdot&\cdot&\binom{0}{33}\end{pmatrix}$$

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

$$\left\langle\mathbf{v}^2_q\right\rangle=\begin{pmatrix}1&-1&1\\1&-2&1\\1&-1&1\end{pmatrix}\;1,\ \tfrac{1}{\sqrt{2}},\ \tfrac{1}{\sqrt{6}}$$

$$\left\langle\mathbf{v}^1_q\right\rangle=\begin{pmatrix}1&-1&\cdot\\1&0&-1\\\cdot&1&-1\end{pmatrix}\;\tfrac{1}{\sqrt{2}},\ \tfrac{1}{\sqrt{2}}$$

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

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Relating $\mathbf{V}^k_q$ to $\mathbf{E}_{m',m}$ by $({}_{m'}{}^k{}_m)$ arrays:

$$\mathbf{V}^k_0=\sum_m\left({}_{m}{}^{k}{}_{m}\right)\mathbf{E}_{m\,m}\qquad \mathbf{V}^k_q=\sum_m\left({}_{m+q}{}^{k}{}_{m}\right)\mathbf{E}_{m+q\;m}\qquad \tilde{\mathbf{V}}^k_q=\sum_m\left({}_{m+q}{}^{k}{}_{m}\right)\mathbf{E}_{m\;m+q}$$

Relating $\mathbf{V}_q^k$ to $\mathbf{E}_{m',m}$ by $\left(_{m'}{}^{k}{}_{m}\right)$ arrays:

$$\mathbf{V}_0^k = \sum_m \left({}^{k}_{m\, m} \right) \mathbf{E}_{m\, m} \qquad \mathbf{V}_q^k = \sum_m \left({}^{\quad k}_{m+q \quad m} \right) \mathbf{E}_{m+q\ m} \qquad \tilde{\mathbf{V}}_q^k = \sum_m \left({}^{\quad k}_{m+q \quad m} \right) \mathbf{E}_{m\ m+q}$$

Dirac notational derivation of $\mathbf{V}_q^k$ to $\mathbf{E}_{m',m}$ relation by $\left(_{m'}{}^{k}{}_{m}\right)$ arrays:

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

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

AMOP reference links on page 2

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Corrected level diagrams Nitrogen p^3

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

$$=\left(\mathbf{V}^k_0\right)^2+\sum_{q=-k}^{k}\left(\tilde{\mathbf{V}}^k_q\mathbf{V}^k_q+\mathbf{V}^k_q\tilde{\mathbf{V}}^k_q\right)$$

$\left(\mathbf{V}^2_0\right)^2=\frac{1}{6}$

	E_{11}	$-2E_{22}$	$+E_{33}$
E_{11}	$E_{11}E_{11}$	$-2E_{11}E_{22}$	$+E_{11}E_{33}$
$-2E_{22}$	$-2E_{22}E_{11}$	$+4E_{22}E_{22}$	$-2E_{22}E_{33}$
$+E_{33}$	$+E_{33}E_{11}$	$-2E_{33}E_{22}$	$+E_{33}E_{33}$

$\tilde{\mathbf{V}}^2_1\mathbf{V}^2_1=\frac{1}{2}$

	$-E_{12}$	$+E_{23}$
$-E_{21}$	$+E_{21}E_{12}$	$-E_{21}E_{23}$
$+E_{32}$	$-E_{32}E_{12}$	$+E_{32}E_{23}$

$\mathbf{V}^2_1\tilde{\mathbf{V}}^2_1=\frac{1}{2}$

	$-E_{21}$	$+E_{32}$
$-E_{12}$	$+E_{12}E_{21}$	$-E_{12}E_{32}$
$+E_{23}$	$-E_{23}E_{12}$	$+E_{23}E_{32}$

$\tilde{\mathbf{V}}^2_2\mathbf{V}^2_2=E_{31}E_{13}$

$\mathbf{V}^2_2\tilde{\mathbf{V}}^2_2=E_{13}E_{31}$

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

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

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

ℓ=1 p=shell $\mathbf{V}^k{}_q$:

QTCA Unit 8 Ch.25 *Tensor tables begins on p. 9*

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Corrected level diagrams Nitrogen p^3

= [2,1] tableau basis and U(3) irep (from p. 29)

$E_{jk} =$

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\left\vert \begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle \begin{smallmatrix}11\\2\end{smallmatrix}\right\vert$	$\overset{(11)\,(22)}{2+1}$	$\overset{(12)}{1}$	$\overset{(23)}{1}$	$\overset{(13)}{-\sqrt{\tfrac{1}{2}}}$	$\overset{(13)}{\sqrt{\tfrac{3}{2}}}$	·	·	·
$\left\langle \begin{smallmatrix}12\\2\end{smallmatrix}\right\vert$	$\overset{(21)}{1}$	$\overset{(11)\,(22)}{1+2}$	·	$\overset{(23)}{\sqrt{\tfrac{1}{2}}}$	$\overset{(23)}{\sqrt{\tfrac{3}{2}}}$	·	$\overset{(13)}{-1}$	·
$\left\langle \begin{smallmatrix}11\\3\end{smallmatrix}\right\vert$	$\overset{(32)}{1}$	·	$\overset{(11)\,(33)}{2+1}$	$\overset{(12)}{\sqrt{2}}$	·	$\overset{(13)}{1}$	·	·
$\left\langle \begin{smallmatrix}12\\3\end{smallmatrix}\right\vert$	$\overset{(31)}{-\sqrt{\tfrac{1}{2}}}$	$\overset{(32)}{\sqrt{\tfrac{1}{2}}}$	$\overset{(21)}{\sqrt{2}}$	$\overset{(11)\,(22)\,(33)}{1+1+1}$	·	$\overset{(23)}{\sqrt{\tfrac{1}{2}}}$	$\overset{(12)}{\sqrt{2}}$	$\overset{(13)}{\sqrt{\tfrac{1}{2}}}$
$\left\langle \begin{smallmatrix}13\\2\end{smallmatrix}\right\vert$	$\overset{(31)}{\sqrt{\tfrac{3}{2}}}$	$\overset{(32)}{\sqrt{\tfrac{3}{2}}}$	·	·	$\overset{(11)\,(22)\,(33)}{1+1+1}$	$\overset{(23)}{\sqrt{\tfrac{3}{2}}}$	·	$\overset{(13)}{\sqrt{\tfrac{3}{2}}}$
$\left\langle \begin{smallmatrix}13\\3\end{smallmatrix}\right\vert$	·	·	$\overset{(31)}{1}$	$\overset{(32)}{\sqrt{\tfrac{1}{2}}}$	$\overset{(32)}{\sqrt{\tfrac{3}{2}}}$	$\overset{(11)\,(33)}{1+2}$	·	$\overset{(12)}{1}$
$\left\langle \begin{smallmatrix}22\\3\end{smallmatrix}\right\vert$	·	$\overset{(31)}{-1}$	·	$\overset{(21)}{\sqrt{2}}$	·	·	$\overset{(22)\,(33)}{2+1}$	$\overset{(23)}{1}$
$\left\langle \begin{smallmatrix}23\\3\end{smallmatrix}\right\vert$	·	·	·	$\overset{(31)}{\sqrt{\tfrac{1}{2}}}$	$\overset{(31)}{\sqrt{\tfrac{3}{2}}}$	$\overset{(21)}{1}$	$\overset{(32)}{1}$	$\overset{(22)\,(33)}{1+2}$

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

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

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

[2,1] tableau basis and matrices of $\mathbf{v}^1$ dipole

$E_{jk} =$

	$M=2$: $\left\|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$M=1$: $\left\|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$M=1$: $\left\|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$M=0$: $\left\|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$M=0$: $\left\|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$M=-1$: $\left\|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$M=-1$: $\left\|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$M=-2$: $\left\|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\|$	(21) 1	(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\|$	(32) 1	·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\|$	(31) $-\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{1}{2}}$	(21) $\sqrt{2}$	(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\|$	(31) $\sqrt{\frac{3}{2}}$	(32) $\sqrt{\frac{3}{2}}$	·	·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\|$	·	·	(31) 1	(32) $\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{3}{2}}$	(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\|$	·	(31) -1	·	(21) $\sqrt{2}$	·	·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\|$	·	·	·	(31) $\sqrt{\frac{1}{2}}$	(31) $\sqrt{\frac{3}{2}}$	(21) 1	(32) 1	(22) (33) $1+2$

dipole (k=1) angular momentum **L**-*operators*

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

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

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$E_{jk} =$

	$M=2$: $\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$M=1$: $\left\vert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$M=1$: $\left\vert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$M=0$: $\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$M=0$: $\left\vert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$M=-1$: $\left\vert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$M=-1$: $\left\vert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$M=-2$: $\left\vert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\tfrac{1}{2}}$	(13) $\sqrt{\tfrac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\vert$	(21) 1	(11) (22) $1+2$	·	(23) $\sqrt{\tfrac{1}{2}}$	(23) $\sqrt{\tfrac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\vert$	(32) 1	·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\vert$	(31) $-\sqrt{\tfrac{1}{2}}$	(32) $\sqrt{\tfrac{1}{2}}$	(21) $\sqrt{2}$	(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\tfrac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\tfrac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\vert$	(31) $\sqrt{\tfrac{3}{2}}$	(32) $\sqrt{\tfrac{3}{2}}$	·	·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\tfrac{3}{2}}$	·	(13) $\sqrt{\tfrac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\vert$	·	·	(31) 1	(32) $\sqrt{\tfrac{1}{2}}$	(32) $\sqrt{\tfrac{3}{2}}$	(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\vert$	·	(31) -1	·	(21) $\sqrt{2}$	·	·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\vert$	·	·	·	(31) $\sqrt{\tfrac{1}{2}}$	(31) $\sqrt{\tfrac{3}{2}}$	(21) 1	(32) 1	(22) (33) $1+2$

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

dipole (k=1) angular momentum **L***-operators*

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

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

[2,1] *tableau basis and matrices of* $\mathbf{v}^1$ *dipole*

$E_{jk} =$

	M=2	*M=1*		*M=0*		*M=-1*		*M=-2*
	$\left\lvert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\lvert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\rvert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\rvert$	(21) 1	(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\rvert$	(32) 1	·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\rvert$	(31) $-\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{1}{2}}$	(21) $\sqrt{2}$	(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\rvert$	(31) $\sqrt{\frac{3}{2}}$	(32) $\sqrt{\frac{3}{2}}$	·	·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\rvert$	·	·	(31) 1	(32) $\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{3}{2}}$	(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\rvert$	·	(31) -1	·	(21) $\sqrt{2}$	·	·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\rvert$	·	·	·	(31) $\sqrt{\frac{1}{2}}$	(31) $\sqrt{\frac{3}{2}}$	(21) 1	(32) 1	(22) (33) $1+2$

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

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

dipole (k=1) angular momentum **L***-operators*

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

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

$\square\square_{\square}$ = [2,1] *tableau basis and matrices of* $\mathbf{v}^1$ *dipole*

$E_{jk}=$

	M=2 $\left\|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	M=1 $\left\|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	M=1 $\left\|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	M=0 $\left\|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	M=0 $\left\|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	M=-1 $\left\|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	M=-1 $\left\|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	M=-2 $\left\|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\|$	(21) 1	(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\|$	(32) 1	·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\|$	(31) $-\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{1}{2}}$	(21) $\sqrt{2}$	(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\|$	(31) $\sqrt{\frac{3}{2}}$	(32) $\sqrt{\frac{3}{2}}$	·	·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\|$	·	·	(31) 1	(32) $\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{3}{2}}$	(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\|$	·	(31) -1	·	(21) $\sqrt{2}$	·	·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\|$	·	·	·	(31) $\sqrt{\frac{1}{2}}$	(31) $\sqrt{\frac{3}{2}}$	(21) 1	(32) 1	(22) (33) $1+2$

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

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

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

dipole (k=1) angular momentum **L**-*operators*

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

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

[2,1] *tableau basis and matrices of* $\mathbf{v}^1$ *dipole*

$E_{jk} =$

	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
	$\left\|{}^{11}_{2}\right\rangle$	$\left\|{}^{12}_{2}\right\rangle$	$\left\|{}^{11}_{3}\right\rangle$	$\left\|{}^{12}_{3}\right\rangle$	$\left\|{}^{13}_{2}\right\rangle$	$\left\|{}^{13}_{3}\right\rangle$	$\left\|{}^{22}_{3}\right\rangle$	$\left\|{}^{23}_{3}\right\rangle$
$\left\langle{}^{11}_{2}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle{}^{12}_{2}\right\|$	(21) 1	(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle{}^{11}_{3}\right\|$	(32) 1	·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle{}^{12}_{3}\right\|$	(31) $-\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{1}{2}}$	(21) $\sqrt{2}$	(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle{}^{13}_{2}\right\|$	(31) $\sqrt{\frac{3}{2}}$	(32) $\sqrt{\frac{3}{2}}$	·	·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle{}^{13}_{3}\right\|$	·	·	(31) 1	(32) $\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{3}{2}}$	(11) (33) $1+2$	·	(12) 1
$\left\langle{}^{22}_{3}\right\|$	·	(31) -1	·	(21) $\sqrt{2}$	·	·	(22) (33) $2+1$	(23) 1
$\left\langle{}^{23}_{3}\right\|$	·	·	·	(31) $\sqrt{\frac{1}{2}}$	(31) $\sqrt{\frac{3}{2}}$	(21) 1	(32) 1	(22) (33) $1+2$

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

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

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

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

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

dipole (k=1) angular momentum **L**-*operators*

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

Squared *angular momentum* **L•L**-*operators*

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

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

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

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

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

dipole (k=1) angular momentum **L**-*operators*

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

Squared *angular momentum* **L•L**-*operators*

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

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

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

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

$$= \quad \tfrac{1}{2} \quad + \tfrac{1}{2} \quad + \quad 1 \quad + 0 \;=\; 2$$

$[2,1]$ *tableau basis and matrices of* $\mathbf{v}^1$ *dipole*

$$E_{jk} =$$

	$M=2$: $\left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$M=1$: $\left|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$M=1$: $\left|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$M=0$: $\left|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$M=0$: $\left|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$M=-1$: $\left|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$M=-1$: $\left|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$M=-2$: $\left|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right|$	(21) 1	(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right|$	(32) 1	·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right|$	(31) $-\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{1}{2}}$	(21) $\sqrt{2}$	(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right|$	(31) $\sqrt{\frac{3}{2}}$	(32) $\sqrt{\frac{3}{2}}$	·	·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right|$	·	·	(31) 1	(32) $\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{3}{2}}$	(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right|$	·	(31) -1	·	(21) $\sqrt{2}$	·	·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right|$	·	·	·	(31) $\sqrt{\frac{1}{2}}$	(31) $\sqrt{\frac{3}{2}}$	(21) 1	(32) 1	(22) (33) $1+2$

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

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

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

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

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

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

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

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

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

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

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

dipole (k=1) angular momentum **L***-operators*

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

Squared *angular momentum* **L•L***-operators*

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

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

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

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

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

dipole (k=1) angular momentum **L***-operators*

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

Squared *angular momentum* **L•L***-operators*

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

$$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right|V^1\cdot V^1\left|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle = \left(2\binom{1}{11}+\binom{1}{22}\right)^2+\binom{1}{21}^2+\binom{1}{23}^2+2\binom{1}{13}^2$$
$$=\tfrac{1}{2}(2\cdot 1-0)^2+\left(\tfrac{1}{\sqrt{2}}\right)^2+\left(\tfrac{1}{\sqrt{2}}\right)^2+2\left(\tfrac{1}{\sqrt{2}}\right)^2 \;=\; 3$$

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

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

$\square\square\!/\!\square$ = [2,1] *tableau basis and matrices of* $\mathbf{v}^1$ *dipole*

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

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

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

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

dipole (k=1) angular momentum **L**-*operators*

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

Squared *angular momentum* **L•L**-*operators*

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

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

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

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

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

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

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

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

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

$$= \tfrac{-1}{2}\left(1\cdot 1 + 1\cdot 1\right) = -1$$

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

[2,1] = [2,1] *tableau basis and matrices of* $\mathbf{v}^1$ *dipole*

$E_{jk}=$	*M=2* $\left\|{11 \atop 2}\right\rangle$	*M=1* $\left\|{12 \atop 2}\right\rangle$	*M=1* $\left\|{11 \atop 3}\right\rangle$	*M=0* $\left\|{12 \atop 3}\right\rangle$	*M=0* $\left\|{13 \atop 2}\right\rangle$	*M=-1* $\left\|{13 \atop 3}\right\rangle$	*M=-1* $\left\|{22 \atop 3}\right\rangle$	*M=-2* $\left\|{23 \atop 3}\right\rangle$
$\left\langle{11 \atop 2}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	.	.	.
$\left\langle{12 \atop 2}\right\|$	(21) 1	(11) (22) $1+2$	.	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	.	(13) -1	.
$\left\langle{11 \atop 3}\right\|$	(32) 1	.	(11) (33) $2+1$	(12) $\sqrt{2}$	.	(13) 1	.	.
$\left\langle{12 \atop 3}\right\|$	(31) $-\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{1}{2}}$	(21) $\sqrt{2}$	(11) (22) (33) $1+1+1$	.	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle{13 \atop 2}\right\|$	(31) $\sqrt{\frac{3}{2}}$	(32) $\sqrt{\frac{3}{2}}$	.	.	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	.	(13) $\sqrt{\frac{3}{2}}$
$\left\langle{13 \atop 3}\right\|$	.	.	(31) 1	(32) $\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{3}{2}}$	(11) (33) $1+2$	.	(12) 1
$\left\langle{22 \atop 3}\right\|$	.	(31) -1	.	(21) $\sqrt{2}$	.	.	(22) (33) $2+1$	(23) 1
$\left\langle{23 \atop 3}\right\|$	.	.	.	(31) $\sqrt{\frac{1}{2}}$	(31) $\sqrt{\frac{3}{2}}$	(21) 1	(32) 1	(22) (33) $1+2$

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

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

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

dipole (k=1) angular momentum **L***-operators*

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

Squared *angular momentum* **L•L***-operators*

$$\left\langle {11 \atop 2} \middle| V^1 \cdot V^1 \middle| {11 \atop 2} \right\rangle = \left(2\binom{1}{11} + \binom{1}{22}\right)^2 + \binom{1}{21}^2 + \binom{1}{23}^2 + 2\binom{1}{13}^2$$
$$= \tfrac{1}{2}\left(2\cdot 1 - 0\right)^2 + \left(\tfrac{1}{\sqrt{2}}\right)^2 + \left(\tfrac{1}{\sqrt{2}}\right)^2 + 2\left(\tfrac{1}{\sqrt{2}}\right)^2 = 3$$

$$\left\langle {12 \atop 2} \middle| V^1 \cdot V^1 \middle| {12 \atop 2} \right\rangle = \left(\binom{1}{11} + 2\binom{1}{22}\right)^2 + \binom{1}{21}^2 + 2\binom{1}{23}^2 + \binom{1}{13}^2$$
$$= \tfrac{1}{2}\left(1\cdot 1 + 2\cdot 0\right)^2 + \left(\tfrac{1}{\sqrt{2}}\right)^2 + 2\left(\tfrac{1}{\sqrt{2}}\right)^2 + 0$$
$$= \tfrac{1}{2} + \tfrac{1}{2} + 1 + 0 = 2$$

$$\left\langle {11 \atop 3} \middle| V^1 \cdot V^1 \middle| {11 \atop 3} \right\rangle = \left(2\binom{1}{11} + \binom{1}{33}\right)^2 + 2\binom{1}{21}^2 + \binom{1}{23}^2 + \binom{1}{13}^2$$
$$= \tfrac{1}{2}\left(2\cdot 1 - 1\cdot 1\right)^2 + 2\left(\tfrac{1}{\sqrt{2}}\right)^2 + \left(\tfrac{1}{\sqrt{2}}\right)^2 + 0$$
$$= \tfrac{1}{2} + 1 + \tfrac{1}{2} + 0 = 2$$

$$\left\langle {12 \atop 2} \middle| V^1 \cdot V^1 \middle| {11 \atop 3} \right\rangle = +\binom{1}{21}\binom{1}{32} + \binom{1}{23}\binom{1}{12}$$
$$= \tfrac{-1}{2}\left(1\cdot 1 + 1\cdot 1\right) = -1$$

	$\begin{smallmatrix}1 & 1\\ 2 & \end{smallmatrix}$			*eigenvalues*	
$\begin{smallmatrix}1 & 1\\ 2 & \end{smallmatrix}$	3			3	
		$\begin{smallmatrix}1 & 2\\ 2 & \end{smallmatrix}$	$\begin{smallmatrix}1 & 1\\ 3 & \end{smallmatrix}$		
$\begin{smallmatrix}1 & 2\\ 2 & \end{smallmatrix}$		2	-1	1	0
$\begin{smallmatrix}1 & 1\\ 3 & \end{smallmatrix}$		-1	2	0	3

$[2,1]$ tableau basis and matrices of $\mathbf{v}^1$ dipole

$E_{jk} =$

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

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

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

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

dipole (k=1) angular momentum **L***-operators*

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

Squared *angular momentum* **L•L***-operators*

$$\left\langle \begin{smallmatrix}11\\2\end{smallmatrix} \middle| V^1 \cdot V^1 \middle| \begin{smallmatrix}11\\2\end{smallmatrix} \right\rangle = \left(2\binom{1}{11} + \binom{1}{22}\right)^2 + \binom{1}{21}^2 + \binom{1}{23}^2 + 2\binom{1}{13}^2$$
$$= \tfrac{1}{2}\left(2\cdot 1 - 0\right)^2 + \left(\tfrac{1}{\sqrt{2}}\right)^2 + \left(\tfrac{1}{\sqrt{2}}\right)^2 + 2\left(\tfrac{1}{\sqrt{2}}\right)^2 = 3$$

$$\left\langle \begin{smallmatrix}12\\2\end{smallmatrix} \middle| V^1 \cdot V^1 \middle| \begin{smallmatrix}12\\2\end{smallmatrix} \right\rangle = \left(\binom{1}{11} + 2\binom{1}{22}\right)^2 + \binom{1}{21}^2 + 2\binom{1}{23}^2 + \binom{1}{13}^2$$
$$= \tfrac{1}{2}\left(1\cdot 1 + 2\cdot 0\right)^2 + \left(\tfrac{1}{\sqrt{2}}\right)^2 + 2\left(\tfrac{1}{\sqrt{2}}\right)^2 + 0$$
$$= \tfrac{1}{2} + \tfrac{1}{2} + 1 + 0 = 2$$

$$\left\langle \begin{smallmatrix}11\\3\end{smallmatrix} \middle| V^1 \cdot V^1 \middle| \begin{smallmatrix}11\\3\end{smallmatrix} \right\rangle = \left(2\binom{1}{11} + \binom{1}{33}\right)^2 + 2\binom{1}{21}^2 + \binom{1}{23}^2 + \binom{1}{13}^2$$
$$= \tfrac{1}{2}\left(2\cdot 1 - 1\cdot 1\right)^2 + 2\left(\tfrac{1}{\sqrt{2}}\right)^2 + \left(\tfrac{1}{\sqrt{2}}\right)^2 + 0$$
$$= \tfrac{1}{2} + 1 + \tfrac{1}{2} + 0 = 2$$

$$\left\langle \begin{smallmatrix}12\\2\end{smallmatrix} \middle| V^1 \cdot V^1 \middle| \begin{smallmatrix}11\\3\end{smallmatrix} \right\rangle = +\binom{1}{21}\binom{1}{32} + \binom{1}{23}\binom{1}{12}$$
$$= \tfrac{-1}{2}\left(1\cdot 1 + 1\cdot 1\right) = -1$$

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

eigenvalues		**L•L** *eigenvalues* $j(j+1)$		
3		6		$(j=2)$
1	0	2	0	$(j=1)$
0	3	0	6	$(j=2)$

AMOP reference links on page 2

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-½) 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 $\mathbf{e}_{jk}$ operator expressions for *(e-e)*-interaction matrix

Tensor tables are $(2\ell+1)$-by-$(2\ell+1)$ arrays $\left({}_{p}{}^{k}{}_{q}\right)$ giving $\mathbf{V}_q^k$ in terms of $\mathbf{E}_{p,q}$.
- Relating $\mathbf{V}_q^k$ to $\mathbf{E}_{m',m}$ by $\left({}_{m'}{}^{k}{}_{m}\right)$ arrays
- Atomic p-shell *ee*-interaction in elementary operator form

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

➡ [2,1] tableau basis (from p.29) and matrices of $\mathbf{v}^2$ and $\mathbf{v}^2\bullet\mathbf{v}^2$ quadrupole
- ${}^4S$, ${}^2P$, and ${}^2D$ energy calculation of quartet and doublet (spin-½) p^3 orbits

Corrected level diagrams Nitrogen p^3

$\square\square$ = [2,1] *tableau basis and U(3) irep (from p. 29)*

$E_{jk} =$

	$M=2$: $\left\vert{11 \atop 2}\right\rangle$	$M=1$: $\left\vert{12 \atop 2}\right\rangle$	$M=1$: $\left\vert{11 \atop 3}\right\rangle$	$M=0$: $\left\vert{12 \atop 3}\right\rangle$	$M=0$: $\left\vert{13 \atop 2}\right\rangle$	$M=-1$: $\left\vert{13 \atop 3}\right\rangle$	$M=-1$: $\left\vert{22 \atop 3}\right\rangle$	$M=-2$: $\left\vert{23 \atop 3}\right\rangle$
$\left\langle{11 \atop 2}\right\vert$	$\overset{(11)\ (22)}{2+1}$	$\overset{(12)}{1}$	$\overset{(23)}{1}$	$\overset{(13)}{-\sqrt{\tfrac{1}{2}}}$	$\overset{(13)}{\sqrt{\tfrac{3}{2}}}$	·	·	·
$\left\langle{12 \atop 2}\right\vert$	$\overset{(21)}{1}$	$\overset{(11)\ (22)}{1+2}$	·	$\overset{(23)}{\sqrt{\tfrac{1}{2}}}$	$\overset{(23)}{\sqrt{\tfrac{3}{2}}}$	·	$\overset{(13)}{-1}$	·
$\left\langle{11 \atop 3}\right\vert$	$\overset{(32)}{1}$	·	$\overset{(11)\ (33)}{2+1}$	$\overset{(12)}{\sqrt{2}}$	·	$\overset{(13)}{1}$	·	·
$\left\langle{12 \atop 3}\right\vert$	$\overset{(31)}{-\sqrt{\tfrac{1}{2}}}$	$\overset{(32)}{\sqrt{\tfrac{1}{2}}}$	$\overset{(21)}{\sqrt{2}}$	$\overset{(11)\ (22)\ (33)}{1+1+1}$	·	$\overset{(23)}{\sqrt{\tfrac{1}{2}}}$	$\overset{(12)}{\sqrt{2}}$	$\overset{(13)}{\sqrt{\tfrac{1}{2}}}$
$\left\langle{13 \atop 2}\right\vert$	$\overset{(31)}{\sqrt{\tfrac{3}{2}}}$	$\overset{(32)}{\sqrt{\tfrac{3}{2}}}$	·	·	$\overset{(11)\ (22)\ (33)}{1+1+1}$	$\overset{(23)}{\sqrt{\tfrac{3}{2}}}$	·	$\overset{(13)}{\sqrt{\tfrac{3}{2}}}$
$\left\langle{13 \atop 3}\right\vert$	·	·	$\overset{(31)}{1}$	$\overset{(32)}{\sqrt{\tfrac{1}{2}}}$	$\overset{(32)}{\sqrt{\tfrac{3}{2}}}$	$\overset{(11)\ (33)}{1+2}$	·	$\overset{(12)}{1}$
$\left\langle{22 \atop 3}\right\vert$	·	$\overset{(31)}{-1}$	·	$\overset{(21)}{\sqrt{2}}$	·	·	$\overset{(22)\ (33)}{2+1}$	$\overset{(23)}{1}$
$\left\langle{23 \atop 3}\right\vert$	·	·	·	$\overset{(31)}{\sqrt{\tfrac{1}{2}}}$	$\overset{(31)}{\sqrt{\tfrac{3}{2}}}$	$\overset{(21)}{1}$	$\overset{(32)}{1}$	$\overset{(22)\ (33)}{1+2}$

$\ell=1$ (condensed format)

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

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

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

[2,1] *tableau basis and matrices of* $\mathbf{v}^2$ *quadrupole*

$E_{jk} =$

	$M=2$: $\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$M=1$: $\left\vert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$M=1$: $\left\vert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$M=0$: $\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$M=0$: $\left\vert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$M=-1$: $\left\vert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$M=-1$: $\left\vert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$M=-2$: $\left\vert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\vert$	(21) 1	(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\vert$	(32) 1	·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\vert$	(31) $-\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{1}{2}}$	(21) $\sqrt{2}$	(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\vert$	(31) $\sqrt{\frac{3}{2}}$	(32) $\sqrt{\frac{3}{2}}$	·	·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\vert$	·	·	(31) 1	(32) $\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{3}{2}}$	(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\vert$	·	(31) -1	·	(21) $\sqrt{2}$	·	·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\vert$	·	·	·	(31) $\sqrt{\frac{1}{2}}$	(31) $\sqrt{\frac{3}{2}}$	(21) 1	(32) 1	(22) (33) $1+2$

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

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

ℓ=1 (condensed format)

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

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

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

[2,1] *tableau basis and matrices of* $\mathbf{v}^2$ *quadrupole*

$E_{jk} =$

	M=2 $\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	*M=1* $\left\vert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	*M=0* $\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	*M=-1* $\left\vert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	*M=-2* $\left\vert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\vert$	(21) 1	(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\vert$	(32) 1	·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\vert$	(31) $-\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{1}{2}}$	(21) $\sqrt{2}$	(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\vert$	(31) $\sqrt{\frac{3}{2}}$	(32) $\sqrt{\frac{3}{2}}$	·	·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\vert$	·	·	(31) 1	(32) $\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{3}{2}}$	(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\vert$	·	(31) -1	·	(21) $\sqrt{2}$	·	·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\vert$	·	·	·	(31) $\sqrt{\frac{1}{2}}$	(31) $\sqrt{\frac{3}{2}}$	(21) 1	(32) 1	(22) (33) $1+2$

ℓ=1 (condensed format)

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

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

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

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

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

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

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

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

□□/□ = [2,1] *tableau basis and matrices of* $\mathbf{v}^2$ *quadrupole*

$E_{jk} =$

	M=2	M=1		M=0		M=-1		M=-2
	$\left\vert\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\vert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\vert$	(21) 1	(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\vert$	(32) 1	·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\vert$	(31) $-\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{1}{2}}$	(21) $\sqrt{2}$	(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\vert$	(31) $\sqrt{\frac{3}{2}}$	(32) $\sqrt{\frac{3}{2}}$	·	·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\vert$	·	·	(31) 1	(32) $\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{3}{2}}$	(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\vert$	·	(31) -1	·	(21) $\sqrt{2}$	·	·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\vert$	·	·	·	(31) $\sqrt{\frac{1}{2}}$	(31) $\sqrt{\frac{3}{2}}$	(21) 1	(32) 1	(22) (33) $1+2$

ℓ=1 (condensed format)

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

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

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

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

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

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

[2,1] = [2,1] *tableau basis and matrices of* $\mathbf{v}^2$ *quadrupole*

$E_{jk} =$

	$M=2$: $\left\vert{}^{11}_{2}\right\rangle$	$M=1$: $\left\vert{}^{12}_{2}\right\rangle$	$M=1$: $\left\vert{}^{11}_{3}\right\rangle$	$M=0$: $\left\vert{}^{12}_{3}\right\rangle$	$M=0$: $\left\vert{}^{13}_{2}\right\rangle$	$M=-1$: $\left\vert{}^{13}_{3}\right\rangle$	$M=-1$: $\left\vert{}^{22}_{3}\right\rangle$	$M=-2$: $\left\vert{}^{23}_{3}\right\rangle$
$\left\langle{}^{11}_{2}\right\vert$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle{}^{12}_{2}\right\vert$	(21) 1	(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle{}^{11}_{3}\right\vert$	(32) 1	·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle{}^{12}_{3}\right\vert$	(31) $-\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{1}{2}}$	(21) $\sqrt{2}$	(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle{}^{13}_{2}\right\vert$	(31) $\sqrt{\frac{3}{2}}$	(32) $\sqrt{\frac{3}{2}}$	·	·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle{}^{13}_{3}\right\vert$	·	·	(31) 1	(32) $\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{3}{2}}$	(11) (33) $1+2$	·	(12) 1
$\left\langle{}^{22}_{3}\right\vert$	·	(31) -1	·	(21) $\sqrt{2}$	·	·	(22) (33) $2+1$	(23) 1
$\left\langle{}^{23}_{3}\right\vert$	·	·	·	(31) $\sqrt{\frac{1}{2}}$	(31) $\sqrt{\frac{3}{2}}$	(21) 1	(32) 1	(22) (33) $1+2$

ℓ=1 (condensed format)

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

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

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

$$\left\langle {}^{11}_{2} \middle| V^2 \cdot V^2 \middle| {}^{11}_{2} \right\rangle = \left(2\binom{2}{11}+\binom{2}{22}\right)^2 + \binom{2}{21}\binom{2}{12} + \binom{2}{32}\binom{2}{23} + 2\binom{2}{31}\binom{2}{13}$$
$$= \tfrac{1}{6}\left(2\cdot 1 - 2\right)^2 + \tfrac{1}{\sqrt{2}}\cdot\tfrac{1}{\sqrt{2}} + \tfrac{1}{\sqrt{2}}\cdot\tfrac{1}{\sqrt{2}} + 2\cdot 1\cdot 1 = 3$$

$$\left\langle {}^{12}_{2} \middle| V^2 \cdot V^2 \middle| {}^{12}_{2} \right\rangle = \left(\binom{2}{11}+2\binom{2}{22}\right)^2 + \binom{2}{21}\binom{2}{12} + 2\binom{2}{32}\binom{2}{23} + \binom{2}{31}\binom{2}{13}$$
$$= \tfrac{1}{6}\left(1\cdot 1 - 2\cdot 2\right)^2 + \tfrac{1}{\sqrt{2}}\cdot\tfrac{1}{\sqrt{2}} + 2\tfrac{1}{\sqrt{2}}\cdot\tfrac{1}{\sqrt{2}} + 1\cdot 1$$
$$= \tfrac{3}{2} + \tfrac{1}{2} + 1 + 1 = 4$$

$$\left\langle {}^{11}_{3} \middle| V^2 \cdot V^2 \middle| {}^{11}_{3} \right\rangle = \left(2\binom{2}{11}+\binom{2}{33}\right)^2 + \binom{2}{21}\binom{2}{12} + 2\binom{2}{32}\binom{2}{23} + \binom{2}{31}\binom{2}{13}$$
$$= \tfrac{1}{6}\left(2\cdot 1 + 1\cdot 1\right)^2 + 2\tfrac{1}{\sqrt{2}}\cdot\tfrac{1}{\sqrt{2}} + \tfrac{1}{\sqrt{2}}\cdot\tfrac{1}{\sqrt{2}} + 1\cdot 1$$
$$= \tfrac{3}{2} + 1 + \tfrac{1}{2} + 1 = 4$$

$$\left\langle {}^{12}_{2} \middle| V^2 \cdot V^2 \middle| {}^{11}_{3} \right\rangle = +\binom{2}{21}\binom{2}{32} + \binom{2}{23}\binom{2}{12}$$
$$= \tfrac{-1}{2}\left(1\cdot 1 + 1\cdot 1\right) = -1$$

$\square\square_{\square}$ = [2,1] *tableau basis and matrices of* $\mathbf{v}^2$ *quadrupole*

$E_{jk} =$

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

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

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

$$\left\langle \mathbf{v}^0_0 \right\rangle = \begin{pmatrix} \binom{0}{11} & \cdot & \cdot \\ \cdot & \binom{0}{22} & \cdot \\ \cdot & \cdot & \binom{0}{33} \end{pmatrix} \qquad \left\langle \mathbf{v}^0_0 \right\rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix}$$

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

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

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

$$\left\langle \begin{smallmatrix}12\\2\end{smallmatrix} \middle| V^2 \cdot V^2 \middle| \begin{smallmatrix}11\\3\end{smallmatrix} \right\rangle = +\binom{2}{21}\binom{2}{32} + \binom{2}{23}\binom{2}{12}$$
$$= \tfrac{-1}{2}\left(1\cdot 1 + 1\cdot 1\right) = -1$$

	$\begin{smallmatrix}1\,1\\2\end{smallmatrix}$		
$\begin{smallmatrix}1\,1\\2\end{smallmatrix}$	3	$\begin{smallmatrix}1\,2\\2\end{smallmatrix}$	$\begin{smallmatrix}1\,1\\3\end{smallmatrix}$
	$\begin{smallmatrix}1\,2\\2\end{smallmatrix}$	4	-1
	$\begin{smallmatrix}1\,1\\3\end{smallmatrix}$	-1	4

[2,1] *tableau basis and matrices of* $\mathbf{v}^2$ *quadrupole*

$E_{jk} =$

	M=2	*M=1*		*M=0*		*M=-1*		*M=-2*
	$\left\vert \begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	$\left\vert \begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle \begin{smallmatrix}11\\2\end{smallmatrix}\right\vert$	(11) (22) 2 + 1	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle \begin{smallmatrix}12\\2\end{smallmatrix}\right\vert$	(21) 1	(11) (22) 1 + 2	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle \begin{smallmatrix}11\\3\end{smallmatrix}\right\vert$	(32) 1	·	(11) (33) 2 + 1	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle \begin{smallmatrix}12\\3\end{smallmatrix}\right\vert$	(31) $-\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{1}{2}}$	(21) $\sqrt{2}$	(11) (22) (33) 1 + 1 + 1	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle \begin{smallmatrix}13\\2\end{smallmatrix}\right\vert$	(31) $\sqrt{\frac{3}{2}}$	(32) $\sqrt{\frac{3}{2}}$	·	·	(11) (22) (33) 1 + 1 + 1	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle \begin{smallmatrix}13\\3\end{smallmatrix}\right\vert$	·	·	(31) 1	(32) $\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{3}{2}}$	(11) (33) 1 + 2	·	(12) 1
$\left\langle \begin{smallmatrix}22\\3\end{smallmatrix}\right\vert$	·	(31) -1	·	(21) $\sqrt{2}$	·	·	(22) (33) 2 + 1	(23) 1
$\left\langle \begin{smallmatrix}23\\3\end{smallmatrix}\right\vert$	·	·	·	(31) $\sqrt{\frac{1}{2}}$	(31) $\sqrt{\frac{3}{2}}$	(21) 1	(32) 1	(22) (33) 1 + 2

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

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

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

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

$$\left\vert {}^2D_{M=2}\right\rangle = \left\vert \begin{smallmatrix}1\,1\\2\end{smallmatrix}\right\rangle$$
$$\left\vert {}^2D_{M=1}\right\rangle = \tfrac{1}{\sqrt{2}}\left\vert \begin{smallmatrix}1\,2\\2\end{smallmatrix}\right\rangle + \tfrac{1}{\sqrt{2}}\left\vert \begin{smallmatrix}1\,1\\3\end{smallmatrix}\right\rangle$$
$$\left\vert {}^2P_{M=1}\right\rangle = \tfrac{1}{\sqrt{2}}\left\vert \begin{smallmatrix}1\,2\\2\end{smallmatrix}\right\rangle - \tfrac{1}{\sqrt{2}}\left\vert \begin{smallmatrix}1\,1\\3\end{smallmatrix}\right\rangle$$

$$\left\langle \begin{smallmatrix}12\\2\end{smallmatrix}\right\vert V^2\cdot V^2 \left\vert \begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle = +\binom{2}{21}\binom{2}{32}+\binom{2}{23}\binom{2}{12}$$
$$= \tfrac{-1}{2}\left(1\cdot 1+1\cdot 1\right) = -1$$

	$\begin{smallmatrix}1\,1\\2\end{smallmatrix}$	$\begin{smallmatrix}1\,2\\2\end{smallmatrix}$	$\begin{smallmatrix}1\,1\\3\end{smallmatrix}$
$\begin{smallmatrix}1\,1\\2\end{smallmatrix}$	3		
$\begin{smallmatrix}1\,2\\2\end{smallmatrix}$		4	-1
$\begin{smallmatrix}1\,1\\3\end{smallmatrix}$		-1	4

Q•Q *eigenvalues*

3 *(j=2)*

3 0 *(j=2)*

0 5 *(j=1)*

AMOP
reference links
on page 2

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-½) 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 $\mathbf{e}_{jk}$ operator expressions for *(e-e)*-interaction matrix

Tensor tables are $(2\ell+1)$-by-$(2\ell+1)$ arrays $\left({}_p{}^k{}_q\right)$ giving $\mathbf{V}_q^k$ in terms of $\mathbf{E}_{p,q}$.
- Relating $\mathbf{V}_q^k$ to $\mathbf{E}_{m',m}$ by $\left({}_{m'}{}^k{}_m\right)$ arrays
- Atomic p-shell *ee*-interaction in elementary operator form

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

[2,1] tableau basis (from p.29) and matrices of $\mathbf{v}^2$ and $\mathbf{v}^2\bullet\mathbf{v}^2$ quadrupole
- ➡ ${}^4S$,${}^2P$, and ${}^2D$ energy calculation of quartet and doublet (spin-½) p^3 orbits

Corrected level diagrams Nitrogen p^3

[2,1] *tableau matrices of* $\mathbf{v}^2$ *quadrupole:* ^4S, ^2P, *and* ^2D *energy calculation*

$E_{jk}=$

	M=2 $\left\|\begin{smallmatrix}11\\2\end{smallmatrix}\right\rangle$	*M=1* $\left\|\begin{smallmatrix}12\\2\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}11\\3\end{smallmatrix}\right\rangle$	*M=0* $\left\|\begin{smallmatrix}12\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}13\\2\end{smallmatrix}\right\rangle$	*M=-1* $\left\|\begin{smallmatrix}13\\3\end{smallmatrix}\right\rangle$	$\left\|\begin{smallmatrix}22\\3\end{smallmatrix}\right\rangle$	*M=-2* $\left\|\begin{smallmatrix}23\\3\end{smallmatrix}\right\rangle$
$\left\langle\begin{smallmatrix}11\\2\end{smallmatrix}\right\|$	(11) (22) $2+1$	(12) 1	(23) 1	(13) $-\sqrt{\frac{1}{2}}$	(13) $\sqrt{\frac{3}{2}}$	·	·	·
$\left\langle\begin{smallmatrix}12\\2\end{smallmatrix}\right\|$	(21) 1	(11) (22) $1+2$	·	(23) $\sqrt{\frac{1}{2}}$	(23) $\sqrt{\frac{3}{2}}$	·	(13) -1	·
$\left\langle\begin{smallmatrix}11\\3\end{smallmatrix}\right\|$	(32) 1	·	(11) (33) $2+1$	(12) $\sqrt{2}$	·	(13) 1	·	·
$\left\langle\begin{smallmatrix}12\\3\end{smallmatrix}\right\|$	(31) $-\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{1}{2}}$	(21) $\sqrt{2}$	(11) (22) (33) $1+1+1$	·	(23) $\sqrt{\frac{1}{2}}$	(12) $\sqrt{2}$	(13) $\sqrt{\frac{1}{2}}$
$\left\langle\begin{smallmatrix}13\\2\end{smallmatrix}\right\|$	(31) $\sqrt{\frac{3}{2}}$	(32) $\sqrt{\frac{3}{2}}$	·	·	(11) (22) (33) $1+1+1$	(23) $\sqrt{\frac{3}{2}}$	·	(13) $\sqrt{\frac{3}{2}}$
$\left\langle\begin{smallmatrix}13\\3\end{smallmatrix}\right\|$	·	·	(31) 1	(32) $\sqrt{\frac{1}{2}}$	(32) $\sqrt{\frac{3}{2}}$	(11) (33) $1+2$	·	(12) 1
$\left\langle\begin{smallmatrix}22\\3\end{smallmatrix}\right\|$	·	(31) -1	·	(21) $\sqrt{2}$	·	·	(22) (33) $2+1$	(23) 1
$\left\langle\begin{smallmatrix}23\\3\end{smallmatrix}\right\|$	·	·	·	(31) $\sqrt{\frac{1}{2}}$	(31) $\sqrt{\frac{3}{2}}$	(21) 1	(32) 1	(22) (33) $1+2$

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

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

$$\left\langle \mathbf{v}^0_0 \right\rangle = \begin{pmatrix} \binom{0}{11} & \cdot & \cdot \\ \cdot & \binom{0}{22} & \cdot \\ \cdot & \cdot & \binom{0}{33} \end{pmatrix} \qquad \left\langle \mathbf{v}^0_0 \right\rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix}$$

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

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

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

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

	$\begin{smallmatrix}1&1\\2\end{smallmatrix}$		
$\begin{smallmatrix}1&1\\2\end{smallmatrix}$	3	$\begin{smallmatrix}1&2\\2\end{smallmatrix}$	$\begin{smallmatrix}1&1\\3\end{smallmatrix}$
	$\begin{smallmatrix}1&2\\2\end{smallmatrix}$	4	-1
	$\begin{smallmatrix}1&1\\3\end{smallmatrix}$	-1	4

Q•Q ***eigenvalues***

3

3	0
0	5

^2P

^2D

Predicated ^2P,^2D levels

^4S

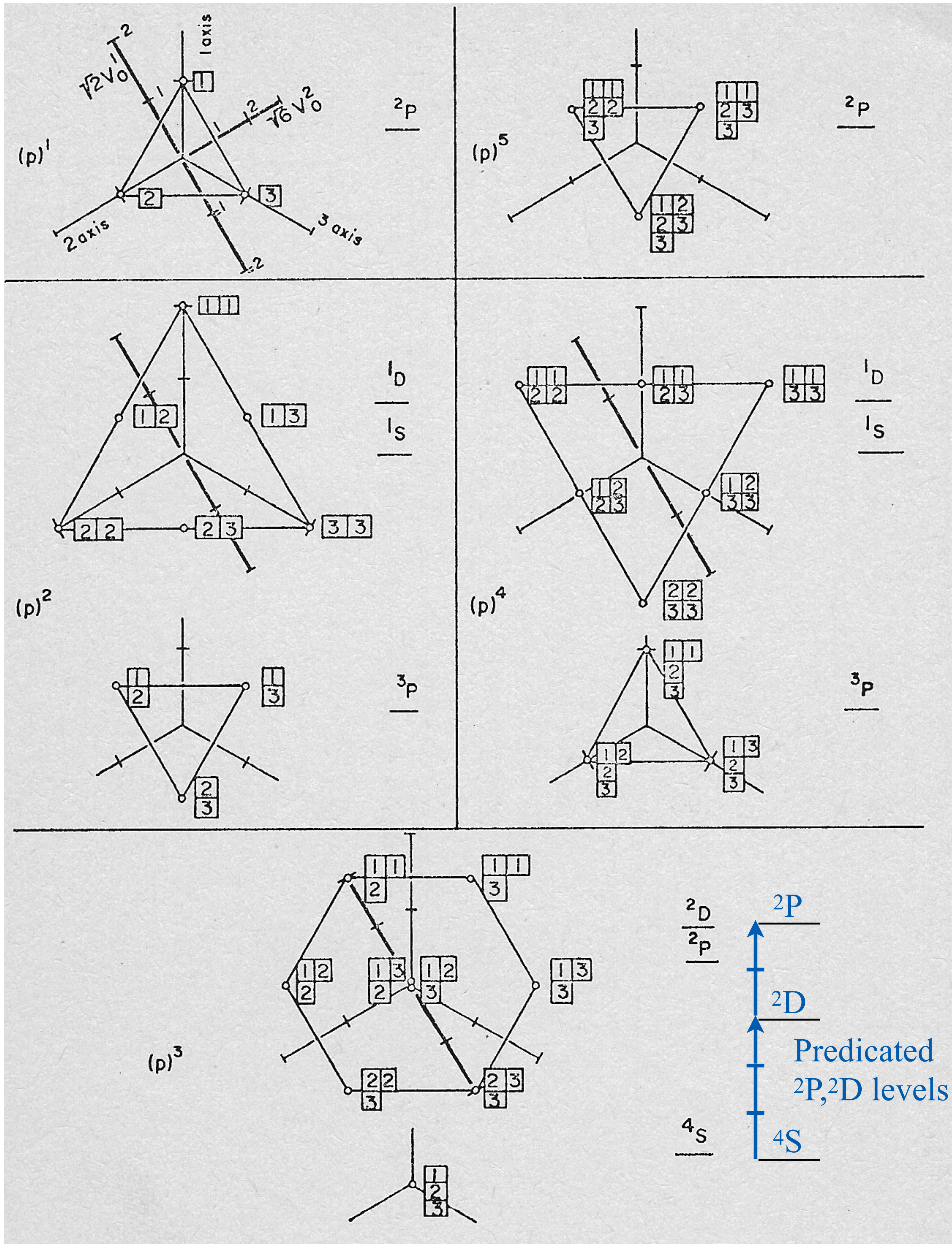


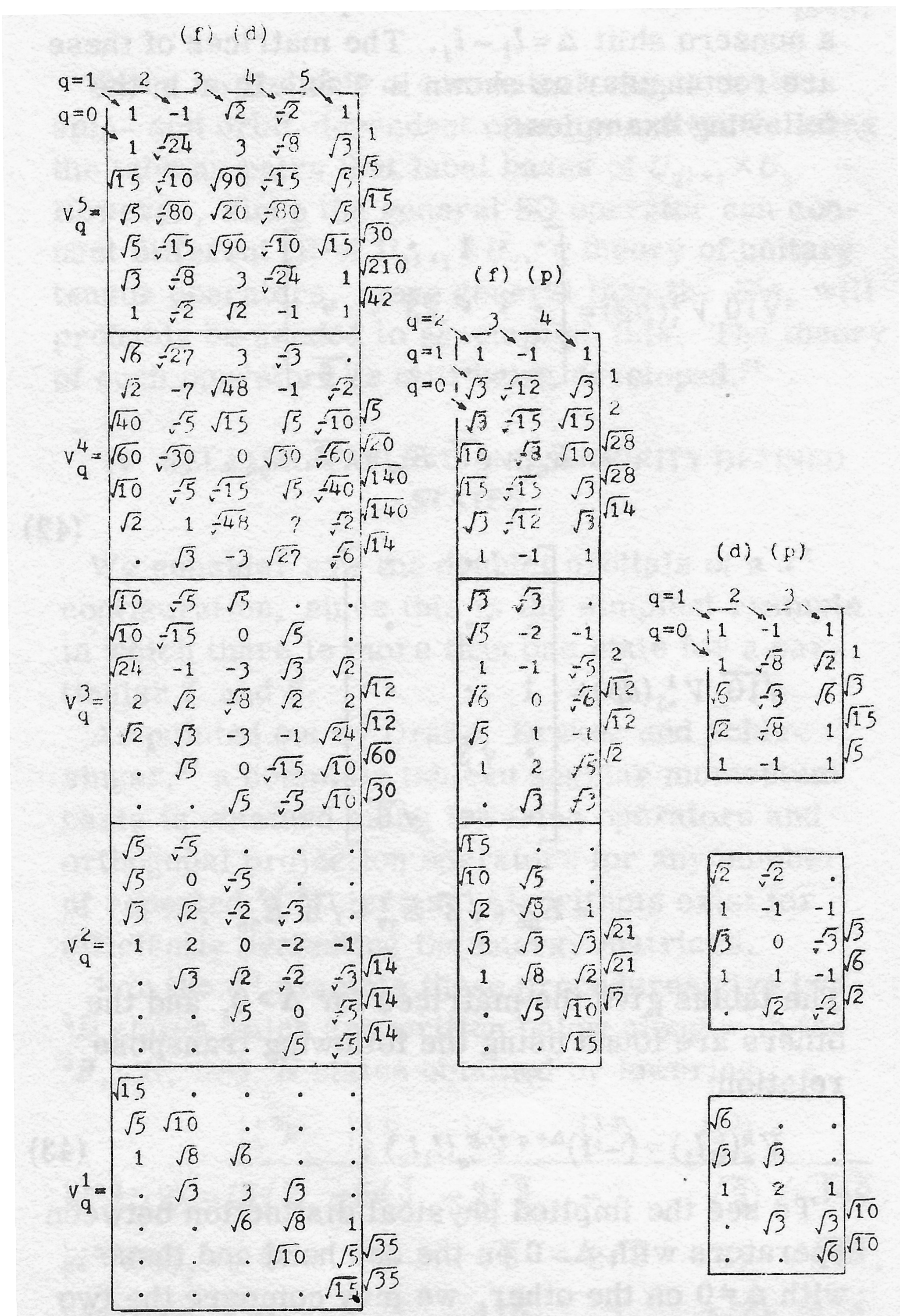
Fig.8 Weight or Moment Diagrams of Atomic $(p)^n$ States
Each tableau is located at point $(x_1\ x_2\ x_3)$ in a cartesian co-ordinate system for which x_n is the number of n's in the tableau. An alternative co-ordinate system is $(v_0^2,\ v_0^1,\ v_0^0)$ defined by Eq.16 which gives the zz-quadrupole 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 ??



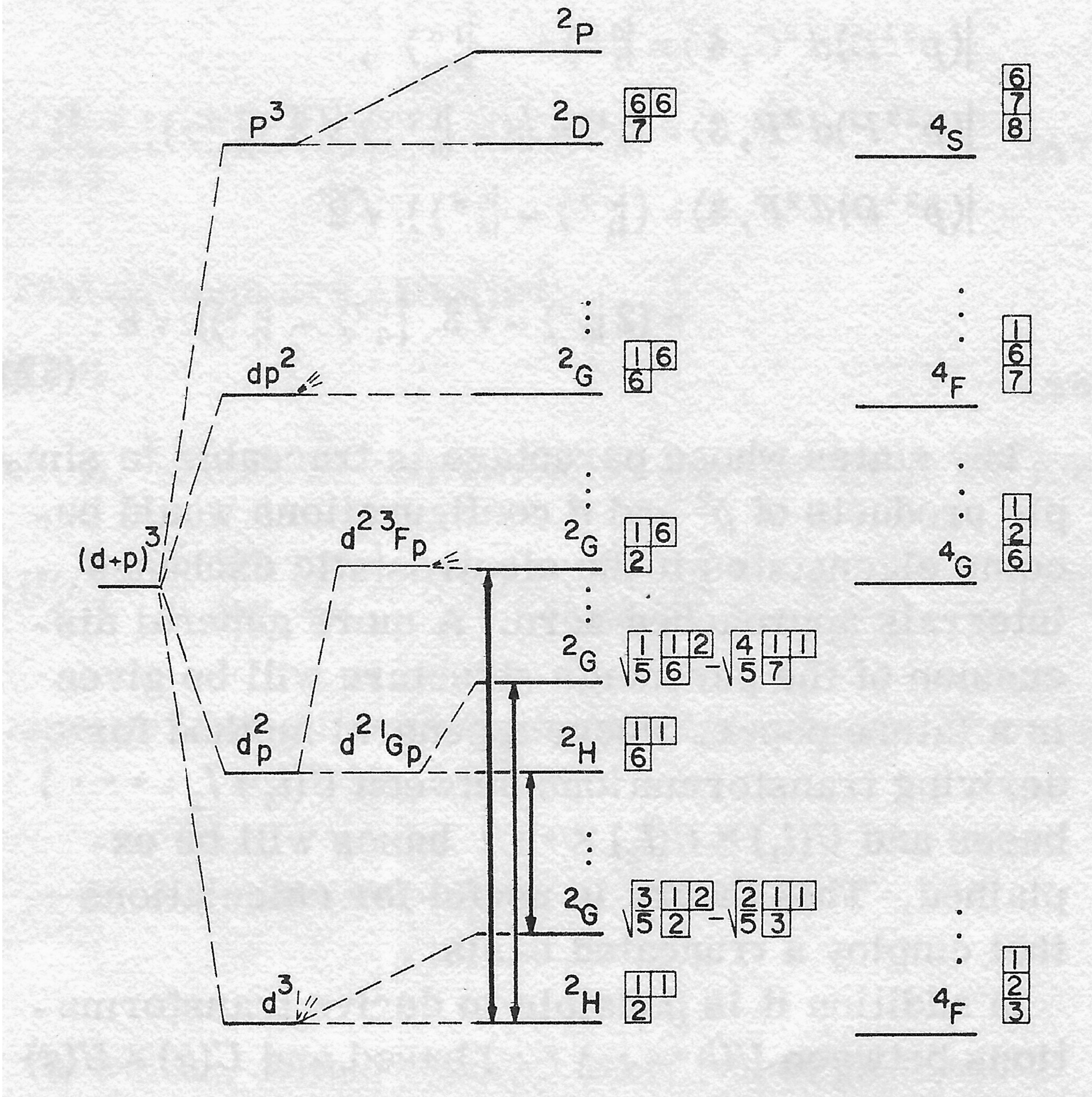
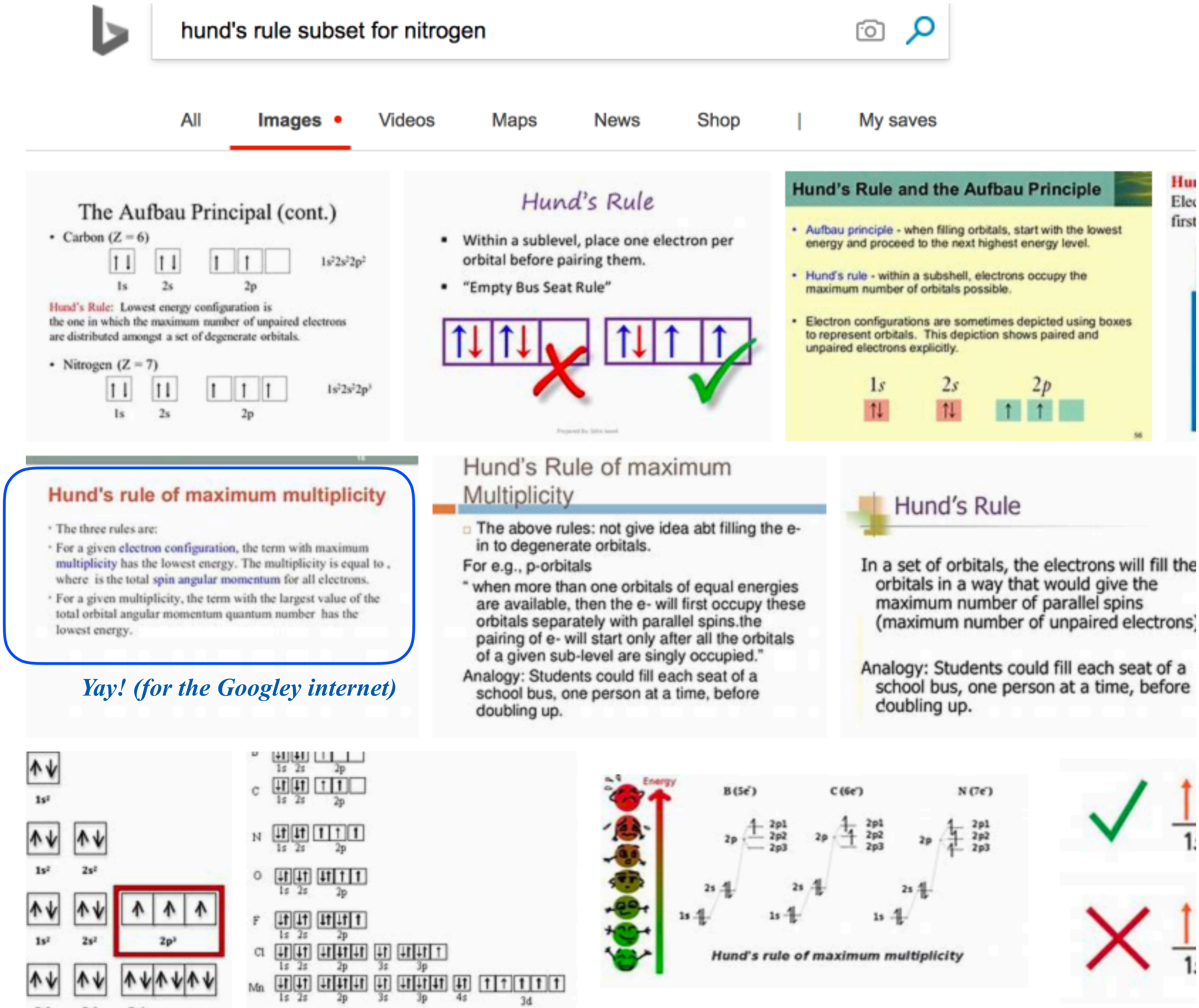


FIG. 6. Example of unitary tableau notation for multiple-shell states. The calculation of the dipole operator using the jawbone formula between states of definite spin and orbit as shown is given in Eq. (48).

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



Yay! (for the Googley internet)

Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

	$\left\vert\begin{smallmatrix}1&1\\2&\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}1&2\\2&\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}1&1\\3&\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}1&2\\3&\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}1&3\\2&\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}1&3\\3&\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}2&2\\3&\end{smallmatrix}\right\rangle$	$\left\vert\begin{smallmatrix}2&3\\3&\end{smallmatrix}\right\rangle$
	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
$\left\langle\begin{smallmatrix}1&1\\2&\end{smallmatrix}\right\vert$	$2^{(11)}+1^{(22)}$	$1^{(12)}$	$1^{(23)}$	$-\sqrt{\frac{1}{2}}^{(13)}$	$\sqrt{\frac{3}{2}}^{(13)}$			
$\left\langle\begin{smallmatrix}1&2\\2&\end{smallmatrix}\right\vert$		$1^{(11)}+2^{(22)}$		$\sqrt{\frac{1}{2}}^{(23)}$	$\sqrt{\frac{3}{2}}^{(23)}$		$-1^{(13)}$	
$\left\langle\begin{smallmatrix}1&1\\3&\end{smallmatrix}\right\vert$			$2^{(11)}+1^{(33)}$	$\sqrt{2}^{(12)}$		$1^{(13)}$		
$\left\langle\begin{smallmatrix}1&2\\3&\end{smallmatrix}\right\vert$				$1^{(11)}+1^{(22)}+1^{(33)}$		$\sqrt{\frac{1}{2}}^{(23)}$	$\sqrt{2}^{(12)}$	$\sqrt{\frac{1}{2}}^{(13)}$
$\left\langle\begin{smallmatrix}1&3\\2&\end{smallmatrix}\right\vert$					$1^{(11)}+1^{(22)}+1^{(33)}$	$\sqrt{\frac{3}{2}}^{(23)}$		$\sqrt{\frac{3}{2}}^{(13)}$
$\left\langle\begin{smallmatrix}1&3\\3&\end{smallmatrix}\right\vert$						$1^{(11)}+2^{(33)}$		$1^{(12)}$
$\left\langle\begin{smallmatrix}2&2\\3&\end{smallmatrix}\right\vert$							$2^{(22)}+1^{(33)}$	$1^{(23)}$
$\left\langle\begin{smallmatrix}2&3\\3&\end{smallmatrix}\right\vert$								$1^{(22)}+2^{(33)}$

$=\langle E_{ij}\rangle$

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:

$$\mathbf{V}_2^2 = E_{13}\ ,\quad -2\mathbf{V}_1^2 = \sqrt{2}(E_{12}-E_{23})\ ,\quad 2\mathbf{V}_{-1}^2 = \sqrt{2}(E_{21}-E_{32})\ ,\quad 2\mathbf{V}_{-2}^2 = E_{31}\ ,$$

$$-2\mathbf{V}_1^1 = \sqrt{2}(E_{12}+E_{23}) \equiv L_+,\quad 2\mathbf{V}_{-1}^1 = \sqrt{2}(E_{21}+E_{32}) \equiv L_-\ .$$

Tableau calculation of 3-electron $\ell=1$ orbital p^3-states and their $\mathbf{V}^k{}_q$ matrices

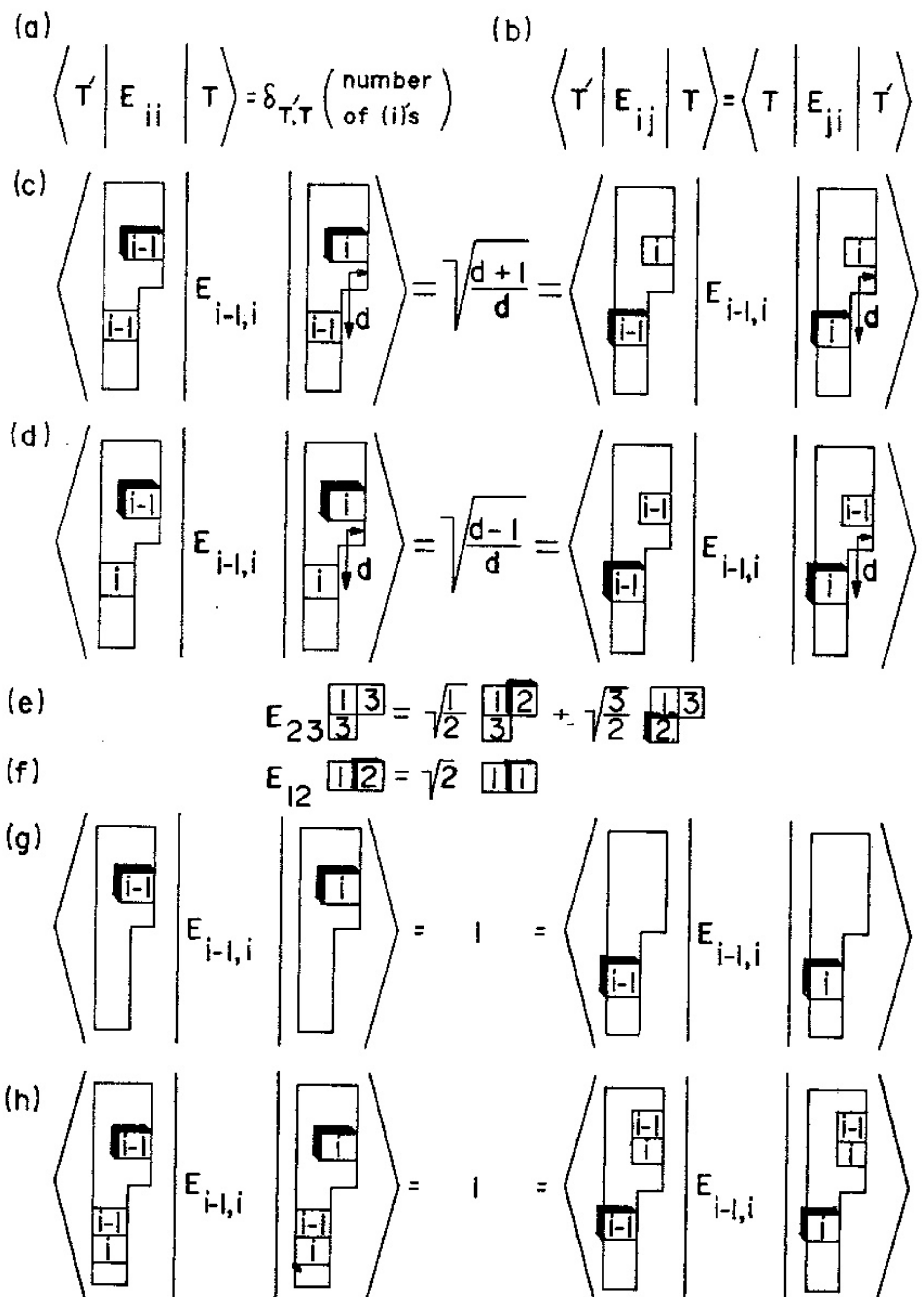
Start with highest angular momentum (L=2) p^3 state: $\left|{}^2D,{}^{L=2}_{M=2}\right\rangle = \begin{smallmatrix}\boxed{1}\boxed{1}\\\boxed{2}\end{smallmatrix}$ (Fermi spin-mate $\begin{smallmatrix}\boxed{\uparrow}\boxed{\uparrow}\\\boxed{\downarrow}\end{smallmatrix}$)

Then apply lowering operator $L_- \equiv \sqrt{2}(E_{21}+E_{32})$

$$\left|{}^2D^{L=2}_{M=1}\right\rangle = \tfrac{1}{2}L_-\left|{}^2D^{L=2}_{M=2}\right\rangle = \tfrac{1}{2}\sqrt{2}(E_{21}+E_{32})\left|\begin{smallmatrix}1&1\\2&\end{smallmatrix}\right\rangle$$

$$= = \frac{1}{\sqrt{2}}\left(\left|\begin{smallmatrix}1&2\\2&\end{smallmatrix}\right\rangle + \left|\begin{smallmatrix}1&1\\3&\end{smallmatrix}\right\rangle\right)$$

Here this is done using Tableau "Jawbone" formula.



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

$$\left|{}^2P^{L=1}_{M=1}\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\begin{smallmatrix}1&2\\2&\end{smallmatrix}\right\rangle - \left|\begin{smallmatrix}1&1\\3&\end{smallmatrix}\right\rangle\right)$$

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

$$\left\langle{}^2P^{L=1}_{M=1}\right|V^k_0\left|{}^2D^{L=2}_{M=1}\right\rangle =$$

$$\frac{1}{\sqrt{2}}\left(\left\langle\begin{smallmatrix}1&2\\2&\end{smallmatrix}\right| + \left\langle\begin{smallmatrix}1&1\\3&\end{smallmatrix}\right|\right)\left[\binom{k}{11}E_{11}+\binom{k}{22}E_{22}+\binom{k}{33}E_{33}\right]\left(\left|\begin{smallmatrix}1&2\\2&\end{smallmatrix}\right\rangle - \left|\begin{smallmatrix}1&1\\3&\end{smallmatrix}\right\rangle\right)$$

$$= \quad \tfrac{1}{2}\left[-\binom{2}{11}E_{11}+2\binom{2}{22}E_{22}-\binom{2}{33}\right] \quad = -\sqrt{\tfrac{3}{2}} \quad \text{for}: \ k=2$$

$$= \quad \tfrac{1}{2}\left[-\binom{1}{11}E_{11}+2\binom{1}{22}E_{22}-\binom{1}{33}\right] \quad = 0 \quad \text{for}: \ k=1$$

$$= \quad \tfrac{1}{2}\left[-\binom{0}{11}E_{11}+2\binom{0}{22}E_{22}-\binom{0}{33}\right] \quad = 0 \quad \text{for}: \ k=0$$

$$\left|1,2,3\right\rangle \equiv \left|1\right\rangle_{particle-a}\left|2\right\rangle_{particle-b}\left|3\right\rangle_{particle-c} \equiv \left|1\right\rangle_{a}\left|2\right\rangle_{b}\left|3\right\rangle_{c}$$

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

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

$e_{12}e_{21}=e_{11}$ $\quad |1\rangle\langle 2\|2\rangle\langle 1| = |1\rangle\langle 1|$

$e_{12}e_{22}=e_{12}$ $\quad |1\rangle\langle 2\|2\rangle\langle 2| = |1\rangle\langle 2|$

Elementary matrix algebra $\quad \vdots$

$e_{jk}e_{pq}=\delta_{pk}e_{jq}$ $\quad |j\rangle\langle k\|p\rangle\langle q| = \delta_{pk}|j\rangle\langle q|$

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 (ℓ=1) representation of L_x, L_y, and L_z

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

Elementary operator form of L_x, L_y, and L_z

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

…and of raise-lower operators L_+ and L_-

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