AMOP reference links on following page

2.12.18 class 9.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Wigner D^J_{mn} irreps of U(2)~R(3) give atomic and molecular eigenfunctions $\Psi_{m,n}$ of 3D rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ and angular momentum uncertainty effects.

Review 1. *Angular momentum raise-n-lower operators* $\mathbf{S}_+$ and $\mathbf{S}_-$ Review 2. Angular momentum commutation

Review 3. *SU(2)⊂U(2) oscillators vs. R(3)⊂O(3) rotors*

Angular momentum magnitude and Θ^J_m-uncertainty cone polar angles

Generating higher-j representations D^j_{mn} of R(3) rotation and U(2) from spinor $D^{1/2}$ irreps

Evaluating D^j_{mn} representations

Applications of D^j_{mn} representations

Atomic wave functions. $D^L_{m0}\sim Y^L_m$ *Spherical harmonics*

$D^{L=1}_{m0}\sim Y^1_m$ *p-waves* $D^{L=2}_{m0}\sim Y^2_m$ *d-waves* $D^L_{00}\sim P^L$ *Legendre waves*

Molecular D^j_{mn} wave functions in "Mock-Mach" lab-vs-body state space $|^J_{mn}\rangle$

$\mathbf{P}^j_{mn}$ *projector and* $D^j_{mn}(\alpha,\beta,\gamma)$ *wave function*

D^J_{mn} *transform* $\mathbf{R}_{(\alpha,\beta,\gamma)}|^J_{mn}\rangle=\Sigma_{m'}D^J_{m'n}(\alpha,\beta,\gamma)|^J_{m'n}\rangle$ *in lab-space,* $\bar{\mathbf{R}}_{(\alpha,\beta,\gamma)}$ *in body-space.*

D^2_{mn} *transform in lab-space (Generalized Stern-Gerlach beam polarization)*

Θ^J_m-cone properties of lab transforms: J=20, J=10, J=30.

Θ^J_m-analysis of high J atomic beams

Θ^J_m-properties of high J molecular lab-vs-body states $|^J_{mn}\rangle$

Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar* $\mathbf{T}_0^0$ *or tensor* $\mathbf{T}_q^2$ *operators*

Rotational Energy Surfaces (RE or RES) of symmetric rotor and eigensolutions

Rotational Energy Surfaces (RE or RES) of asymmetric rotor (for following class)

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

Web Resources - front page

UAF Physics UTube channel

2014 AMOP

2017 Group Theory for QM

2018 AMOP

Frame Transformation Relations And Multipole Transitions In Symmetric Polyatomic Molecules - RMP-1978 (Alt Scanned version)
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
AMOP Ch 32 Molecular Symmetry and Dynamics - 2019
AMOP Ch 0 Space-Time Symmetry - 2019

RESONANCE AND REVIVALS

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

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

**In development - a Web based AMOP Reference page, with more options/control over display*

Review 1. *Angular momentum raise-n-lower operators* $\mathbf{S}_+$ and $\mathbf{S}_-$

$\mathbf{s}_+ = \mathbf{s}_X + i\mathbf{s}_Y$ and $\mathbf{s}_- = \mathbf{s}_X - i\mathbf{s}_Y = \mathbf{s}_+^\dagger$

Review Class 8 p92

Starting with *j=1/2* we see that $\mathbf{S}_+$ is an *elementary projection operator* $\mathbf{e}_{12} = |1\rangle\langle 2| = \mathbf{P}_{12}$

$$\langle \mathbf{s}_+ \rangle^{\frac{1}{2}} = D^{\frac{1}{2}}(\mathbf{s}_+) = D^{\frac{1}{2}}(\mathbf{s}_X + i\mathbf{s}_Y) = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} + i \begin{pmatrix} 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \mathbf{P}_{12}$$

Such operators can be upgraded to *creation-destruction operator* combinations $\mathbf{a}^\dagger\mathbf{a}$

$$\mathbf{s}_+ = \mathbf{a}_1^\dagger \mathbf{a}_2 = \mathbf{a}_\uparrow^\dagger \mathbf{a}_\downarrow \quad , \qquad \mathbf{s}_- = \left(\mathbf{a}_1^\dagger \mathbf{a}_2\right)^\dagger = \mathbf{a}_2^\dagger \mathbf{a}_1 = \mathbf{a}_\downarrow^\dagger \mathbf{a}_\uparrow$$

Hamilton-Pauli-Jordan representation of $\mathbf{s}_Z$ is: $\langle \mathbf{s}_Z \rangle^{\left(\frac{1}{2}\right)} = D^{\left(\frac{1}{2}\right)}(\mathbf{s}_Z) = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$

This suggests an $\mathbf{a}^\dagger\mathbf{a}$ form for $\mathbf{s}_Z$.

$$\mathbf{s}_Z = \tfrac{1}{2}\left(\mathbf{a}_1^\dagger \mathbf{a}_1 - \mathbf{a}_2^\dagger \mathbf{a}_2\right) = \tfrac{1}{2}\left(\mathbf{a}_\uparrow^\dagger \mathbf{a}_\uparrow - \mathbf{a}_\downarrow^\dagger \mathbf{a}_\downarrow\right)$$

Let $\mathbf{a}_1^\dagger = \mathbf{a}_\uparrow^\dagger$ create up-spin ↑

$$|1\rangle = |\uparrow\rangle = \left| \begin{matrix} 1/2 \\ +1/2 \end{matrix} \right\rangle = \mathbf{a}_1^\dagger|0\rangle = \mathbf{a}_\uparrow^\dagger|0\rangle$$

destroys dn-spin ↓

creates up-spin ↑

to raise angular momentum by one $\hbar$ unit

$$\mathbf{a}_\uparrow^\dagger \mathbf{a}_\downarrow |\downarrow\rangle = |\uparrow\rangle \quad \text{or:} \quad \mathbf{a}_1^\dagger \mathbf{a}_2 |2\rangle = |1\rangle$$

Let $\mathbf{a}_2^\dagger = \mathbf{a}_\downarrow^\dagger$ create dn-spin ↓

$$|2\rangle = |\downarrow\rangle = \left| \begin{matrix} 1/2 \\ -1/2 \end{matrix} \right\rangle = \mathbf{a}_2^\dagger|0\rangle = \mathbf{a}_\downarrow^\dagger|0\rangle$$

$\mathbf{s}_- = \mathbf{a}_2^\dagger \mathbf{a}_1 = \mathbf{a}_\downarrow^\dagger \mathbf{a}_\uparrow$ destroys up-spin ↑

creates dn-spin ↓

to lower angular momentum by one $\hbar$ unit

$$\mathbf{a}_\downarrow^\dagger \mathbf{a}_\uparrow |\uparrow\rangle = |\downarrow\rangle \quad \text{or:} \quad \mathbf{a}_2^\dagger \mathbf{a}_1 |1\rangle = |2\rangle$$

Review 2. *Angular momentum commutation relations*

Given Hamilton-Jordan-Pauli product relations : $\sigma_\alpha \sigma_\beta = \delta_{\alpha\beta} + i\varepsilon_{\alpha\beta\gamma}\sigma_\gamma$ with: $\mathbf{s}_\alpha = \sigma_\alpha / 2$

Commutator formulae for $\mathbf{s}_\alpha$: $\mathbf{s}_\alpha \mathbf{s}_\beta - \mathbf{s}_\beta \mathbf{s}_\alpha = [\mathbf{s}_\alpha, \mathbf{s}_\beta] = i\,\varepsilon_{\alpha\beta\gamma}\mathbf{s}_\gamma$

$\sigma_X \sigma_Y = i\sigma_Z$ implies: $[\mathbf{s}_X, \mathbf{s}_Y] = i\mathbf{s}_Z$

$\sigma_Z \sigma_X = i\sigma_Y$ implies: $[\mathbf{s}_Z, \mathbf{s}_X] = i\mathbf{s}_Y$

$\sigma_Y \sigma_Z = i\sigma_X$ implies: $[\mathbf{s}_Y, \mathbf{s}_Z] = i\mathbf{s}_X$

Key Lie theorem:

$\mathbf{s}_Z$ and $\mathbf{s}_\pm = \mathbf{s}_X \pm i\mathbf{s}_Y$ obey *eigen-commutation relations*. $[\mathbf{s}_Z, \mathbf{s}_+] = (+1)\mathbf{s}_+$ and: $[\mathbf{s}_Z, \mathbf{s}_-] = (-1)\mathbf{s}_-$

Proof using elementary matrix operator multiplication: $\mathbf{e}_{jk}\,\mathbf{e}_{mn} = \delta_{km}\,\mathbf{e}_{jn}$ with: $\mathbf{s}_+ = \mathbf{e}_{12}$ and: $\mathbf{s}_- = \mathbf{e}_{21}$

Also: $\mathbf{s}_Z = (\mathbf{e}_{11} - \mathbf{e}_{22})/2 \approx \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}$ $\quad \approx \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ $\quad \approx \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

$\mathbf{e}_{jk}\,\mathbf{e}_{mn} = \delta_{km}\,\mathbf{e}_{jn}$ gives: $[\overbrace{(\mathbf{e}_{11} - \mathbf{e}_{22})/2}^{\mathbf{s}_Z}, \overbrace{\mathbf{e}_{12}}^{\mathbf{s}_+}] = \overbrace{+\mathbf{e}_{12}}^{\mathbf{s}_+}$ and: $[\overbrace{(\mathbf{e}_{11} - \mathbf{e}_{22})/2}^{\mathbf{s}_Z}, \overbrace{\mathbf{e}_{21}}^{\mathbf{s}_-}] = \overbrace{-\mathbf{e}_{21}}^{-\mathbf{s}_-}$

Then there are *up-down commutation relations*: $[\mathbf{s}_+, \mathbf{s}_-] = [\mathbf{e}_{12}, \mathbf{e}_{21}] = \mathbf{e}_{11} - \mathbf{e}_{22} = 2\mathbf{s}_Z$

General eigen-commutation theorem:

$n_1 = j + m$

$n_2 = j - m$

If Hamiltonian $\mathbf{H}$ (or any operator such as $\mathbf{s}_Z$) eigen-commutes with $\mathbf{a}_m$ and $\mathbf{a}^\dagger_n$, that is:

$[\mathbf{H}, \mathbf{a}^\dagger_n] = \omega_n\,\mathbf{a}^\dagger_n$ and $[\mathbf{H}, \mathbf{a}_m] = \omega_m \mathbf{a}_m$, then $\mathbf{H}$ is a combination $\omega_n \mathbf{a}^\dagger_n \mathbf{a}_n$ of number operators.

$$\mathbf{H} = \sum_{n=1}^{2} \omega_n \mathbf{a}^\dagger_n \mathbf{a}_n = \omega_1 \mathbf{a}^\dagger_1 \mathbf{a}_1 + \omega_2 \mathbf{a}^\dagger_2 \mathbf{a}_2 \approx \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix}$$

U(2) Oscillator eigensolutions:

$$\mathbf{H}|n_1 n_2\rangle = \sum_{n=1}^{2} \omega_n \mathbf{a}^\dagger_n \mathbf{a}_n |n_1 n_2\rangle = (\omega_1 n_1 + \omega_2 n_2)|n_1 n_2\rangle = (\omega_1 (j+m) + \omega_2 (j-m))\left|{}^{j}_{m}\right\rangle$$

Review 3. *SU(2)⊂U(2) oscillators vs. R(3)⊂O(3) rotors*

Review Class 8 p 104

U(2) boson oscillator states $|n_1,n_2\rangle$ = R(3) spin or rotor states $\left|\begin{smallmatrix} j \\ m \end{smallmatrix}\right\rangle$

Oscillator total quanta: $\upsilon=(n_1+n_2)$ Rotor total momenta: $j=\upsilon/2$ and z-momenta: $m=(n_1-n_2)/2$

$$\left|n_1 n_2\right\rangle = \frac{\left(\mathbf{a}_1^\dagger\right)^{n_1}\left(\mathbf{a}_2^\dagger\right)^{n_2}}{\sqrt{n_1!\,n_2!}}\left|0\;0\right\rangle = \frac{\left(\mathbf{a}_1^\dagger\right)^{j+m}\left(\mathbf{a}_2^\dagger\right)^{j-m}}{\sqrt{(j+m)!\,(j-m)!}}\left|0\;0\right\rangle = \left|\begin{smallmatrix} j \\ m \end{smallmatrix}\right\rangle$$

$j=\upsilon/2=(n_1+n_2)/2$

$m=(n_1-n_2)/2$

$n_1=j+m$

$n_2=j-m$

U(2) boson oscillator states = *U(2)* spinor states

$$\left|n_\uparrow n_\downarrow\right\rangle = \frac{\left(\mathbf{a}_\uparrow^\dagger\right)^{n_1}\left(\mathbf{a}_\downarrow^\dagger\right)^{n_2}}{\sqrt{n_\uparrow!\,n_\downarrow!}}\left|0\;0\right\rangle = \frac{\left(\mathbf{a}_\uparrow^\dagger\right)^{j+m}\left(\mathbf{a}_\downarrow^\dagger\right)^{j-m}}{\sqrt{(j+m)!\,(j-m)!}}\left|0\;0\right\rangle = \left|\begin{smallmatrix} j \\ m \end{smallmatrix}\right\rangle$$

Oscillator $\mathbf{a}^\dagger\mathbf{a}$ give $\mathbf{s}_\pm$ matrices.

$$\mathbf{a}_1^\dagger\mathbf{a}_2\left|n_1 n_2\right\rangle = \sqrt{n_1+1}\sqrt{n_2}\left|n_1+1\;n_2-1\right\rangle \Rightarrow \mathbf{s}_+\left|\begin{smallmatrix} j \\ m \end{smallmatrix}\right\rangle = \sqrt{j+m+1}\sqrt{j-m}\left|\begin{smallmatrix} j \\ m+1 \end{smallmatrix}\right\rangle$$

$$\mathbf{a}_2^\dagger\mathbf{a}_1\left|n_1 n_2\right\rangle = \sqrt{n_1}\sqrt{n_2+1}\left|n_1-1\;n_2+1\right\rangle \Rightarrow \mathbf{s}_-\left|\begin{smallmatrix} j \\ m \end{smallmatrix}\right\rangle = \sqrt{j+m}\sqrt{j-m+1}\left|\begin{smallmatrix} j \\ m-1 \end{smallmatrix}\right\rangle$$

1/2-difference of number-ops is $\mathbf{s}_Z$ eigenvalue.

$$\left.\begin{array}{l}\mathbf{a}_1^\dagger\mathbf{a}_1\left|n_1 n_2\right\rangle = n_1\left|n_1 n_2\right\rangle \\ \mathbf{a}_2^\dagger\mathbf{a}_2\left|n_1 n_2\right\rangle = n_2\left|n_1 n_2\right\rangle\end{array}\right\} \mathbf{s}_Z\left|\begin{smallmatrix} j \\ m \end{smallmatrix}\right\rangle = \tfrac{1}{2}\left(\mathbf{a}_1^\dagger\mathbf{a}_1 - \mathbf{a}_2^\dagger\mathbf{a}_2\right)\left|\begin{smallmatrix} j \\ m \end{smallmatrix}\right\rangle = \frac{n_1-n_2}{2}\left|\begin{smallmatrix} j \\ m \end{smallmatrix}\right\rangle = m\left|\begin{smallmatrix} j \\ m \end{smallmatrix}\right\rangle$$

j=1 vector $\mathbf{s}_+$ ...*and* $\mathbf{s}_Z$

$$D^1(\mathbf{s}_+) = D^1(\mathbf{s}_X + i\mathbf{s}_Y) = \begin{pmatrix} \cdot & \frac{\sqrt{2}}{2} & \cdot \\ \frac{\sqrt{2}}{2} & \cdot & \frac{\sqrt{2}}{2} \\ \cdot & \frac{\sqrt{2}}{2} & \cdot \end{pmatrix} + i\begin{pmatrix} \cdot & -i\frac{\sqrt{2}}{2} & \cdot \\ i\frac{\sqrt{2}}{2} & \cdot & -i\frac{\sqrt{2}}{2} \\ \cdot & i\frac{\sqrt{2}}{2} & \cdot \end{pmatrix} = \begin{pmatrix} \cdot & \sqrt{2} & \cdot \\ 0 & \cdot & \sqrt{2} \\ \cdot & 0 & \cdot \end{pmatrix}, \qquad D^1(\mathbf{s}_Z) = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$$

j=3/2 spinor $\mathbf{s}_+$ ...*and* $\mathbf{s}_Z$

$$D^{\frac{3}{2}}(\mathbf{s}_+) = \begin{pmatrix} \cdot & \sqrt{3} & \cdot & \cdot \\ 0 & \cdot & \sqrt{4} & \cdot \\ \cdot & 0 & \cdot & \sqrt{3} \\ \cdot & \cdot & 0 & \cdot \end{pmatrix} = \left(D^{\frac{3}{2}}(\mathbf{s}_-)\right)^\dagger, \qquad D^{\frac{3}{2}}(\mathbf{s}_Z) = \begin{pmatrix} \frac{3}{2} & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{2} & \cdot & \cdot \\ \cdot & \cdot & -\frac{1}{2} & \cdot \\ \cdot & \cdot & \cdot & -\frac{3}{2} \end{pmatrix}$$

j=2 tensor $\mathbf{s}_+$ ...*and* $\mathbf{s}_Z$

$$D^2(\mathbf{s}_+) = \begin{pmatrix} \cdot & \sqrt{4} & \cdot & \cdot & \cdot \\ 0 & \cdot & \sqrt{3} & \cdot & \cdot \\ \cdot & 0 & \cdot & \sqrt{3} & \cdot \\ \cdot & \cdot & 0 & \cdot & \sqrt{4} \\ \cdot & \cdot & \cdot & 0 & \cdot \end{pmatrix} = \left(D^2(\mathbf{s}_-)\right)^\dagger, \qquad D^2(\mathbf{s}_Z) = \begin{pmatrix} 2 & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot & -1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & -2 \end{pmatrix}$$

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D^J_{mn} *transform* $\mathbf{R}(\alpha,\beta,\gamma)|^J_{mn}\rangle=\Sigma_{m'}D^J_{m'n}(\alpha,\beta,\gamma)|^J_{m'n}\rangle$ *in lab-space,* $\bar{\mathbf{R}}(\alpha,\beta,\gamma)$ *in body-space.*

D^2_{mn} *transform in lab-space (Generalized Stern-Gerlach beam polarization)*

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Rotational Energy Surfaces (RE or RES) of symmetric rotor and eigensolutions

Rotational Energy Surfaces (RE or RES) of asymmetric rotor (for following class)

Angular momentum magnitude and uncertainty

$\mathbf{s}_\pm = \mathbf{s}_X \pm i\mathbf{s}_Y$

$\mathbf{s}_+ = \mathbf{a}_1^\dagger \mathbf{a}_2$

$\mathbf{s}_- = \mathbf{a}_2^\dagger \mathbf{a}_1$

$\mathbf{s}_Z = \frac{1}{2}\left(\mathbf{a}_1^\dagger \mathbf{a}_1 - \mathbf{a}_2^\dagger \mathbf{a}_2\right)$

Angular momentum squared $\mathbf{s}\bullet\mathbf{s}$ and Z-component $\mathbf{s}_Z$ share eigenstates

$$\mathbf{s}\bullet\mathbf{s} = \mathbf{s}_X{}^2 + \mathbf{s}_Y{}^2 + \mathbf{s}_Z{}^2 = (\mathbf{s}_+\mathbf{s}_- + \mathbf{s}_-\mathbf{s}_+)/2 + \mathbf{s}_Z{}^2$$

Angular momentum magnitude and uncertainty

$\mathbf{s}_{\pm} = \mathbf{s}_X \pm i\mathbf{s}_Y$

$\mathbf{s}_{+} = \mathbf{a}_1^{\dagger}\mathbf{a}_2$

$\mathbf{s}_{-} = \mathbf{a}_2^{\dagger}\mathbf{a}_1$

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Angular momentum squared $\mathbf{s}\bullet\mathbf{s}$ and Z-component $\mathbf{s}_Z$ share eigenstates

$$\mathbf{s}\bullet\mathbf{s} = \mathbf{s}_X^2 + \mathbf{s}_Y^2 + \mathbf{s}_Z^2 = (\mathbf{s}_+\mathbf{s}_- + \mathbf{s}_-\mathbf{s}_+)/2 + \mathbf{s}_Z^2$$

j=1/2 fundamental matrices square up not to *(1/2)*^{2} *=1/4* but to *3/4*.

$$D^{\frac{1}{2}}\left(\mathbf{S}_X^2 + \mathbf{S}_Y^2 + \mathbf{S}_Z^2\right) = \frac{1}{4}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\cdot\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\cdot\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\cdot\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Angular momentum magnitude and uncertainty

$$\mathbf{s}_{\pm}=\mathbf{s}_X \pm i\mathbf{s}_Y$$
$$\mathbf{s}_{+}=\mathbf{a}_1^\dagger \mathbf{a}_2$$
$$\mathbf{s}_{-}=\mathbf{a}_2^\dagger \mathbf{a}_1$$
$$\mathbf{s}_Z=\tfrac{1}{2}\left(\mathbf{a}_1^\dagger \mathbf{a}_1-\mathbf{a}_2^\dagger \mathbf{a}_2\right)$$

Angular momentum squared $\mathbf{s}\bullet\mathbf{s}$ and Z-component $\mathbf{s}_Z$ share eigenstates

$$\mathbf{s}\bullet\mathbf{s}=\mathbf{s}_X^2+\mathbf{s}_Y^2+\mathbf{s}_Z^2=(\mathbf{s}_+\mathbf{s}_-+\mathbf{s}_-\mathbf{s}_+)/2+\mathbf{s}_Z^2$$

j=1/2 fundamental matrices square up not to *(1/2)*^{2} *=1/4* but to *3/4*.

$$D^{\frac{1}{2}}\left(\mathbf{S}_X^2+\mathbf{S}_Y^2+\mathbf{S}_Z^2\right)=\frac{1}{4}\begin{pmatrix}0&1\\1&0\end{pmatrix}\cdot\begin{pmatrix}0&1\\1&0\end{pmatrix}+\frac{1}{4}\begin{pmatrix}0&-i\\i&0\end{pmatrix}\cdot\begin{pmatrix}0&-i\\i&0\end{pmatrix}+\frac{1}{4}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\cdot\begin{pmatrix}1&0\\0&-1\end{pmatrix}=\frac{3}{4}\begin{pmatrix}1&0\\0&1\end{pmatrix}$$

In terms of **a**-operators the squared momentum operator is

$$\mathbf{s}\bullet\mathbf{s}=\tfrac{1}{4}\left[2\mathbf{a}_1^\dagger\mathbf{a}_2\mathbf{a}_2^\dagger\mathbf{a}_1+2\mathbf{a}_2^\dagger\mathbf{a}_1\mathbf{a}_1^\dagger\mathbf{a}_2+\left(\mathbf{a}_1^\dagger\mathbf{a}_1-\mathbf{a}_2^\dagger\mathbf{a}_2\right)\left(\mathbf{a}_1^\dagger\mathbf{a}_1-\mathbf{a}_2^\dagger\mathbf{a}_2\right)\right]$$

Angular momentum magnitude and uncertainty

$\mathbf{s}_{\pm}=\mathbf{s}_X \pm i\mathbf{s}_Y$

$\mathbf{s}_+=\mathbf{a}_1^\dagger \mathbf{a}_2$

$\mathbf{s}_-=\mathbf{a}_2^\dagger \mathbf{a}_1$

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Angular momentum squared $\mathbf{s}\bullet\mathbf{s}$ and Z-component $\mathbf{s}_Z$ share eigenstates

$$\mathbf{s}\bullet\mathbf{s} = \mathbf{s}_X^2 + \mathbf{s}_Y^2 + \mathbf{s}_Z^2 = (\mathbf{s}_+\mathbf{s}_- + \mathbf{s}_-\mathbf{s}_+)/2 + \mathbf{s}_Z^2$$

j=1/2 fundamental matrices square up not to *(1/2)*^{2} *=1/4* but to *3/4*.

$$D^{\frac{1}{2}}\left(\mathbf{S}_X^2+\mathbf{S}_Y^2+\mathbf{S}_Z^2\right)=\frac{1}{4}\begin{pmatrix}0&1\\1&0\end{pmatrix}\cdot\begin{pmatrix}0&1\\1&0\end{pmatrix}+\frac{1}{4}\begin{pmatrix}0&-i\\i&0\end{pmatrix}\cdot\begin{pmatrix}0&-i\\i&0\end{pmatrix}+\frac{1}{4}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\cdot\begin{pmatrix}1&0\\0&-1\end{pmatrix}=\frac{3}{4}\begin{pmatrix}1&0\\0&1\end{pmatrix}$$

In terms of **a**-operators the squared momentum operator is

$$\mathbf{s}\bullet\mathbf{s}=\frac{1}{4}\left[2\mathbf{a}_1^\dagger\mathbf{a}_2\mathbf{a}_2^\dagger\mathbf{a}_1+2\mathbf{a}_2^\dagger\mathbf{a}_1\mathbf{a}_1^\dagger\mathbf{a}_2+\left(\mathbf{a}_1^\dagger\mathbf{a}_1-\mathbf{a}_2^\dagger\mathbf{a}_2\right)\left(\mathbf{a}_1^\dagger\mathbf{a}_1-\mathbf{a}_2^\dagger\mathbf{a}_2\right)\right]$$

Using $\mathbf{a}_m\mathbf{a}^\dagger_n = \mathbf{a}^\dagger_n\,\mathbf{a}_m + \delta_{mn}\mathbf{1}$ gives $\mathbf{s}\bullet\mathbf{s}$ as number operators.

(Normal order: *left←creation*, *destruct→right*.)

Angular momentum magnitude and uncertainty

$\mathbf{s}_\pm = \mathbf{s}_X \pm i\mathbf{s}_Y$

$\mathbf{s}_+ = \mathbf{a}_1^\dagger \mathbf{a}_2$

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Has <u>very</u> simple j-formula…

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Magnitude $|\mathbf{J}| = \sqrt{j(j+1)}$ of angular momentum $\mathbf{s}=\mathbf{J}$:
(approaches $j+½$ for large j)

$$\left|\mathbf{s}\right|\left|{j \atop m}\right\rangle = \sqrt{\mathbf{s}\bullet\mathbf{s}}\left|{j \atop m}\right\rangle = \sqrt{j\left(j+1\right)}\left|{j \atop m}\right\rangle \cong \left(j+\tfrac{1}{2}\right)\left|{j \atop m}\right\rangle$$

Wigner D^J_{mn} irreps of U(2)~R(3) give atomic and molecular eigenfunctions $\Psi_{m,n}$ of 3D rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ and angular momentum uncertainty effects.

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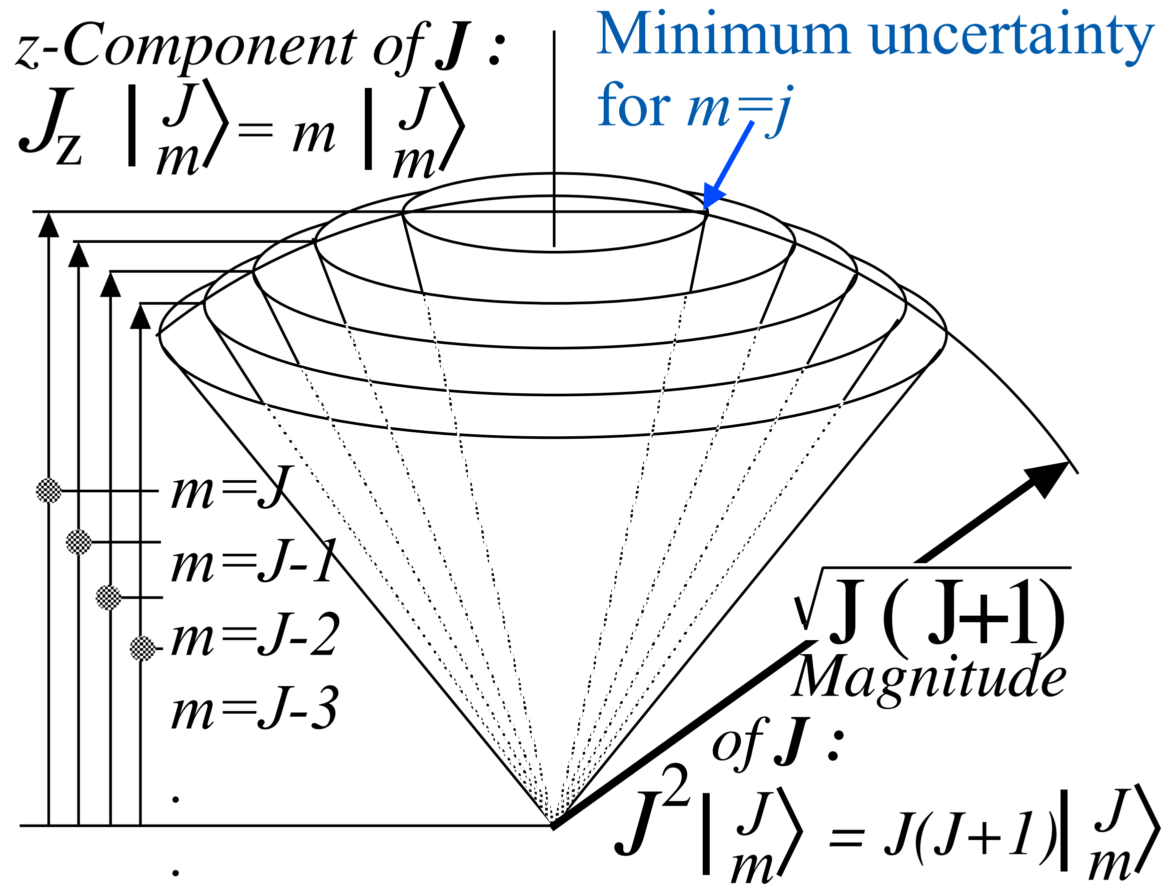

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For j=m=½

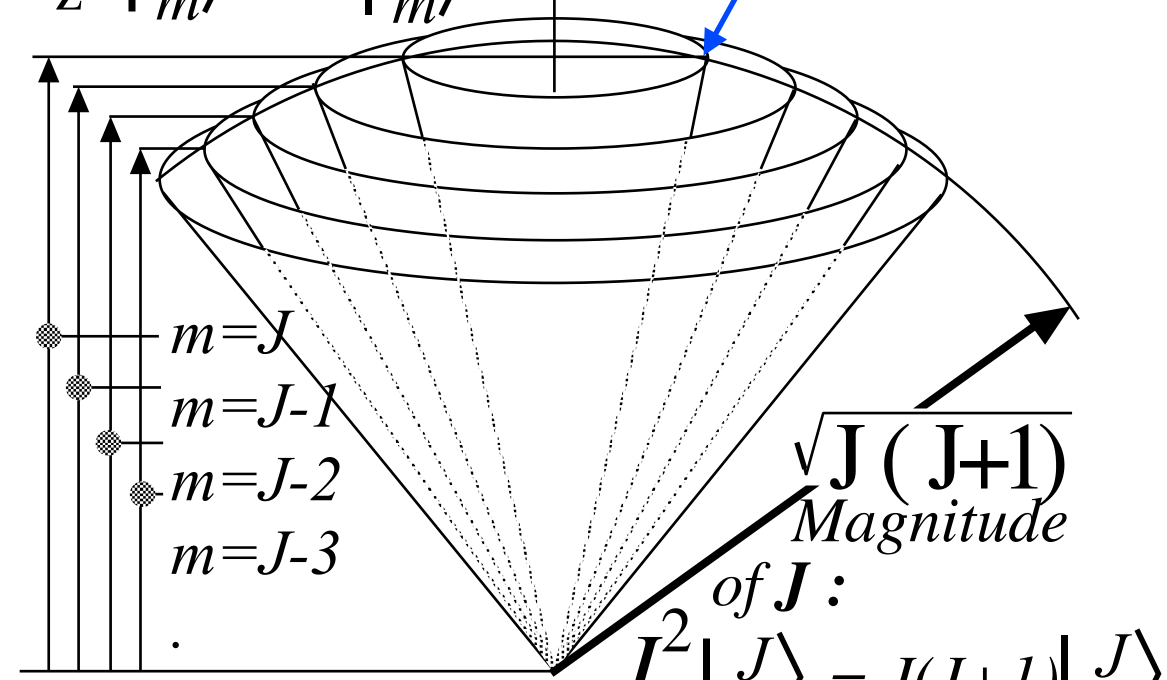
$$\Theta^{1/2}_{1/2} = \arccos\left(\frac{\frac{1}{2}}{\sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right)}}\right) = \cos^{-1}\frac{1}{2\frac{\sqrt{3}}{2}} = 54.7°$$

Greatest posible uncertainty

z-Component of ***J*** *:*

$$J_z \left|\begin{matrix}J\\m\end{matrix}\right\rangle = m \left|\begin{matrix}J\\m\end{matrix}\right\rangle$$

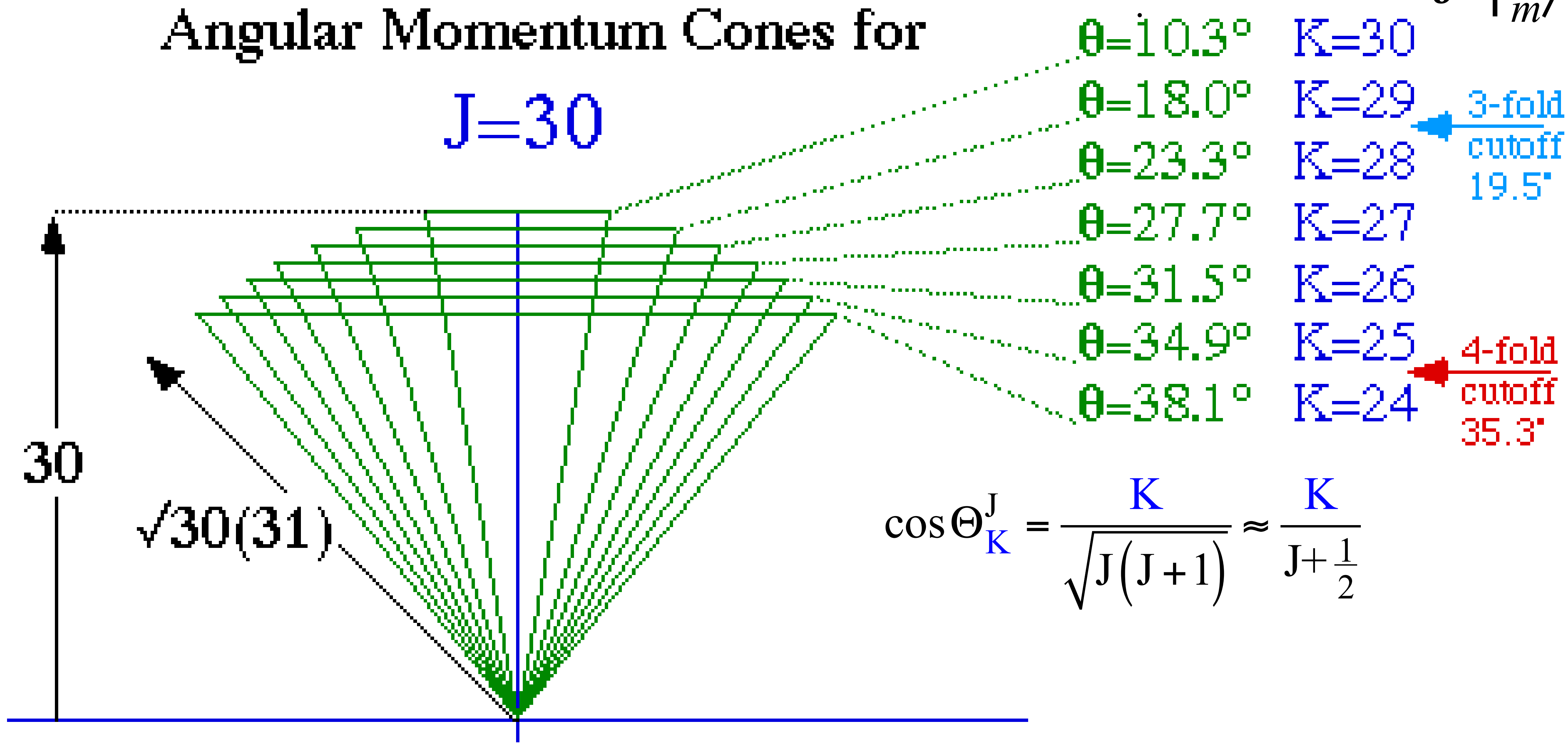
Minimum uncertainty for *m=j*



Magnitude of ***J*** *:*

$$J^2 \left|\begin{matrix}J\\m\end{matrix}\right\rangle = J(J+1) \left|\begin{matrix}J\\m\end{matrix}\right\rangle$$

Angular Momentum Cones for J=30



$$\cos\Theta^J_K = \frac{K}{\sqrt{J(J+1)}} \approx \frac{K}{J+\frac{1}{2}}$$

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A fundamental (spin-1/2) Euler transformation $\mathbf{R}(\alpha\beta\gamma)$ given in three notations.

$$\begin{pmatrix} \langle 1|1'\rangle & \langle 1|2'\rangle \\ \langle 2|1'\rangle & \langle 2|2'\rangle \end{pmatrix} = \begin{pmatrix} \langle 1|\mathbf{R}(\alpha\beta\gamma)|1\rangle & \langle 1|\mathbf{R}(\alpha\beta\gamma)|2\rangle \\ \langle 2|\mathbf{R}(\alpha\beta\gamma)|1\rangle & \langle 2|\mathbf{R}(\alpha\beta\gamma)|2\rangle \end{pmatrix} = \begin{pmatrix} D^{1/2}_{11}(\alpha\beta\gamma) & D^{1/2}_{12}(\alpha\beta\gamma) \\ D^{1/2}_{21}(\alpha\beta\gamma) & D^{1/2}_{22}(\alpha\beta\gamma) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} & -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} \\ e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} & e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} \end{pmatrix}$$

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Corresponding transformation of the fundamental creation operators

$$\mathbf{a}^\dagger_{1'} = D^{1/2}_{11}(\alpha\beta\gamma)\mathbf{a}^\dagger_1 + D^{1/2}_{21}(\alpha\beta\gamma)\mathbf{a}^\dagger_2 = e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2}\mathbf{a}^\dagger_1 + e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2}\mathbf{a}^\dagger_2$$

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$$\begin{pmatrix} \langle 1|1'\rangle & \langle 1|2'\rangle \\ \langle 2|1'\rangle & \langle 2|2'\rangle \end{pmatrix} = \begin{pmatrix} \langle 1|\mathbf{R}(\alpha\beta\gamma)|1\rangle & \langle 1|\mathbf{R}(\alpha\beta\gamma)|2\rangle \\ \langle 2|\mathbf{R}(\alpha\beta\gamma)|1\rangle & \langle 2|\mathbf{R}(\alpha\beta\gamma)|2\rangle \end{pmatrix} = \begin{pmatrix} D^{1/2}_{11}(\alpha\beta\gamma) & D^{1/2}_{12}(\alpha\beta\gamma) \\ D^{1/2}_{21}(\alpha\beta\gamma) & D^{1/2}_{22}(\alpha\beta\gamma) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} & -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} \\ e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} & e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} \end{pmatrix}$$

Corresponding transformation of the fundamental creation operators

$$\mathbf{a}^\dagger_{1'} = D^{1/2}_{11}(\alpha\beta\gamma)\mathbf{a}^\dagger_1 + D^{1/2}_{21}(\alpha\beta\gamma)\mathbf{a}^\dagger_2 = e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2}\mathbf{a}^\dagger_1 + e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2}\mathbf{a}^\dagger_2$$

$$\mathbf{a}^\dagger_{2'} = D^{1/2}_{12}(\alpha\beta\gamma)\mathbf{a}^\dagger_1 + D^{1/2}_{22}(\alpha\beta\gamma)\mathbf{a}^\dagger_2 = -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2}\mathbf{a}^\dagger_1 + e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2}\mathbf{a}^\dagger_2$$

Problem: Find corresponding transformation $D^{(j)}(\alpha\beta\gamma)$ matrix for a ($\upsilon=2j$)-oscillator state

($\upsilon=2j$)-quantum state is rotated to a new "prime" basis.

$$\mathbf{R}(\alpha\beta\gamma)\left|{}^{j}_{n}\right\rangle = \frac{\left(\mathbf{a}^\dagger_{1'}\right)^{j+n}\left(\mathbf{a}^\dagger_{2'}\right)^{j-n}}{\sqrt{(j+n)!(j-n)!}}\left|0\,0\right\rangle = \frac{\left(D_{11}\mathbf{a}^\dagger_1 + D_{21}\mathbf{a}^\dagger_2\right)^{j+n}\left(D_{21}\mathbf{a}^\dagger_1 + D_{22}\mathbf{a}^\dagger_2\right)^{j-n}}{\sqrt{(j+n)!(j-n)!}}\left|0\,0\right\rangle$$

Generating irreducible representations of R(3) and U(2) rotations $\mathbf{R}(\alpha\beta\gamma)$

A fundamental (spin-1/2) Euler transformation $\mathbf{R}(\alpha\beta\gamma)$ given in three notations.

$$\begin{pmatrix} \langle 1|1'\rangle & \langle 1|2'\rangle \\ \langle 2|1'\rangle & \langle 2|2'\rangle \end{pmatrix} = \begin{pmatrix} \langle 1|\mathbf{R}(\alpha\beta\gamma)|1\rangle & \langle 1|\mathbf{R}(\alpha\beta\gamma)|2\rangle \\ \langle 2|\mathbf{R}(\alpha\beta\gamma)|1\rangle & \langle 2|\mathbf{R}(\alpha\beta\gamma)|2\rangle \end{pmatrix} = \begin{pmatrix} D^{1/2}_{11}(\alpha\beta\gamma) & D^{1/2}_{12}(\alpha\beta\gamma) \\ D^{1/2}_{21}(\alpha\beta\gamma) & D^{1/2}_{22}(\alpha\beta\gamma) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} & -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} \\ e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} & e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} \end{pmatrix}$$

Corresponding transformation of the fundamental creation operators

$$\mathbf{a}^\dagger_{1'} = D^{1/2}_{11}(\alpha\beta\gamma)\mathbf{a}^\dagger_1 + D^{1/2}_{21}(\alpha\beta\gamma)\mathbf{a}^\dagger_2 = e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2}\mathbf{a}^\dagger_1 + e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2}\mathbf{a}^\dagger_2$$

$$\mathbf{a}^\dagger_{2'} = D^{1/2}_{12}(\alpha\beta\gamma)\mathbf{a}^\dagger_1 + D^{1/2}_{22}(\alpha\beta\gamma)\mathbf{a}^\dagger_2 = -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2}\mathbf{a}^\dagger_1 + e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2}\mathbf{a}^\dagger_2$$

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Binomial expansion is a double sum over binomial coefficients: $\binom{n}{k} = \frac{n!}{k!(n-k)!}$

$$\mathbf{R}(\alpha\beta\gamma)\left|{}^{j}_{n}\right\rangle = \frac{\sum_\ell \sum_k \binom{j+n}{\ell}\left(D_{11}\mathbf{a}^\dagger_1\right)^\ell\left(D_{21}\mathbf{a}^\dagger_2\right)^{j+n-\ell}\binom{j-n}{k}\left(D_{12}\mathbf{a}^\dagger_1\right)^k\left(D_{22}\mathbf{a}^\dagger_2\right)^{j-n-k}}{\sqrt{(j+n)!(j-n)!}}|0\,0\rangle \qquad = \sqrt{(j+n)!(j-n)!}\sum_\ell \sum_k \frac{\left(D_{11}\mathbf{a}^\dagger_1\right)^\ell\left(D_{21}\mathbf{a}^\dagger_2\right)^{j+n-\ell}\left(D_{12}\mathbf{a}^\dagger_1\right)^k\left(D_{22}\mathbf{a}^\dagger_2\right)^{j-n-k}}{\ell!(j+n-\ell)!k!(j-n-k)!}|0\,0\rangle$$

Generating irreducible representations of R(3) and U(2) rotations $\mathbf{R}(\alpha\beta\gamma)$

A fundamental (spin-1/2) Euler transformation $\mathbf{R}(\alpha\beta\gamma)$ given in three notations.

$$\begin{pmatrix} \langle 1|1'\rangle & \langle 1|2'\rangle \\ \langle 2|1'\rangle & \langle 2|2'\rangle \end{pmatrix} = \begin{pmatrix} \langle 1|\mathbf{R}(\alpha\beta\gamma)|1\rangle & \langle 1|\mathbf{R}(\alpha\beta\gamma)|2\rangle \\ \langle 2|\mathbf{R}(\alpha\beta\gamma)|1\rangle & \langle 2|\mathbf{R}(\alpha\beta\gamma)|2\rangle \end{pmatrix} = \begin{pmatrix} D^{1/2}_{11}(\alpha\beta\gamma) & D^{1/2}_{12}(\alpha\beta\gamma) \\ D^{1/2}_{21}(\alpha\beta\gamma) & D^{1/2}_{22}(\alpha\beta\gamma) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} & -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} \\ e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} & e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} \end{pmatrix}$$

Corresponding transformation of the fundamental creation operators

$$\mathbf{a}^\dagger_{1'} = D^{1/2}_{11}(\alpha\beta\gamma)\mathbf{a}^\dagger_1 + D^{1/2}_{21}(\alpha\beta\gamma)\mathbf{a}^\dagger_2 = e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2}\mathbf{a}^\dagger_1 + e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2}\mathbf{a}^\dagger_2$$

$$\mathbf{a}^\dagger_{2'} = D^{1/2}_{12}(\alpha\beta\gamma)\mathbf{a}^\dagger_1 + D^{1/2}_{22}(\alpha\beta\gamma)\mathbf{a}^\dagger_2 = -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2}\mathbf{a}^\dagger_1 + e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2}\mathbf{a}^\dagger_2$$

Problem: Find corresponding transformation $D^{(j)}(\alpha\beta\gamma)$ matrix for a $(\upsilon=2j)$-oscillator state

$(\upsilon=2j)$-quantum state is rotated to a new "prime" basis.

$$\mathbf{R}(\alpha\beta\gamma)\left|{}^{j}_{n}\right\rangle = \frac{(\mathbf{a}^\dagger_{1'})^{j+n}(\mathbf{a}^\dagger_{2'})^{j-n}}{\sqrt{(j+n)!(j-n)!}}|0\,0\rangle = \frac{(D_{11}\mathbf{a}^\dagger_1 + D_{21}\mathbf{a}^\dagger_2)^{j+n}(D_{21}\mathbf{a}^\dagger_1 + D_{22}\mathbf{a}^\dagger_2)^{j-n}}{\sqrt{(j+n)!(j-n)!}}|0\,0\rangle$$

Binomial expansion is a double sum over binomial coefficients: $\binom{n}{k} = \frac{n!}{k!(n-k)!}$

$$\mathbf{R}(\alpha\beta\gamma)\left|{}^{j}_{n}\right\rangle = \frac{\sum_\ell \sum_k \binom{j+n}{\ell}(D_{11}\mathbf{a}^\dagger_1)^\ell(D_{21}\mathbf{a}^\dagger_2)^{j+n-\ell}\binom{j-n}{k}(D_{12}\mathbf{a}^\dagger_1)^k(D_{22}\mathbf{a}^\dagger_2)^{j-n-k}}{\sqrt{(j+n)!(j-n)!}}|0\,0\rangle = \sqrt{(j+n)!(j-n)!}\frac{\sum_\ell \sum_k (D_{11}\mathbf{a}^\dagger_1)^\ell(D_{21}\mathbf{a}^\dagger_2)^{j+n-\ell}(D_{12}\mathbf{a}^\dagger_1)^k(D_{22}\mathbf{a}^\dagger_2)^{j-n-k}}{\ell!(j+n-\ell)!k!(j-n-k)!}|0\,0\rangle$$

Let $\mathbf{a}^\dagger$-operator powers be $j\pm m$ forms : $j+m=\ell+k$, $j-m=2j-\ell-k$ so $\ell=j+m-k$ and $j+n-\ell=n-m+k$

$$= \sqrt{(j+n)!(j-n)!}\frac{\sum_\ell \sum_k (D_{11})^\ell(D_{21})^{j+n-\ell}(D_{12})^k(D_{22})^{j-n-k}}{\ell!(j+n-\ell)!k!(j-n-k)!}(\mathbf{a}^\dagger_1)^{\ell+k}(\mathbf{a}^\dagger_2)^{2j-\ell-k}|0\,0\rangle = \sqrt{(j+n)!(j-n)!}\frac{\sum_m \sum_k (D_{11})^{j+m-k}(D_{21})^{n-m+k}(D_{12})^k(D_{22})^{j-n-k}}{(j+m-k)!(n-m+k)!k!(j-n-k)!}(\mathbf{a}^\dagger_1)^{j+m}(\mathbf{a}^\dagger_2)^{j-m}|0\,0\rangle$$

Generating irreducible representations of R(3) and U(2) rotations $\mathbf{R}(\alpha\beta\gamma)$

A fundamental (spin-1/2) Euler transformation $\mathbf{R}(\alpha\beta\gamma)$ given in three notations.

$$\begin{pmatrix} \langle 1|1'\rangle & \langle 1|2'\rangle \\ \langle 2|1'\rangle & \langle 2|2'\rangle \end{pmatrix} = \begin{pmatrix} \langle 1|\mathbf{R}(\alpha\beta\gamma)|1\rangle & \langle 1|\mathbf{R}(\alpha\beta\gamma)|2\rangle \\ \langle 2|\mathbf{R}(\alpha\beta\gamma)|1\rangle & \langle 2|\mathbf{R}(\alpha\beta\gamma)|2\rangle \end{pmatrix} = \begin{pmatrix} D^{1/2}_{11}(\alpha\beta\gamma) & D^{1/2}_{12}(\alpha\beta\gamma) \\ D^{1/2}_{21}(\alpha\beta\gamma) & D^{1/2}_{22}(\alpha\beta\gamma) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} & -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} \\ e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} & e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} \end{pmatrix}$$

Corresponding transformation of the fundamental creation operators

$$\mathbf{a}^\dagger_{1'} = D^{1/2}_{11}(\alpha\beta\gamma)\mathbf{a}^\dagger_1 + D^{1/2}_{21}(\alpha\beta\gamma)\mathbf{a}^\dagger_2 = e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2}\mathbf{a}^\dagger_1 + e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2}\mathbf{a}^\dagger_2$$

$$\mathbf{a}^\dagger_{2'} = D^{1/2}_{12}(\alpha\beta\gamma)\mathbf{a}^\dagger_1 + D^{1/2}_{22}(\alpha\beta\gamma)\mathbf{a}^\dagger_2 = -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2}\mathbf{a}^\dagger_1 + e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2}\mathbf{a}^\dagger_2$$

Problem: Find corresponding transformation $D^{(j)}(\alpha\beta\gamma)$ matrix for a ($\upsilon=2j$)-oscillator state

($\upsilon=2j$)-quantum state is rotated to a new "prime" basis.

$$\mathbf{R}(\alpha\beta\gamma)\left|{}^{j}_{n}\right\rangle = \frac{\left(\mathbf{a}^\dagger_{1'}\right)^{j+n}\left(\mathbf{a}^\dagger_{2'}\right)^{j-n}}{\sqrt{(j+n)!(j-n)!}}|0\,0\rangle = \frac{\left(D_{11}\mathbf{a}^\dagger_1 + D_{21}\mathbf{a}^\dagger_2\right)^{j+n}\left(D_{21}\mathbf{a}^\dagger_1 + D_{22}\mathbf{a}^\dagger_2\right)^{j-n}}{\sqrt{(j+n)!(j-n)!}}|0\,0\rangle$$

This gives general *irreducible representation of U(2)* :

$$\left\langle {}^{j}_{m}\right|\mathbf{R}(\alpha\beta\gamma)\left|{}^{j}_{n}\right\rangle = D^{j}_{m,n}(\alpha\beta\gamma) = \sqrt{(j+n)!(j-n)!}\sqrt{(j+m)!(j-m)!}\frac{\sum_k \left(D_{11}\right)^{j+m-k}\left(D_{21}\right)^{n-m+k}\left(D_{12}\right)^{k}\left(D_{22}\right)^{j-n-k}}{(j+m-k)!(n-m+k)!k!(j-n-k)!}$$

And general *SU(2) irreducible representation for Euler angles (αβγ)*.

$$\left\langle {}^{j}_{m}\right|\mathbf{R}(\alpha\beta\gamma)\left|{}^{j}_{n}\right\rangle = D^{j}_{m,n}(\alpha\beta\gamma) = \sqrt{(j+n)!(j-n)!}\sqrt{(j+m)!(j-m)!}\frac{\sum_k (-1)^k\left(\cos\frac{\beta}{2}\right)^{2j+m-n-2k}\left(\sin\frac{\beta}{2}\right)^{n-m+2k} e^{-i(m\alpha+n\gamma)}}{(j+m-k)!(n-m+k)!k!(j-n-k)!}$$

k-sum limited by (-*integer*)!=∞ and 0!=1=1!

Wigner D^J_{mn} irreps of U(2)~R(3) give atomic and molecular eigenfunctions $\Psi_{m,n}$ of 3D rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ and angular momentum uncertainty effects.

Review 1. *Angular momentum raise-n-lower operators* $\mathbf{S}_+$ and $\mathbf{S}_-$ Review 2. Angular momentum commutation

Review 3. *SU(2)⊂U(2) oscillators vs. R(3)⊂O(3) rotors*

Angular momentum magnitude and Θ^J_m-uncertainty cone polar angles

Generating higher-j representations D^j_{mn} of R(3) rotation and U(2) from spinor $D^{1/2}$ irreps

Evaluating D^j_{mn} representations

Applications of D^j_{mn} representations

Atomic wave functions. $D^L_{m0}\sim Y^L_m$ *Spherical harmonics*

$D^{L=1}_{m0}\sim Y^1_m$ *p-waves* $D^{L=2}_{m0}\sim Y^2_m$ *d-waves* $D^L_{00}\sim P^L$ *Legendre waves*

Molecular D^j_{mn} wave functions in "Mock-Mach" lab-vs-body state space $|{}^J_{mn}\rangle$

$\mathbf{P}^j_{mn}$ *projector and* $D^j_{mn}(\alpha,\beta,\gamma)$ *wave function*

D^J_{mn} *transform* $\mathbf{R}(\alpha,\beta,\gamma)|{}^J_{mn}\rangle=\Sigma_{m'}D^J_{m'n}(\alpha,\beta,\gamma)|{}^J_{m'n}\rangle$ *in lab-space,* $\bar{\mathbf{R}}(\alpha,\beta,\gamma)$ *in body-space.*

D^2_{mn} *transform in lab-space (Generalized Stern-Gerlach beam polarization)*

Θ^J_m-cone properties of lab transforms: J=20, J=10, J=30.

Θ^J_m-analysis of high J atomic beams

Θ^J_m-properties of high J molecular lab-vs-body states $|{}^J_{mn}\rangle$

Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar* $\mathbf{T}_0^0$ *or tensor* $\mathbf{T}_q^2$ *operators*

Rotational Energy Surfaces (RE or RES) of symmetric rotor and eigensolutions

Rotational Energy Surfaces (RE or RES) of asymmetric rotor (for following class)

Generating irreducible representations of R(3) and U(2) rotations $\mathbf{R}(\alpha\beta\gamma)$

Evaluating *irreducible representation of U(2)* :

$$\left\langle {}^{j}_{m}\right|\mathbf{R}(\alpha\beta\gamma)\left|{}^{j}_{n}\right\rangle = D^{j}_{m,n}(\alpha\beta\gamma) = \sqrt{(j+n)!(j-n)!}\sqrt{(j+m)!(j-m)!}\sum_k \frac{(D_{11})^{j+m-k}(D_{21})^{n-m+k}(D_{12})^{k}(D_{22})^{j-n-k}}{(j+m-k)!(n-m+k)!k!(j-n-k)!}$$

Easily done for *Euler angles* $(\alpha\beta\gamma)$ or *Darboux axis angles* **[φϑΘ]**

$$\begin{pmatrix} D^{1/2}_{11}(\alpha\beta\gamma) & D^{1/2}_{12}(\alpha\beta\gamma) \\ D^{1/2}_{21}(\alpha\beta\gamma) & D^{1/2}_{22}(\alpha\beta\gamma) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} & -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} \\ e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} & e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} \end{pmatrix}$$

or

$$\begin{pmatrix} D^{1/2}_{11}[\varphi\vartheta\Theta] & D^{1/2}_{12}[\varphi\vartheta\Theta] \\ D^{1/2}_{21}[\varphi\vartheta\Theta] & D^{1/2}_{22}[\varphi\vartheta\Theta] \end{pmatrix} = \begin{pmatrix} \cos\frac{\Theta}{2} - i\cos\vartheta\sin\frac{\Theta}{2} & -ie^{-i\varphi}\sin\vartheta\sin\frac{\Theta}{2} \\ -ie^{+i\varphi}\sin\vartheta\sin\frac{\Theta}{2} & \cos\frac{\Theta}{2} + i\cos\vartheta\sin\frac{\Theta}{2} \end{pmatrix}$$

k-Summation Σ_k limits amount to prohibiting a $p!=(-N)!=\infty$ factor in denominator.

$(j+m-k) \geq 0$	$(n-m+k) \geq 0$	$k \geq 0$	$(j-n-k) \geq 0$
or: $k \leq j+m$	or: $k \leq m-n$		or: $k \leq j-n$

Power p on $(D_{ab})^p$ must be zero or greater ($p \geq 0$).

Euler angles $(\alpha\beta\gamma)$ vs *axis angles* **[φϑΘ]** *Lect.5 p7-11*

Generating irreducible representations of R(3) and U(2) rotations $\mathbf{R}(\alpha\beta\gamma)$

Evaluating *irreducible representation of U(2)* :

$$\left\langle {}^{j}_{m}\right|\mathbf{R}(\alpha\beta\gamma)\left|{}^{j}_{n}\right\rangle = D^{j}_{m,n}(\alpha\beta\gamma) = \sqrt{(j+n)!(j-n)!}\sqrt{(j+m)!(j-m)!}\sum_k \frac{(D_{11})^{j+m-k}(D_{21})^{n-m+k}(D_{12})^{k}(D_{22})^{j-n-k}}{(j+m-k)!(n-m+k)!k!(j-n-k)!}$$

Easily done for *Euler angles* $(\alpha\beta\gamma)$ or *Darboux axis angles* $[\varphi\vartheta\Theta]$

$$\begin{pmatrix} D^{1/2}_{11}(\alpha\beta\gamma) & D^{1/2}_{12}(\alpha\beta\gamma) \\ D^{1/2}_{21}(\alpha\beta\gamma) & D^{1/2}_{22}(\alpha\beta\gamma) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} & -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} \\ e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} & e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} \end{pmatrix}$$

or

$$\begin{pmatrix} D^{1/2}_{11}[\varphi\vartheta\Theta] & D^{1/2}_{12}[\varphi\vartheta\Theta] \\ D^{1/2}_{21}[\varphi\vartheta\Theta] & D^{1/2}_{22}[\varphi\vartheta\Theta] \end{pmatrix} = \begin{pmatrix} \cos\frac{\Theta}{2} - i\cos\vartheta\sin\frac{\Theta}{2} & -ie^{-i\varphi}\sin\vartheta\sin\frac{\Theta}{2} \\ -ie^{+i\varphi}\sin\vartheta\sin\frac{\Theta}{2} & \cos\frac{\Theta}{2} + i\cos\vartheta\sin\frac{\Theta}{2} \end{pmatrix}$$

$(j+m-k) \geq 0$ or: $k \leq j+m$

$(n-m+k) \geq 0$ or: $k \geq m-n$

$k \geq 0$

$(j-n-k) \geq 0$ or: $k \leq j-n$

k-Summation Σ_k limits amount to prohibiting a $p!=(-N)!=\infty$ factor in denominator.

Power p on $(D_{ab})^p$ must be zero or greater ($p \geq 0$).

Examples: $D^{j}_{m,n} = D^{8}_{2,4}$ has sum: $\sum_{k=0}^{4}$ 5 terms $k \leq 8+2=10$, $k \geq 2\text{-}4=\text{-}2$, $k \geq 0$, $k \leq 8\text{-}4=4$.

$D^{j}_{m,n} = D^{8}_{-4,4}$ has sum: $\sum_{k=0}^{4}$ 5 terms $k \leq 8\text{-}4=4$, $k \geq 4\text{-}4=0$. $k \geq 0$, $k \leq 8\text{-}4=4$

Generating irreducible representations of R(3) and U(2) rotations $\mathbf{R}(\alpha\beta\gamma)$

Evaluating *irreducible representation of U(2)* :

$$\left\langle {}^{j}_{m}\right|\mathbf{R}(\alpha\beta\gamma)\left|{}^{j}_{n}\right\rangle = D^{j}_{m,n}(\alpha\beta\gamma) = \sqrt{(j+n)!(j-n)!}\sqrt{(j+m)!(j-m)!}\sum_k \frac{(D_{11})^{j+m-k}(D_{21})^{n-m+k}(D_{12})^{k}(D_{22})^{j-n-k}}{(j+m-k)!(n-m+k)!k!(j-n-k)!}$$

Easily done for *Euler angles* $(\alpha\beta\gamma)$ or *Darboux axis angles* $[\varphi\vartheta\Theta]$

$$\begin{pmatrix} D^{1/2}_{11}(\alpha\beta\gamma) & D^{1/2}_{12}(\alpha\beta\gamma) \\ D^{1/2}_{21}(\alpha\beta\gamma) & D^{1/2}_{22}(\alpha\beta\gamma) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} & -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} \\ e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} & e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} \end{pmatrix}$$

or

$$\begin{pmatrix} D^{1/2}_{11}[\varphi\vartheta\Theta] & D^{1/2}_{12}[\varphi\vartheta\Theta] \\ D^{1/2}_{21}[\varphi\vartheta\Theta] & D^{1/2}_{22}[\varphi\vartheta\Theta] \end{pmatrix} = \begin{pmatrix} \cos\frac{\Theta}{2} - i\cos\vartheta\sin\frac{\Theta}{2} & -ie^{-i\varphi}\sin\vartheta\sin\frac{\Theta}{2} \\ -ie^{+i\varphi}\sin\vartheta\sin\frac{\Theta}{2} & \cos\frac{\Theta}{2} + i\cos\vartheta\sin\frac{\Theta}{2} \end{pmatrix}$$

$(j+m-k) \geq 0$ or: $k \leq j+m$

$(n-m+k) \geq 0$ or: $k \geq m-n$

$k \geq 0$

$(j-n-k) \geq 0$ or: $k \leq j-n$

k-Summation Σ_k limits amount to prohibiting a $p!=(-N)!=\infty$ factor in denominator.

Power p on $(D_{ab})^p$ must be zero or greater ($p \geq 0$).

Examples: $D^{j}_{m,n} = D^{8}_{2,4}$ has sum: $\sum_{k=0}^{4}$ 5 terms $k \leq 8+2=10$, $k \geq 2\text{-}4=-2$, $k \geq 0$, $k \leq 8\text{-}4=4$.

$D^{j}_{m,n} = D^{8}_{-4,4}$ has sum: $\sum_{k=0}^{4}$ 5 terms $k \leq 8\text{-}4=4$, $k \geq 4\text{-}4=0$. $k \geq 0$, $k \leq 8\text{-}4=4$

$D^{j}_{m,n} = D^{8}_{-8,4}$ has sum: $\sum_{k=0}^{0}$ 1 term $k \leq 8\text{-}8=0$, $k \geq -8\text{-}4=-12$. $k \geq 0$, $k \leq 8\text{-}4=4$

Generating irreducible representations of R(3) and U(2) rotations $\mathbf{R}(\alpha\beta\gamma)$

Evaluating *irreducible representation of U(2)* :

$$\left\langle {j \atop m} \right| \mathbf{R}(\alpha\beta\gamma) \left| {j \atop n} \right\rangle = D^j_{m,n}(\alpha\beta\gamma) = \sqrt{(j+n)!(j-n)!}\sqrt{(j+m)!(j-m)!}\sum_k \frac{(D_{11})^{j+m-k}(D_{21})^{n-m+k}(D_{12})^{k}(D_{22})^{j-n-k}}{(j+m-k)!(n-m+k)!k!(j-n-k)!}$$

Easily done for *Euler angles* $(\alpha\beta\gamma)$ or

$$\begin{pmatrix} D^{1/2}_{11}(\alpha\beta\gamma) & D^{1/2}_{12}(\alpha\beta\gamma) \\ D^{1/2}_{21}(\alpha\beta\gamma) & D^{1/2}_{22}(\alpha\beta\gamma) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} & -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} \\ e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} & e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} \end{pmatrix}$$

or *Darboux axis angles* $[\varphi\vartheta\Theta]$

$$\begin{pmatrix} D^{1/2}_{11}[\varphi\vartheta\Theta] & D^{1/2}_{12}[\varphi\vartheta\Theta] \\ D^{1/2}_{21}[\varphi\vartheta\Theta] & D^{1/2}_{22}[\varphi\vartheta\Theta] \end{pmatrix} = \begin{pmatrix} \cos\frac{\Theta}{2} - i\cos\vartheta\sin\frac{\Theta}{2} & -ie^{-i\varphi}\sin\vartheta\sin\frac{\Theta}{2} \\ -ie^{+i\varphi}\sin\vartheta\sin\frac{\Theta}{2} & \cos\frac{\Theta}{2} + i\cos\vartheta\sin\frac{\Theta}{2} \end{pmatrix}$$

$(j+m-k) \geq 0$ or: $k \leq j+m$ | $(n-m+k) \geq 0$ or: $k \geq m-n$ | $k \geq 0$ | $(j-n-k) \geq 0$ or: $k \leq j-n$

k-Summation Σ_k limits amount to prohibiting a $p!=(-N)!=\infty$ factor in denominator.

Power p on $(D_{ab})^p$ must be zero or greater ($p \geq 0$).

Examples: $D^j_{m,n} = D^8_{2,4}$ has sum: $\sum_{k=0}^{4}$ 5 terms $k \leq 8+2=10$, $k \geq 2\text{-}4=\text{-}2$, $k \geq 0$, $k \leq 8\text{-}4=4$.

$D^j_{m,n} = D^8_{-4,4}$ has sum: $\sum_{k=0}^{4}$ 5 terms $k \leq 8\text{-}4=4$, $k \geq 4\text{-}4=0$. $k \geq 0$, $k \leq 8\text{-}4=4$

$D^j_{m,n} = D^8_{-8,4}$ has sum: $\sum_{k=0}^{0}$ 1 term $k \leq 8\text{-}8=0$, $k \geq \text{-}8\text{-}4=\text{-}12$. $k \geq 0$, $k \leq 8\text{-}4=4$

$D^j_{m,n} = D^{\frac{1}{2}}_{-\frac{1}{2},\frac{1}{2}}$ has sum: $\sum_{k=0}^{0}$ 1 term $k \leq ½\text{-}½=0$, $k \geq \text{-}½\text{-}½=\text{-}1$. $k \geq 0$, $k \leq ½\text{-}½=0$

Wigner D^J_{mn} irreps of U(2)~R(3) give atomic and molecular eigenfunctions $\Psi_{m,n}$ of 3D rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ and angular momentum uncertainty effects.

Review 1. *Angular momentum raise-n-lower operators* $\mathbf{S}_+$ and $\mathbf{S}_-$ Review 2. Angular momentum commutation

Review 3. *SU(2)⊂U(2) oscillators vs. R(3)⊂O(3) rotors*

Angular momentum magnitude and Θ^J_m*-uncertainty cone polar angles*

Generating higher-j representations D^j_{mn} *of R(3) rotation and U(2) from spinor* $D^{1/2}$ *irreps*

Evaluating D^j_{mn} *representations*

Applications of D^j_{mn} *representations*

Atomic wave functions. $D^L_{m0}\sim Y^L_m$ *Spherical harmonics*

$D^{L=1}_{m0}\sim Y^1_m$ *p-waves* ← $D^{L=2}_{m0}\sim Y^2_m$ *d-waves* $D^L_{00}\sim P^L$ *Legendre waves*

Molecular D^j_{mn} *wave functions in "Mock-Mach" lab-vs-body state space* $|^J_{mn}\rangle$

$\mathbf{P}^j_{mn}$ *projector and* $D^j_{mn}(\alpha,\beta,\gamma)$ *wave function*

D^J_{mn} *transform* $\mathbf{R}_{(\alpha,\beta,\gamma)}|^J_{mn}\rangle=\Sigma_{m'}D^J_{m'n}(\alpha,\beta,\gamma)|^J_{m'n}\rangle$ *in lab-space,* $\bar{\mathbf{R}}_{(\alpha,\beta,\gamma)}$ *in body-space.*

D^2_{mn} *transform in lab-space (Generalized Stern-Gerlach beam polarization)*

Θ^J_m*-cone properties of lab transforms: J=20, J=10, J=30.*

Θ^J_m*-analysis of high J atomic beams*

Θ^J_m*-properties of high J molecular lab-vs-body states* $|^J_{mn}\rangle$

Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar* $\mathbf{T}_0^0$ *or tensor* $\mathbf{T}_q^2$ *operators*

Rotational Energy Surfaces (RE or RES) of symmetric rotor and eigensolutions

Rotational Energy Surfaces (RE or RES) of asymmetric rotor (for following class)

Atomic and molecular $D^{J*}_{mn}(\alpha,\beta,\gamma)$-wavefunctions

$$\left\langle {j \atop m} \right| \mathbf{R}(\alpha\beta\gamma) \left| {j \atop n} \right\rangle = D^{j}_{m,n}(\alpha\beta\gamma) = \sqrt{(j+n)!(j-n)!}\sqrt{(j+m)!(j-m)!}\sum_k \frac{(-1)^k \left(\cos\frac{\beta}{2}\right)^{2j+m-n-2k}\left(\sin\frac{\beta}{2}\right)^{n-m+2k} e^{-i(m\alpha+n\gamma)}}{(j+m-k)!(n-m+k)!k!(j-n-k)!}$$

Vector ($j=\ell=1$) representation

$$D^1(\alpha\beta\gamma) = \begin{pmatrix} e^{-i\alpha} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{i\alpha} \end{pmatrix} \begin{pmatrix} \frac{1+\cos\beta}{2} & \frac{-\sin\beta}{\sqrt{2}} & \frac{1-\cos\beta}{2} \\ \frac{\sin\beta}{\sqrt{2}} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}} \\ \frac{1-\cos\beta}{2} & \frac{\sin\beta}{\sqrt{2}} & \frac{1+\cos\beta}{2} \end{pmatrix} \begin{pmatrix} e^{-i\gamma} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{i\gamma} \end{pmatrix} = \begin{pmatrix} e^{-i\alpha}\frac{1+\cos\beta}{2}e^{-i\gamma} & e^{-i\alpha}\frac{-\sin\beta}{\sqrt{2}} & e^{-i\alpha}\frac{1-\cos\beta}{2}e^{i\gamma} \\ \frac{\sin\beta}{\sqrt{2}}e^{-i\gamma} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}}e^{i\gamma} \\ e^{i\alpha}\frac{1-\cos\beta}{2}e^{-i\gamma} & e^{i\alpha}\frac{\sin\beta}{\sqrt{2}} & e^{i\alpha}\frac{1+\cos\beta}{2}e^{i\gamma} \end{pmatrix}$$

Notation Switch:
azimuth angle:
$\alpha \longrightarrow \phi$
polar angle:
$\beta \longrightarrow \theta$

Here half-angle identities were used. $\cos^2\frac{\beta}{2} = \frac{1+\cos\beta}{2}$, $\sin^2\frac{\beta}{2} = \frac{1-\cos\beta}{2}$, $\sin\frac{\beta}{2}\cos\frac{\beta}{2} = \frac{\sin\beta}{2}$,

$$Y^{1*}_{1}(\phi,\theta) = \sqrt{\tfrac{3}{4\pi}}\, e^{-i\phi}\frac{-\sin\theta}{\sqrt{2}} = D^1_{1,0}(\phi,\theta)$$

$$Y^{1*}_{0}(\phi,\theta) = \sqrt{\tfrac{3}{4\pi}} \quad \cos\beta \quad = D^1_{0,0}(\phi,\theta)$$

$$Y^{1*}_{-1}(\phi,\theta) = \sqrt{\tfrac{3}{4\pi}}\, e^{+i\phi}\frac{\sin\theta}{\sqrt{2}} = D^1_{-1,0}(\phi,\theta)$$

Atomic and molecular $D^{J*}_{mn}(\alpha,\beta,\gamma)$-wavefunctions

$$\left\langle {j \atop m}\right|\mathbf{R}(\alpha\beta\gamma)\left|{j \atop n}\right\rangle = D^j_{m,n}(\alpha\beta\gamma) = \sqrt{(j+n)!(j-n)!}\sqrt{(j+m)!(j-m)!}\,\frac{\sum_k (-1)^k \left(\cos\frac{\beta}{2}\right)^{2j+m-n-2k}\left(\sin\frac{\beta}{2}\right)^{n-m+2k} e^{-i(m\alpha+n\gamma)}}{(j+m-k)!(n-m+k)!k!(j-n-k)!}$$

Vector ($j=\ell=1$) representation

$$D^1(\alpha\beta\gamma) = \begin{pmatrix} e^{-i\alpha} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{i\alpha} \end{pmatrix}\begin{pmatrix} \frac{1+\cos\beta}{2} & \frac{-\sin\beta}{\sqrt{2}} & \frac{1-\cos\beta}{2} \\ \frac{\sin\beta}{\sqrt{2}} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}} \\ \frac{1-\cos\beta}{2} & \frac{\sin\beta}{\sqrt{2}} & \frac{1+\cos\beta}{2} \end{pmatrix}\begin{pmatrix} e^{-i\gamma} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{i\gamma} \end{pmatrix} = \begin{pmatrix} e^{-i\alpha}\frac{1+\cos\beta}{2}e^{-i\gamma} & e^{-i\alpha}\frac{-\sin\beta}{\sqrt{2}} & e^{-i\alpha}\frac{1-\cos\beta}{2}e^{i\gamma} \\ \frac{\sin\beta}{\sqrt{2}}e^{-i\gamma} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}}e^{i\gamma} \\ e^{i\alpha}\frac{1-\cos\beta}{2}e^{-i\gamma} & e^{i\alpha}\frac{\sin\beta}{\sqrt{2}} & e^{i\alpha}\frac{1+\cos\beta}{2}e^{i\gamma} \end{pmatrix}$$

Notation Switch:
azimuth angle: $\alpha \to \phi$
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Here half-angle identities were used. $\cos^2\frac{\beta}{2} = \frac{1+\cos\beta}{2}$, $\sin^2\frac{\beta}{2} = \frac{1-\cos\beta}{2}$, $\sin\frac{\beta}{2}\cos\frac{\beta}{2} = \frac{\sin\beta}{2}$,

$$Y^{1*}_1(\phi,\theta) = \sqrt{\tfrac{3}{4\pi}}\,e^{-i\phi}\frac{-\sin\theta}{\sqrt{2}} = D^1_{1,0}(\phi,\theta)$$

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$$Y^{1*}_{-1}(\phi,\theta) = \sqrt{\tfrac{3}{4\pi}}\,e^{+i\phi}\frac{\sin\theta}{\sqrt{2}} = D^1_{-1,0}(\phi,\theta)$$

Center ($n=0$) column with the factor $\sqrt{\frac{2\ell+1}{4\pi}}$ gives set of *spherical harmonics* Y^ℓ_m.

$$Y^\ell_m(\phi\theta) = D^{\ell*}_{m,n=0}(\phi\theta 0)\sqrt{\frac{2\ell+1}{4\pi}}$$

Dipole ($j=\ell=1$) wavefunctions

$$D^{1*}_{1,0}(\phi\theta 0) = -e^{i\phi}\frac{\sin\theta}{\sqrt{2}} = -\frac{\cos\phi\sin\theta + i\cos\phi\sin\theta}{\sqrt{2}} = -\frac{x+iy}{r\sqrt{2}}$$

$$D^{1*}_{0,0}(\phi\theta 0) = \cos\theta = \cos\theta = z/r$$

$$D^{1*}_{-1,0}(\phi\theta 0) = e^{-i\phi}\frac{\sin\theta}{\sqrt{2}} = \frac{\cos\phi\sin\theta - i\cos\phi\sin\theta}{\sqrt{2}} = \frac{x-iy}{r\sqrt{2}}$$

Atomic and molecular $D^{J*}_{mn}(\alpha,\beta,\gamma)$-wavefunctions

$$\left\langle {j \atop m}\right| \mathbf{R}(\alpha\beta\gamma) \left| {j \atop n}\right\rangle = D^{j}_{m,n}(\alpha\beta\gamma) = \sqrt{(j+n)!(j-n)!}\sqrt{(j+m)!(j-m)!}\,\frac{\sum_k (-1)^k \left(\cos\frac{\beta}{2}\right)^{2j+m-n-2k}\left(\sin\frac{\beta}{2}\right)^{n-m+2k} e^{-i(m\alpha+n\gamma)}}{(j+m-k)!(n-m+k)!k!(j-n-k)!}$$

Vector ($j=\ell=1$) representation

$$D^1(\alpha\beta\gamma)=\begin{pmatrix} e^{-i\alpha} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{i\alpha}\end{pmatrix}\begin{pmatrix} \frac{1+\cos\beta}{2} & \frac{-\sin\beta}{\sqrt{2}} & \frac{1-\cos\beta}{2} \\ \frac{\sin\beta}{\sqrt{2}} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}} \\ \frac{1-\cos\beta}{2} & \frac{\sin\beta}{\sqrt{2}} & \frac{1+\cos\beta}{2}\end{pmatrix}\begin{pmatrix} e^{-i\gamma} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{i\gamma}\end{pmatrix}=\begin{pmatrix} e^{-i\alpha}\frac{1+\cos\beta}{2}e^{-i\gamma} & e^{-i\alpha}\frac{-\sin\beta}{\sqrt{2}} & e^{-i\alpha}\frac{1-\cos\beta}{2}e^{i\gamma} \\ \frac{\sin\beta}{\sqrt{2}}e^{-i\gamma} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}}e^{i\gamma} \\ e^{i\alpha}\frac{1-\cos\beta}{2}e^{-i\gamma} & e^{i\alpha}\frac{\sin\beta}{\sqrt{2}} & e^{i\alpha}\frac{1+\cos\beta}{2}e^{i\gamma}\end{pmatrix}$$

Notation Switch:
azimuth angle:
$\alpha \to \phi$
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Here half-angle identities were used. $\cos^2\frac{\beta}{2}=\frac{1+\cos\beta}{2}$, $\sin^2\frac{\beta}{2}=\frac{1-\cos\beta}{2}$, $\sin\frac{\beta}{2}\cos\frac{\beta}{2}=\frac{\sin\beta}{2}$,

$$Y^{1*}_{1}(\phi,\theta)=\sqrt{\tfrac{3}{4\pi}}\,e^{-i\phi}\frac{-\sin\theta}{\sqrt{2}}=D^1_{1,0}(\phi,\theta)$$

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Center ($n=0$) column with the factor $\sqrt{\frac{2\ell+1}{4\pi}}$ gives set of *spherical harmonics* Y^{ℓ}_{m}.

$$Y^{\ell}_{m}(\phi\theta)=D^{\ell*}_{m,n=0}(\phi\theta 0)\sqrt{\frac{2\ell+1}{4\pi}}$$

Dipole ($j=\ell=1$) wavefunctions

$$D^{1*}_{1,0}(\phi\theta 0)=-e^{i\phi}\frac{\sin\theta}{\sqrt{2}}=-\frac{\cos\phi\sin\theta+i\cos\phi\sin\theta}{\sqrt{2}}=-\frac{x+iy}{r\sqrt{2}}$$

$$D^{1*}_{0,0}(\phi\theta 0)=\cos\theta=\cos\theta=z/r$$

$$D^{1*}_{-1,0}(\phi\theta 0)=e^{-i\phi}\frac{\sin\theta}{\sqrt{2}}=\frac{\cos\phi\sin\theta-i\cos\phi\sin\theta}{\sqrt{2}}=\frac{x-iy}{r\sqrt{2}}$$

3-D linear-circular polarization T-matrix:

$$\begin{pmatrix} \left\langle {1 \atop 1}\middle| {1 \atop x}\right\rangle & \left\langle {1 \atop 1}\middle| {1 \atop y}\right\rangle & \left\langle {1 \atop 1}\middle| {1 \atop z}\right\rangle \\ \left\langle {1 \atop 0}\middle| {1 \atop x}\right\rangle & \left\langle {1 \atop 0}\middle| {1 \atop y}\right\rangle & \left\langle {1 \atop 0}\middle| {1 \atop z}\right\rangle \\ \left\langle {1 \atop -1}\middle| {1 \atop x}\right\rangle & \left\langle {1 \atop -1}\middle| {1 \atop y}\right\rangle & \left\langle {1 \atop -1}\middle| {1 \atop z}\right\rangle \end{pmatrix}=\begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \end{pmatrix}$$

Atomic and molecular $D^{J*}_{mn}(\alpha,\beta,\gamma)$-wavefunctions

$$\left\langle {j \atop m} \right| \mathbf{R}(\alpha\beta\gamma) \left| {j \atop n} \right\rangle = D^j_{m,n}(\alpha\beta\gamma) = \sqrt{(j+n)!(j-n)!}\sqrt{(j+m)!(j-m)!}\,\frac{\sum_k (-1)^k \left(\cos\frac{\beta}{2}\right)^{2j+m-n-2k}\left(\sin\frac{\beta}{2}\right)^{n-m+2k} e^{-i(m\alpha+n\gamma)}}{(j+m-k)!(n-m+k)!k!(j-n-k)!}$$

Vector ($j=\ell=1$) representation

$$D^1(\alpha\beta\gamma) = \begin{pmatrix} e^{-i\alpha} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{i\alpha} \end{pmatrix} \begin{pmatrix} \frac{1+\cos\beta}{2} & \frac{-\sin\beta}{\sqrt{2}} & \frac{1-\cos\beta}{2} \\ \frac{\sin\beta}{\sqrt{2}} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}} \\ \frac{1-\cos\beta}{2} & \frac{\sin\beta}{\sqrt{2}} & \frac{1+\cos\beta}{2} \end{pmatrix} \begin{pmatrix} e^{-i\gamma} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{i\gamma} \end{pmatrix} = \begin{pmatrix} e^{-i\alpha}\frac{1+\cos\beta}{2}e^{-i\gamma} & e^{-i\alpha}\frac{-\sin\beta}{\sqrt{2}} & e^{-i\alpha}\frac{1-\cos\beta}{2}e^{i\gamma} \\ \frac{\sin\beta}{\sqrt{2}}e^{-i\gamma} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}}e^{i\gamma} \\ e^{i\alpha}\frac{1-\cos\beta}{2}e^{-i\gamma} & e^{i\alpha}\frac{\sin\beta}{\sqrt{2}} & e^{i\alpha}\frac{1+\cos\beta}{2}e^{i\gamma} \end{pmatrix}$$

Notation Switch:
azimuth angle: $\alpha \to \phi$
polar angle: $\beta \to \theta$

Here half-angle identities were used. $\cos^2\frac{\beta}{2} = \frac{1+\cos\beta}{2}$, $\sin^2\frac{\beta}{2} = \frac{1-\cos\beta}{2}$, $\sin\frac{\beta}{2}\cos\frac{\beta}{2} = \frac{\sin\beta}{2}$,

$$Y^{1*}_1(\phi,\theta) = \sqrt{\tfrac{3}{4\pi}}\, e^{-i\phi}\frac{-\sin\theta}{\sqrt{2}} = D^1_{1,0}(\phi,\theta)$$

$$Y^{1*}_0(\phi,\theta) = \sqrt{\tfrac{3}{4\pi}}\, \cos\beta = D^1_{0,0}(\phi,\theta)$$

$$Y^{1*}_{-1}(\phi,\theta) = \sqrt{\tfrac{3}{4\pi}}\, e^{+i\phi}\frac{\sin\theta}{\sqrt{2}} = D^1_{-1,0}(\phi,\theta)$$

Center ($n=0$) column with the factor $\sqrt{\frac{2\ell+1}{4\pi}}$ gives set of *spherical harmonics Y^ℓ_m*.

$$Y^\ell_m(\phi\theta) = D^{\ell*}_{m,n=0}(\phi\theta 0)\sqrt{\frac{2\ell+1}{4\pi}}$$

Dipole ($j=\ell=1$) wavefunctions

$$D^{1*}_{1,0}(\phi\theta 0) = -e^{i\phi}\frac{\sin\theta}{\sqrt{2}} = -\frac{\cos\phi\sin\theta + i\cos\phi\sin\theta}{\sqrt{2}} = -\frac{x+iy}{r\sqrt{2}}$$

$$D^{1*}_{0,0}(\phi\theta 0) = \cos\theta = \cos\theta = z/r$$

$$D^{1*}_{-1,0}(\phi\theta 0) = e^{-i\phi}\frac{\sin\theta}{\sqrt{2}} = \frac{\cos\phi\sin\theta - i\cos\phi\sin\theta}{\sqrt{2}} = \frac{x-iy}{r\sqrt{2}}$$

3-D linear-circular polarization T-matrix:

$$\begin{pmatrix} \left\langle {1 \atop 1}\middle|{1 \atop x}\right\rangle & \left\langle {1 \atop 1}\middle|{1 \atop y}\right\rangle & \left\langle {1 \atop 1}\middle|{1 \atop z}\right\rangle \\ \left\langle {1 \atop 0}\middle|{1 \atop x}\right\rangle & \left\langle {1 \atop 0}\middle|{1 \atop y}\right\rangle & \left\langle {1 \atop 0}\middle|{1 \atop z}\right\rangle \\ \left\langle {1 \atop -1}\middle|{1 \atop x}\right\rangle & \left\langle {1 \atop -1}\middle|{1 \atop y}\right\rangle & \left\langle {1 \atop -1}\middle|{1 \atop z}\right\rangle \end{pmatrix} = \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \end{pmatrix}$$

Applying T-matrix:

$$\begin{pmatrix} \frac{-1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & 0 & \frac{i}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} \frac{1+\cos\beta}{2} & \frac{-\sin\beta}{\sqrt{2}} & \frac{1-\cos\beta}{2} \\ \frac{\sin\beta}{\sqrt{2}} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}} \\ \frac{1-\cos\beta}{2} & \frac{\sin\beta}{\sqrt{2}} & \frac{1+\cos\beta}{2} \end{pmatrix} \cdot \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \end{pmatrix} = \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \sin\beta \end{pmatrix}$$

$$\begin{pmatrix} \frac{-1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & 0 & \frac{i}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} e^{-i\alpha} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{i\alpha} \end{pmatrix} \cdot \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \end{pmatrix} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} D^1_{x,x}(\alpha\beta\gamma) & D^1_{x,y} & D^1_{x,z} \\ D^1_{y,x} & D^1_{y,y} & D^1_{y,z} \\ D^1_{z,x} & D^1_{z,y} & D^1_{z,z} \end{pmatrix} =$$

T-matrix transforms to linear polarization (xyz) basis

$$\begin{pmatrix} \cos\alpha\cos\beta\cos\gamma - \sin\alpha\sin\gamma & -\cos\alpha\cos\beta\sin\gamma - \sin\alpha\cos\gamma & \cos\alpha\sin\beta \\ \sin\alpha\cos\beta\cos\gamma + \cos\alpha\sin\gamma & -\sin\alpha\cos\beta\sin\gamma + \cos\alpha\cos\gamma & \sin\alpha\sin\beta \\ -\cos\gamma\sin\beta & \sin\gamma\sin\beta & \cos\beta \end{pmatrix}$$

Atomic and molecular $D^{J*}_{mn}(\alpha,\beta,\gamma)$-wavefunctions

Vector ($j=\ell=1$) representation

$$D^1(\alpha\beta\gamma)=\begin{pmatrix} e^{-i\alpha} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{i\alpha}\end{pmatrix}\begin{pmatrix} \frac{1+\cos\beta}{2} & \frac{-\sin\beta}{\sqrt{2}} & \frac{1-\cos\beta}{2} \\ \frac{\sin\beta}{\sqrt{2}} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}} \\ \frac{1-\cos\beta}{2} & \frac{\sin\beta}{\sqrt{2}} & \frac{1+\cos\beta}{2}\end{pmatrix}\begin{pmatrix} e^{-i\gamma} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{i\gamma}\end{pmatrix}=\begin{pmatrix} e^{-i\alpha}\frac{1+\cos\beta}{2}e^{-i\gamma} & e^{-i\alpha}\frac{-\sin\beta}{\sqrt{2}} & e^{-i\alpha}\frac{1-\cos\beta}{2}e^{i\gamma} \\ \frac{\sin\beta}{\sqrt{2}}e^{-i\gamma} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}}e^{i\gamma} \\ e^{i\alpha}\frac{1-\cos\beta}{2}e^{-i\gamma} & e^{i\alpha}\frac{\sin\beta}{\sqrt{2}} & e^{i\alpha}\frac{1+\cos\beta}{2}e^{i\gamma}\end{pmatrix}$$

Notation Switch:
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Here half-angle identities were used. $\cos^2\frac{\beta}{2}=\frac{1+\cos\beta}{2},\ \sin^2\frac{\beta}{2}=\frac{1-\cos\beta}{2},\ \sin\frac{\beta}{2}\cos\frac{\beta}{2}=\frac{\sin\beta}{2},$

$$Y_1^{1*}(\phi,\theta)=\sqrt{\frac{3}{4\pi}}\,e^{-i\phi}\frac{-\sin\theta}{\sqrt{2}}=D^1_{1,0}(\phi,\theta)$$

$$Y_0^{1*}(\phi,\theta)=\sqrt{\frac{3}{4\pi}}\quad\cos\beta\ =D^1_{0,0}(\phi,\theta)$$

$$Y_{-1}^{1*}(\phi,\theta)=\sqrt{\frac{3}{4\pi}}\,e^{+i\phi}\frac{\sin\theta}{\sqrt{2}}\ =D^1_{-1,0}(\phi,\theta)$$

Center ($n=0$) column with the factor $\sqrt{\frac{2\ell+1}{4\pi}}$ gives set of *spherical harmonics Y^ℓ_m*.

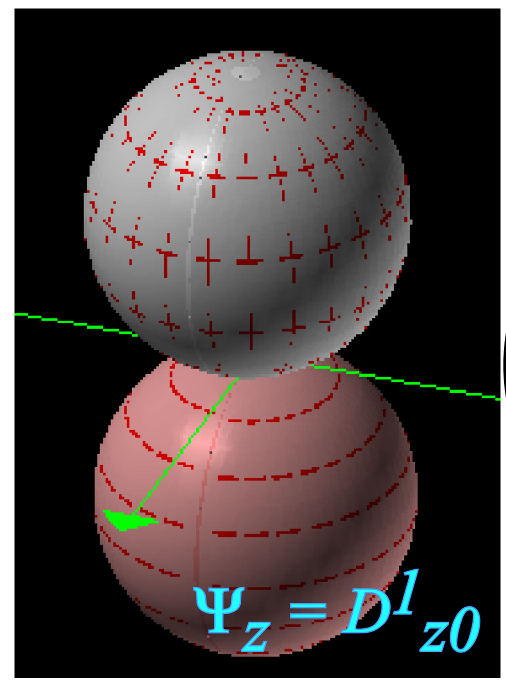
$$Y^\ell_m(\phi\theta)=D^{\ell*}_{m,n=0}(\phi\theta 0)\sqrt{\frac{2\ell+1}{4\pi}}$$

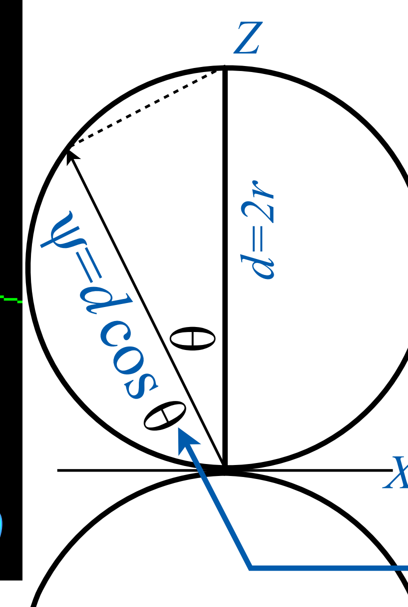
Dipole ($j=\ell=1$) wavefunctions

$$D^{1*}_{1,0}(\phi\theta 0)=-e^{i\phi}\frac{\sin\theta}{\sqrt{2}}=-\frac{\cos\phi\sin\theta+i\cos\phi\sin\theta}{\sqrt{2}}=-\frac{x+iy}{r\sqrt{2}}$$

$$D^{1*}_{0,0}(\phi\theta 0)=\cos\theta\quad=\quad\cos\theta\quad=\ z/r$$

$$D^{1*}_{-1,0}(\phi\theta 0)=e^{-i\phi}\frac{\sin\theta}{\sqrt{2}}=\frac{\cos\phi\sin\theta-i\cos\phi\sin\theta}{\sqrt{2}}=\frac{x-iy}{r\sqrt{2}}$$

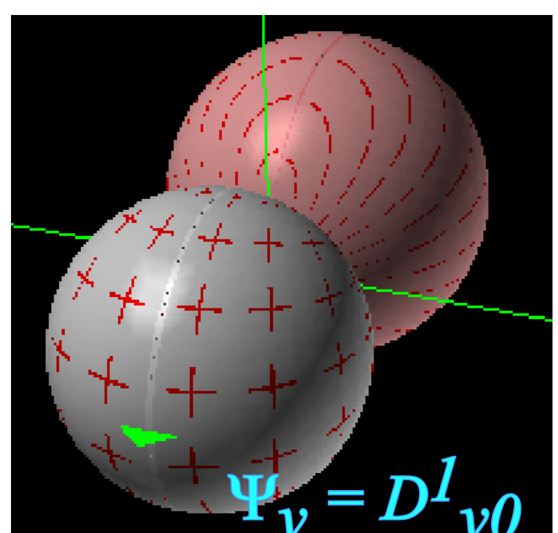


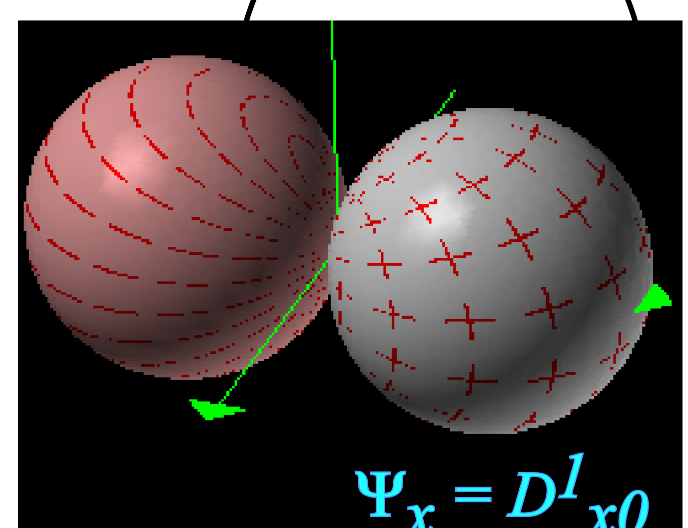


$$\Psi^1_x(\phi,\theta)=D^1_{x,z}(\phi,\theta,0)=\cos\phi\sin\theta$$

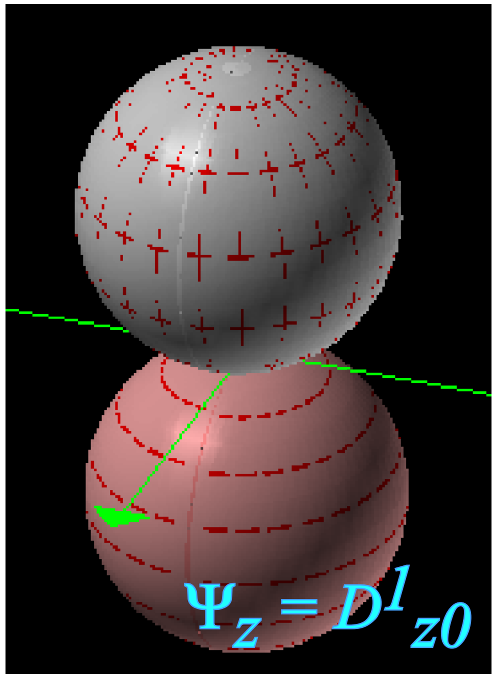
$$\Psi^1_y(\phi,\theta)=D^1_{y,z}(\phi,\theta,0)=\sin\phi\sin\theta$$

$$\Psi^1_z(\phi,\theta)=D^1_{z,z}(\phi,\theta,0)=\cos\theta$$

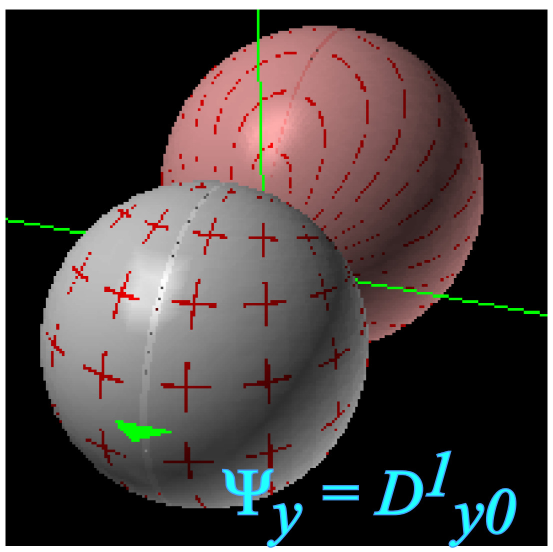


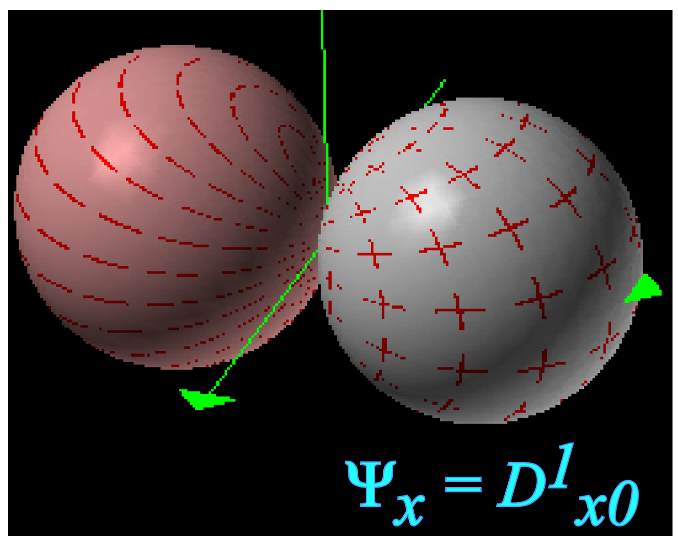


Atomic and molecular $D^{J*}_{mn}(\alpha,\beta,\gamma)$-wavefunctions and probability distributions



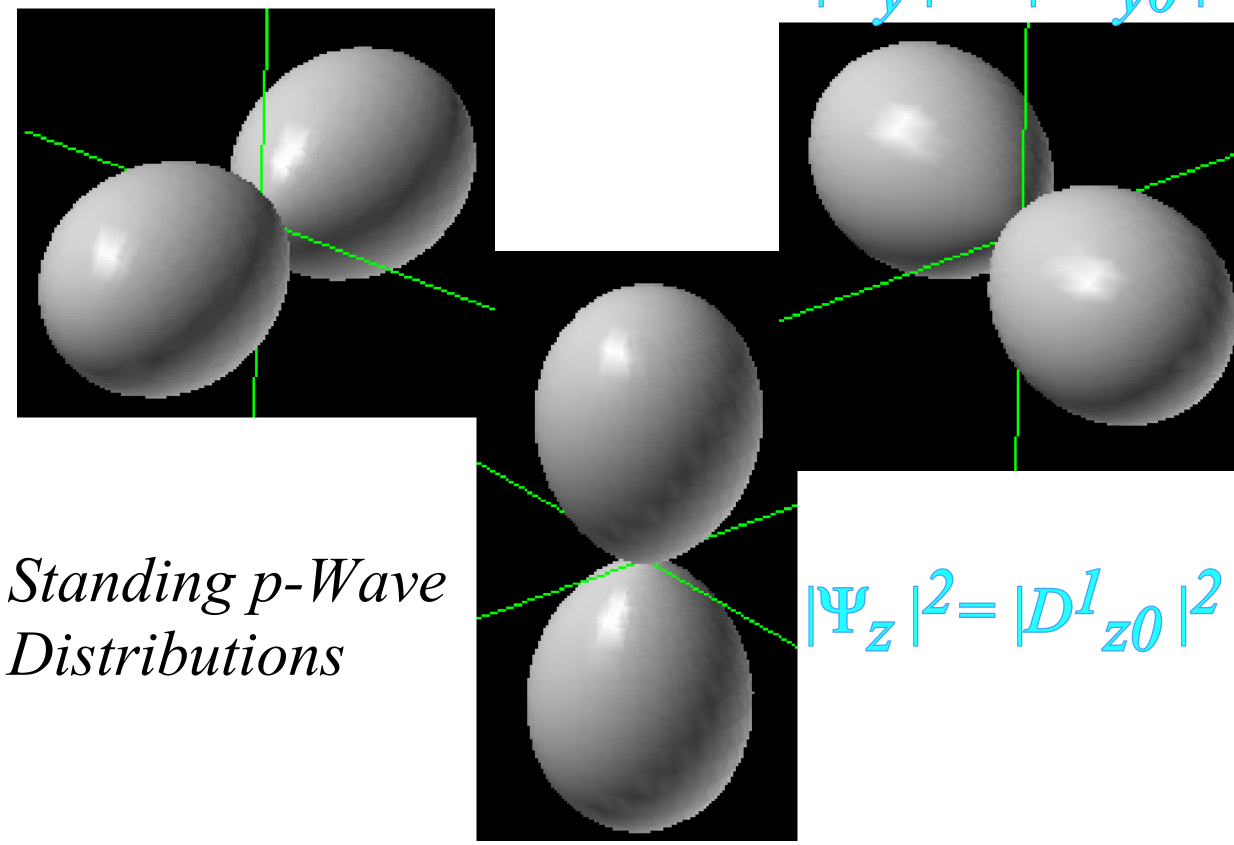
j = 1
Standing
p-Waves





$|\Psi_x|^2 = |D^1_{x0}|^2$

$|\Psi_y|^2 = |D^1_{y0}|^2$



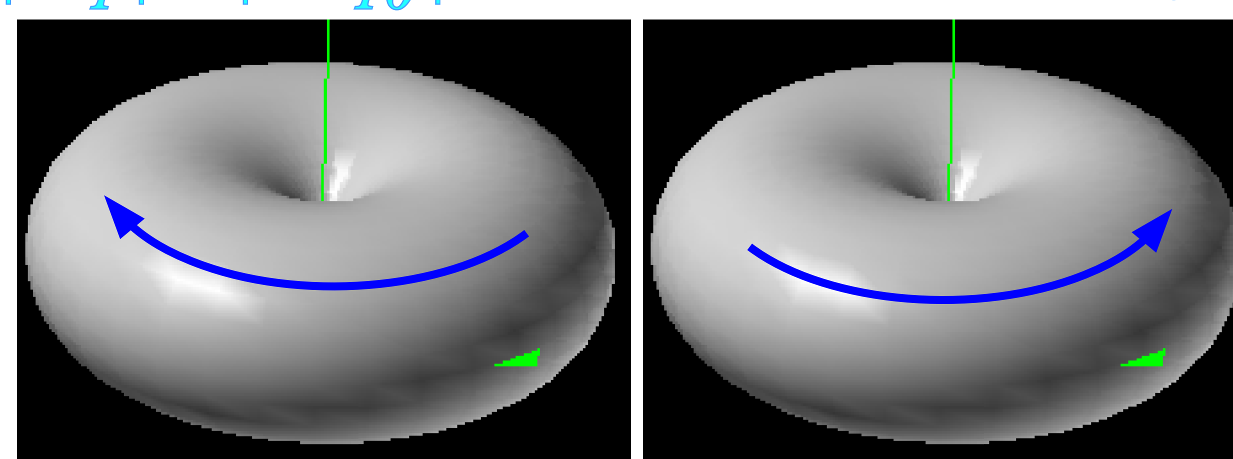
Standing p-Wave Distributions

$|\Psi_z|^2 = |D^1_{z0}|^2$

Moving p-Wave Distributions

$|\Psi_{-1}|^2 = |D^1_{-10}|^2$

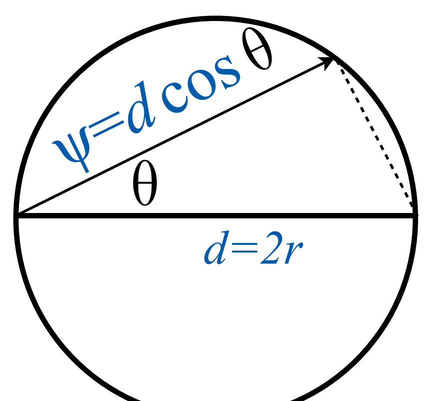
$|\Psi_1|^2 = |D^1_{10}|^2$



$$\Psi^1_x(\phi,\theta) = D^1_{x,z}(\phi,\theta,0) = \cos\phi\sin\theta$$

$$\Psi^1_y(\phi,\theta) = D^1_{y,z}(\phi,\theta,0) = \sin\phi\sin\theta$$

$$\Psi^1_z(\phi,\theta) = D^1_{z,z}(\phi,\theta,0) = \cos\theta$$



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$D^{L=1}_{m0} \sim Y^1_m$ *p-waves* $D^{L=2}_{m0} \sim Y^2_m$ *d-waves* ← $D^L_{00} \sim P^L$ *Legendre waves*

Molecular D^j_{mn} wave functions in "Mock-Mach" lab-vs-body state space $|{}^J_{mn}\rangle$

$\mathbf{P}^j_{mn}$ *projector and $D^j_{mn}(\alpha,\beta,\gamma)$ wave function*

D^J_{mn} *transform* $\mathbf{R}(\alpha,\beta,\gamma)|{}^J_{mn}\rangle=\Sigma_{m'}D^J_{m'n}(\alpha,\beta,\gamma)|{}^J_{m'n}\rangle$ *in lab-space,* $\bar{\mathbf{R}}(\alpha,\beta,\gamma)$ *in body-space.*

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Θ^J_m-analysis of high J atomic beams

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Rotational Energy Surfaces (RE or RES) of symmetric rotor and eigensolutions

Rotational Energy Surfaces (RE or RES) of asymmetric rotor (for following class)

Atomic and molecular $D^{J*}_{mn}(\alpha,\beta,\gamma)$-wavefunctions

Tensor ($j=\ell=2$) representation

$$D^2(\alpha\beta 0)=\left(\begin{array}{cc|c|cc}
e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)^2 & e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & \sqrt{\frac{3}{8}}e^{-i2\alpha}\sin^2\beta & e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{-i2\alpha}\left(\frac{1-\cos\beta}{2}\right)^2 \\
e^{-i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{-i\alpha}\left(\frac{1+\cos\beta}{2}\right)(2\cos\beta-1) & -\sqrt{\frac{3}{2}}e^{-i\alpha}\sin\beta\cos\beta & e^{-i\alpha}\left(\frac{1-\cos\beta}{2}\right)(2\cos\beta+1) & -e^{-i\alpha}\left(\frac{1-\cos\beta}{2}\right)\sin\beta \\
\sqrt{\frac{3}{8}}\sin^2\beta & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \frac{3\cos^2\beta-1}{2} & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \sqrt{\frac{3}{8}}\sin^2\beta \\
e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{i\alpha}\left(\frac{1-\cos\beta}{2}\right)(2\cos\beta+1) & \sqrt{\frac{3}{2}}e^{i\alpha}\sin\beta\cos\beta & e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)(2\cos\beta-1) & -e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta \\
e^{i2\alpha}\left(\frac{1-\cos\beta}{2}\right)^2 & e^{i2\alpha}\left(\frac{1-\cos\beta}{2}\right)\sin\beta & \sqrt{\frac{3}{8}}e^{i2\alpha}\sin^2\beta & e^{i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{i2\alpha}\left(\frac{1+\cos\beta}{2}\right)^2
\end{array}\right)$$

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e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)^2 & e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & \sqrt{\frac{3}{8}}e^{-i2\alpha}\sin^2\beta & e^{-i2\alpha}\left(\frac{1-\cos\beta}{2}\right)\sin\beta & e^{-i2\alpha}\left(\frac{1-\cos\beta}{2}\right)^2 \\
e^{-i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{-i\alpha}\left(\frac{1+\cos\beta}{2}\right)(2\cos\beta-1) & -\sqrt{\frac{3}{2}}e^{-i\alpha}\sin\beta\cos\beta & e^{-i\alpha}\left(\frac{1-\cos\beta}{2}\right)(2\cos\beta+1) & -e^{-i\alpha}\left(\frac{1-\cos\beta}{2}\right)\sin\beta \\
\sqrt{\frac{3}{8}}\sin^2\beta & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \frac{3\cos^2\beta-1}{2} & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \sqrt{\frac{3}{8}}\sin^2\beta \\
e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{i\alpha}\left(\frac{1-\cos\beta}{2}\right)(2\cos\beta+1) & \sqrt{\frac{3}{2}}e^{i\alpha}\sin\beta\cos\beta & e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)(2\cos\beta-1) & -e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta \\
e^{i2\alpha}\left(\frac{1-\cos\beta}{2}\right)^2 & e^{i2\alpha}\left(\frac{1-\cos\beta}{2}\right)\sin\beta & \sqrt{\frac{3}{8}}e^{i2\alpha}\sin^2\beta & e^{i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{i2\alpha}\left(\frac{1+\cos\beta}{2}\right)^2
\end{pmatrix}$$

Notation Switch:
azimuth angle:
$\alpha\to\phi$
polar angle:
$\beta\to\theta$

Spherical *2^k-multipole functions X^k_q* or *X-functions* are *D^**-functions times the k^{th} power of radius *(r^k)*.

$$X^k_q = r^k D^{k*}_{q,0} = \sqrt{\frac{4\pi}{2k+1}}\,r^k Y^k_q$$

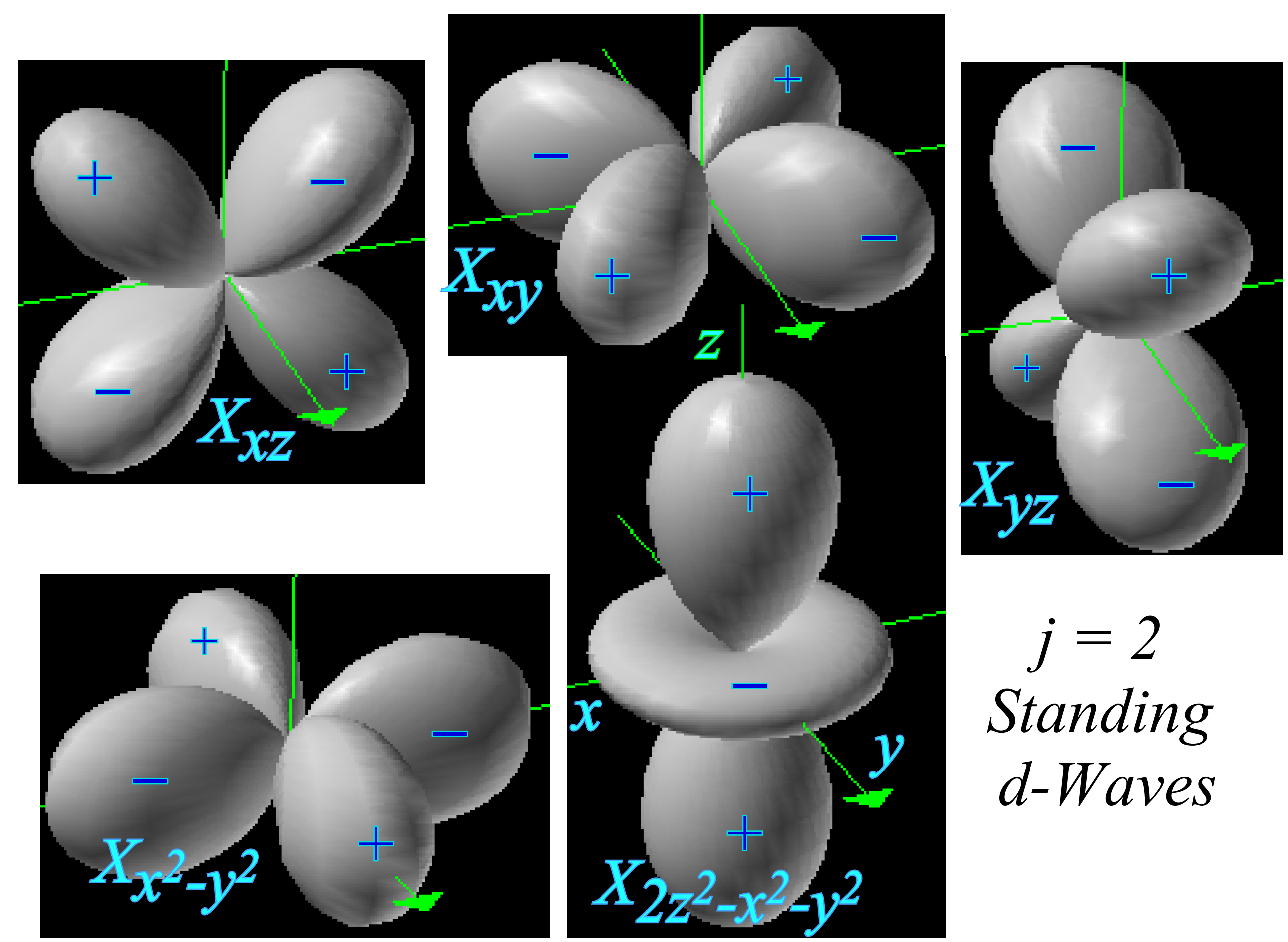
$$\sqrt{4\pi/5}\,Y^{\ell=2}_{m=2}(\phi\theta) = D^{2*}_{2,0}(\phi\theta 0) = \sqrt{\frac{3}{8}}e^{i2\phi}\sin^2\theta = \sqrt{\frac{3}{8}}\frac{(x+iy)^2}{r^2}$$

$$\sqrt{4\pi/5}\,Y^{\ell=2}_{m=1}(\phi\theta) = D^{2*}_{1,0}(\phi\theta 0) = -\sqrt{\frac{3}{2}}e^{i\phi}\sin\theta\cos\theta = -\sqrt{\frac{3}{2}}\frac{(x+iy)z}{r^2}$$

$$\sqrt{4\pi/5}\,Y^{\ell=2}_{m=0}(\phi\theta) = D^{2*}_{0,0}(\phi\theta 0) = \frac{3\cos^2\theta-1}{2} = \frac{3z^2-r^2}{2r^2}$$

$$\sqrt{4\pi/5}\,Y^{\ell=2}_{m=-1}(\phi\theta) = D^{2*}_{-1,0}(\phi\theta 0) = \sqrt{\frac{3}{2}}e^{-i\phi}\sin\theta\cos\theta = \sqrt{\frac{3}{2}}\frac{(x-iy)z}{r^2}$$

$$\sqrt{4\pi/5}\,Y^{\ell=2}_{m=-2}(\phi\theta) = D^{2*}_{-2,0}(\phi\theta 0) = \sqrt{\frac{3}{8}}e^{-i2\phi}\sin^2\theta = \sqrt{\frac{3}{8}}\frac{(x-iy)^2}{r^2}$$



j = 2
Standing d-Waves

Atomic and molecular $D^{J*}_{mn}(\alpha,\beta,\gamma)$-wavefunctions

Tensor ($j=\ell=2$) representation

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$$\sqrt{4\pi/5}\;Y^{\ell=2}_{m=0}(\phi\theta) = D^{2*}_{0,0}(\phi\theta 0) = \frac{3\cos^2\theta-1}{2} = \frac{3z^2-r^2}{2r^2}$$

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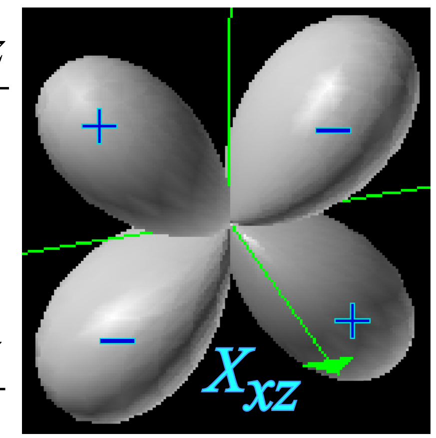
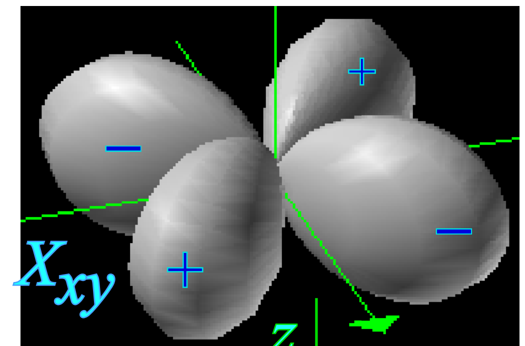
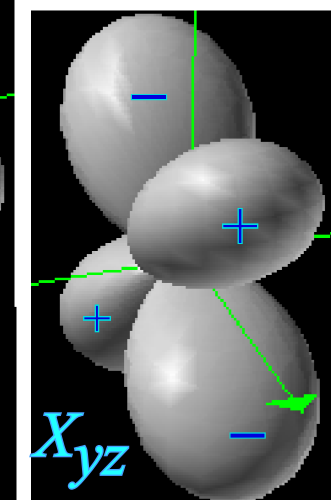
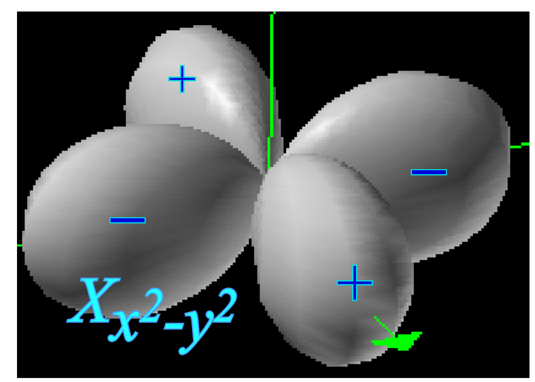
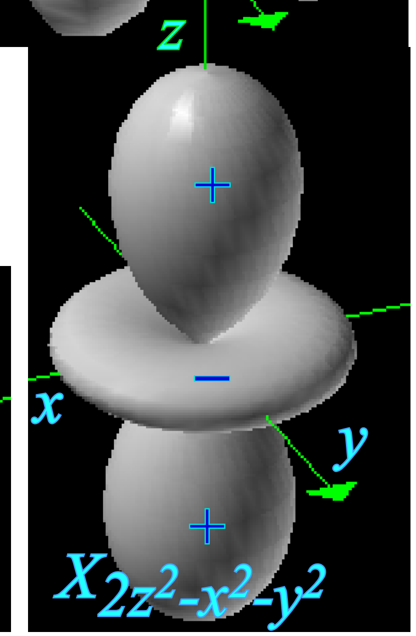
$$\sqrt{4\pi/5}\;Y^{\ell=2}_{m=-2}(\phi\theta) = D^{2*}_{-2,0}(\phi\theta 0) = \sqrt{\frac{3}{8}}e^{-i2\phi}\sin^2\theta = \sqrt{\frac{3}{8}}\frac{(x-iy)^2}{r^2}$$





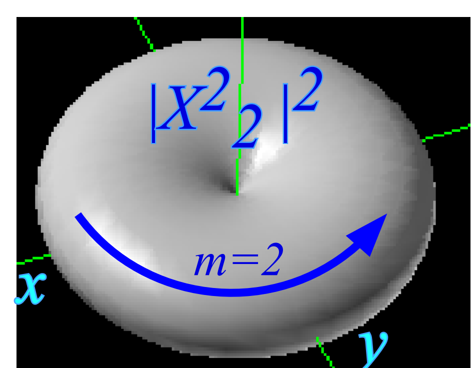


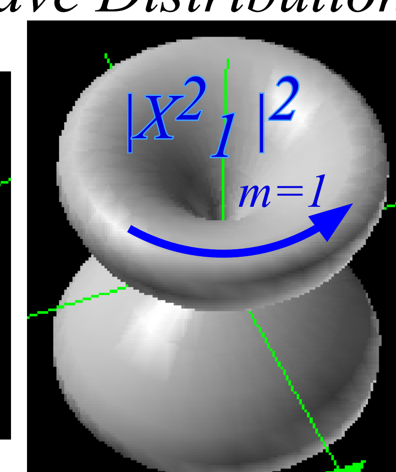


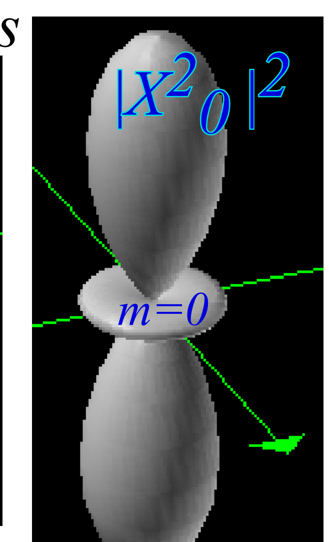


j = 2 Standing d-Waves

j = 2 Moving d-Wave Distributions







Notation Switch:
azimuth angle:
$\alpha \rightarrow \phi$
polar angle:
$\beta \rightarrow \theta$

Wigner D^J_{mn} irreps of U(2)~R(3) give atomic and molecular eigenfunctions $\Psi_{m,n}$ of 3D rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ and angular momentum uncertainty effects.

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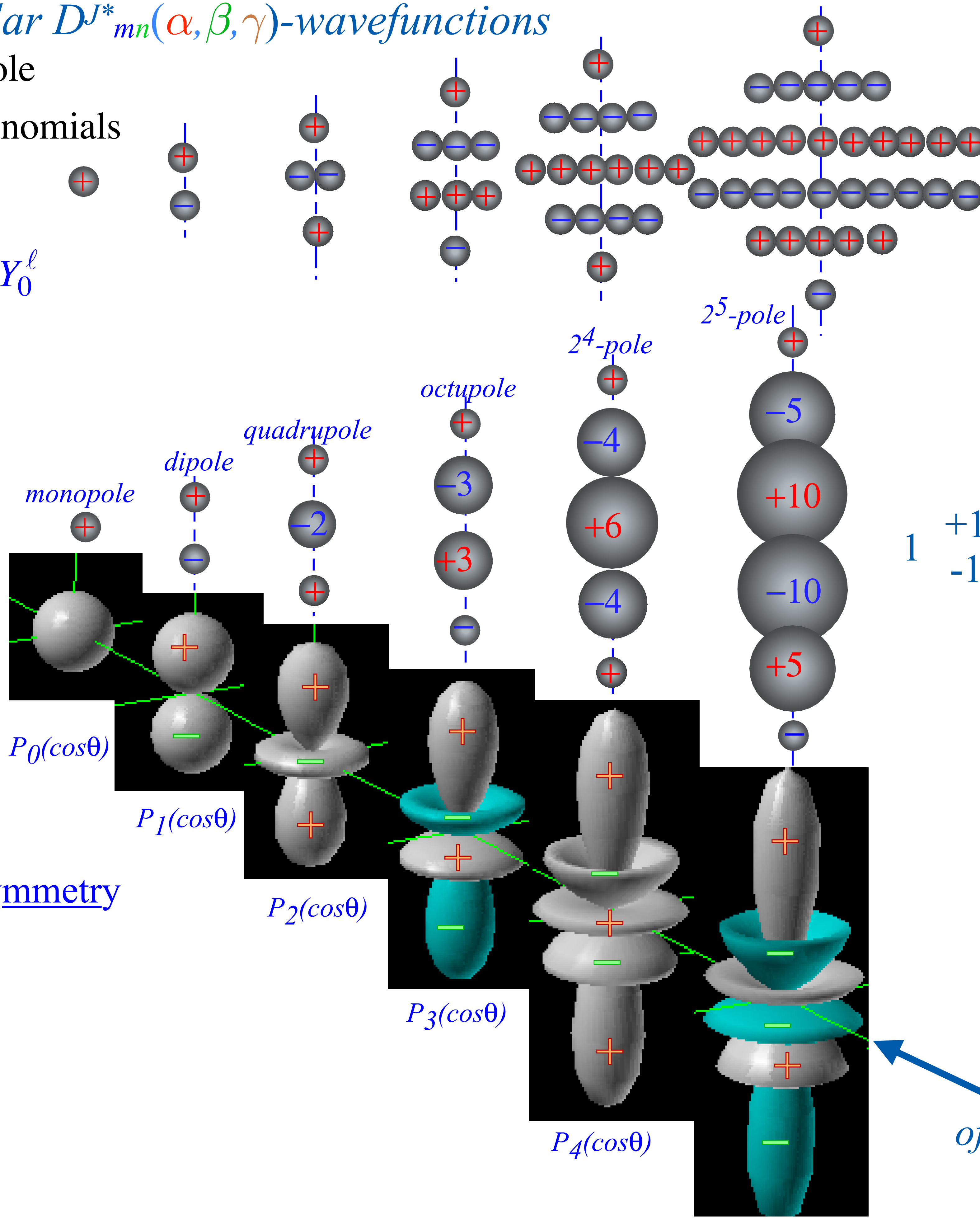
Atomic and molecular $D^{J*}_{mn}(\alpha,\beta,\gamma)$-wavefunctions

Legendre $P_\ell(\Theta)$ Multipole

Symmetric ($m = 0$) Polynomials

$$X_0^\ell = r^\ell D_{0,0}^{\ell*} = \sqrt{\frac{4\pi}{2\ell+1}}\, r^\ell Y_0^\ell$$

$$P_\ell(\Theta) = D_{0,0}^\ell(0,\Theta,0)$$



<u>Notation Switch</u>:

azimuth angle:

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polar angle:

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1

+1 -1

+1 -2 +1

+1 -3 +3 -1

+1 -4 +6 -4 +1

+1 -5 +10 -10 +5 -1

Note Pascal Triangle of (+) and (-) charges

<u>$P_\ell(\cos\theta)$ cylindrical symmetry</u>

If $m=0$ then wave is independent of the azimuth angle ϕ and only function of polar angle θ.

Each charge distribution fits in a tiny space at origin of its $P_\ell(\cos\theta)$ wave

Wigner D^J_{mn} irreps of U(2)~R(3) give atomic and molecular eigenfunctions $\Psi_{m,n}$ of 3D rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ and angular momentum uncertainty effects.

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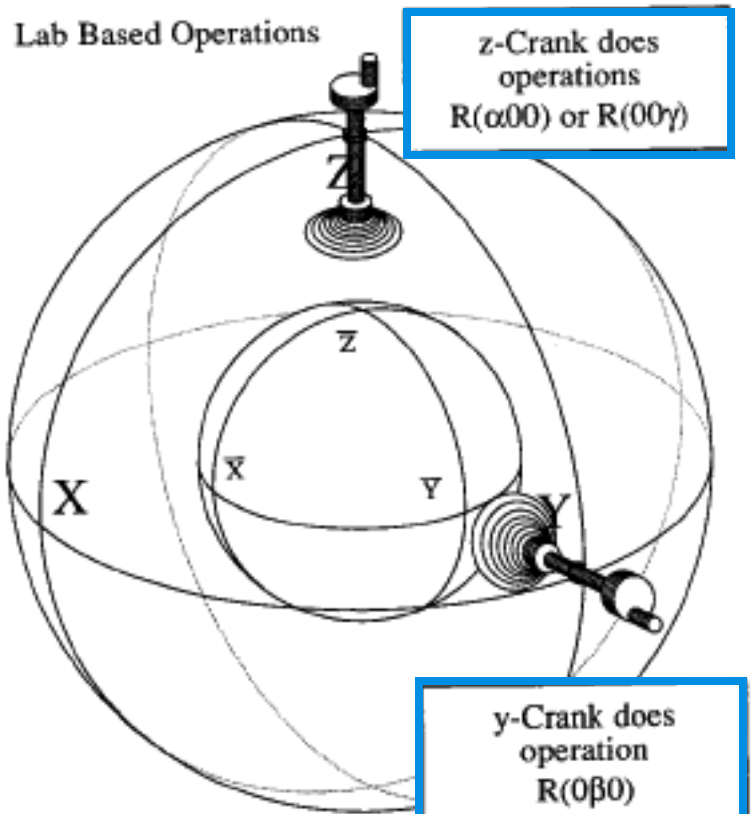
"Mock-Mach" lab-vs-body-defined states $|{}^J_{mn}\rangle = \mathbf{P}_{mn}{}^J |(0,0,0)\rangle = \int d(\alpha,\beta,\gamma) D^{J*}_{mn}(\alpha,\beta,\gamma)\mathbf{R}(\alpha,\beta,\gamma)|(0,0,0)\rangle$

From GroupThLect 25 p.15.

"Give me a place to stand...
and I will move the Earth"
Archimedes 287-212 B.C.E

Ideas of duality/relativity go *way* back (...VanVleck, Casimir..., Mach, Newton, Archimedes...)

Lab-fixed(Extrinsic-Global)**R**,**S**,..*vs.* Body-fixed (Intrinsic-Local)$\bar{\mathbf{R}}$,$\bar{\mathbf{S}}$,..



all **R**,**S**,..
commute with
all $\bar{\mathbf{R}}$,$\bar{\mathbf{S}}$,..

"Mock-Mach" relativity principles

$$\mathbf{R}|1\rangle = \bar{\mathbf{R}}^{-1}|1\rangle$$
$$\mathbf{S}|1\rangle = \bar{\mathbf{S}}^{-1}|1\rangle$$
$$\vdots$$

...for *one* state |1) *only!*

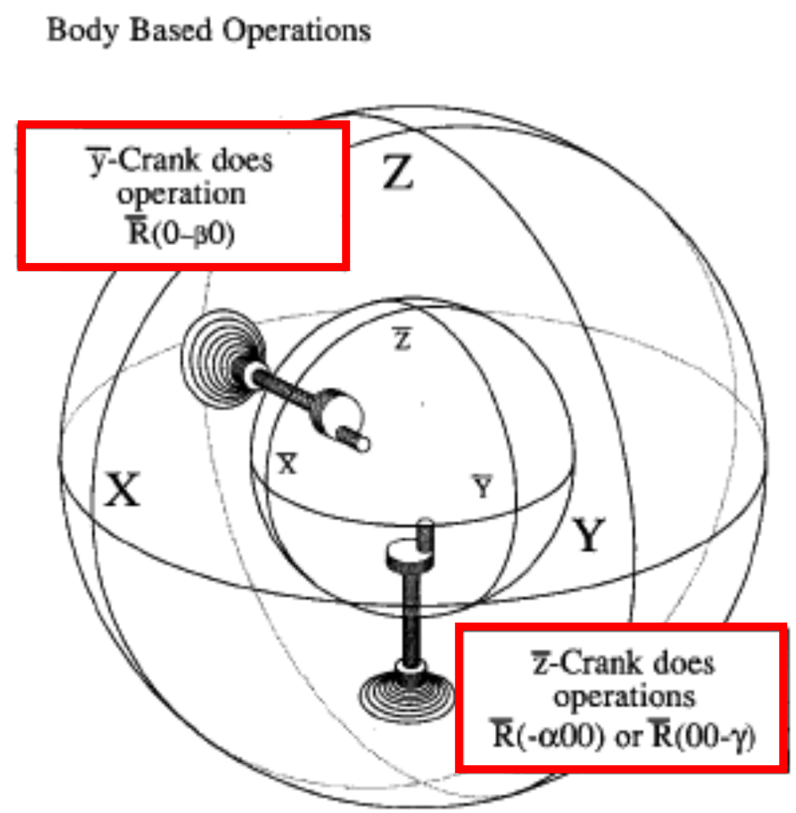


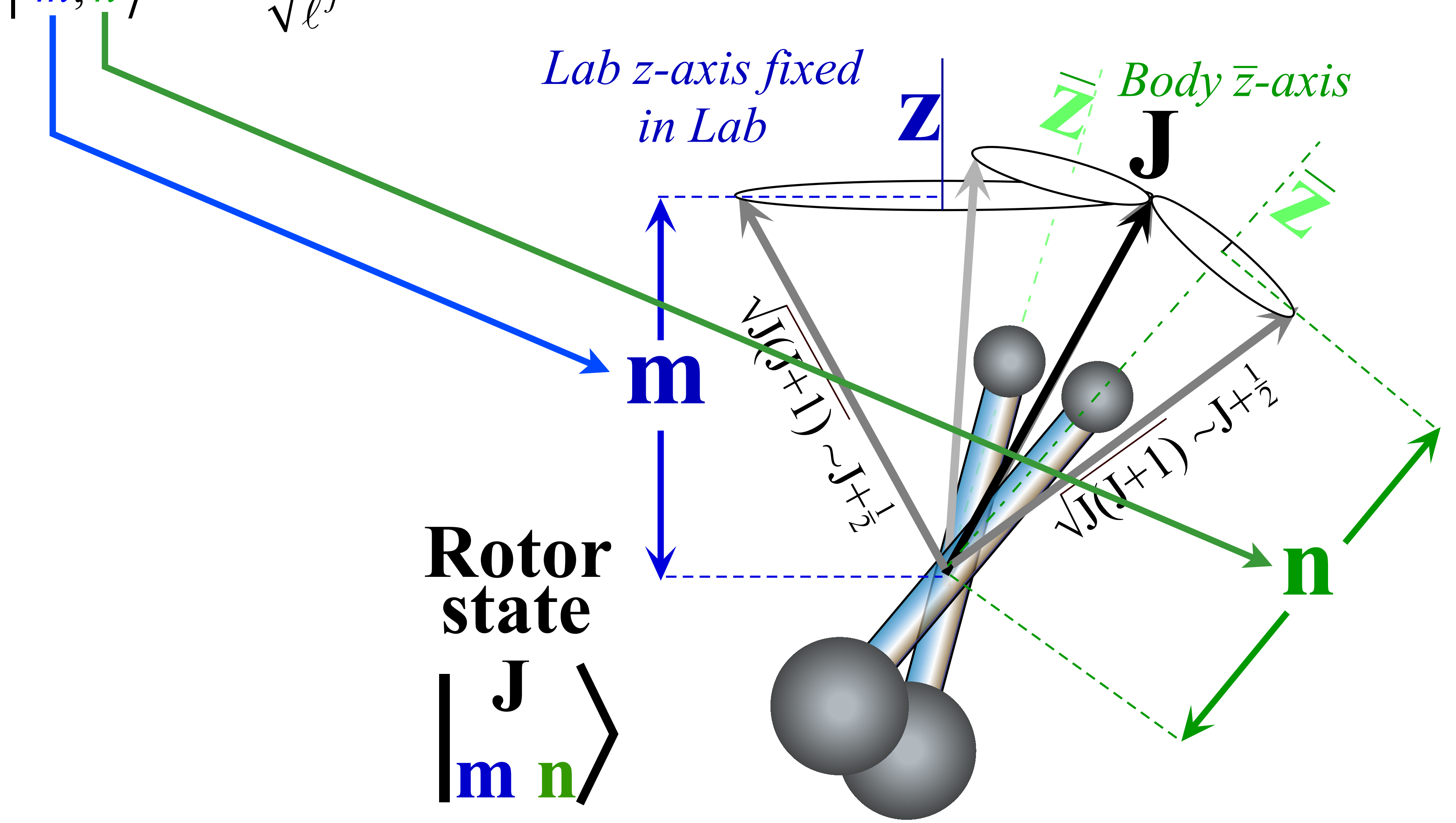
Figure from Ch. 5 of PSDS (Originally in Rev. Mod. Phys. 50, 1, p.37 (1978) Fig. 2)
Ch. 5 of PSDS p328 *RModPhys50p37*

Atomic and molecular $D^{J*}_{mn}(\alpha,\beta,\gamma)$-wavefunctions

"Mock-Mach" lab-vs-body-defined states $\left|{}^{J}_{mn}\right\rangle = \mathbf{P}_{mn}{}^{J}\left|(0,0,0)\right\rangle$

Eigenstates of angular momentum are built from projected initial position states $|000\rangle$.

$$\left|\begin{matrix} j \\ m,n \end{matrix}\right\rangle = \frac{\mathbf{P}^{j}_{m,n}\left|000\right\rangle}{\sqrt{\ell^{j}}}$$



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Molecular D^j_{mn} *wave functions in "Mock-Mach" lab-vs-body state space* $|^J_{mn}\rangle$

$\mathbf{P}^j_{mn}$ *projector and* $D^j_{mn}(\alpha,\beta,\gamma)$ *wave function*

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Rotational Energy Surfaces (RE or RES) of asymmetric rotor (for following class)

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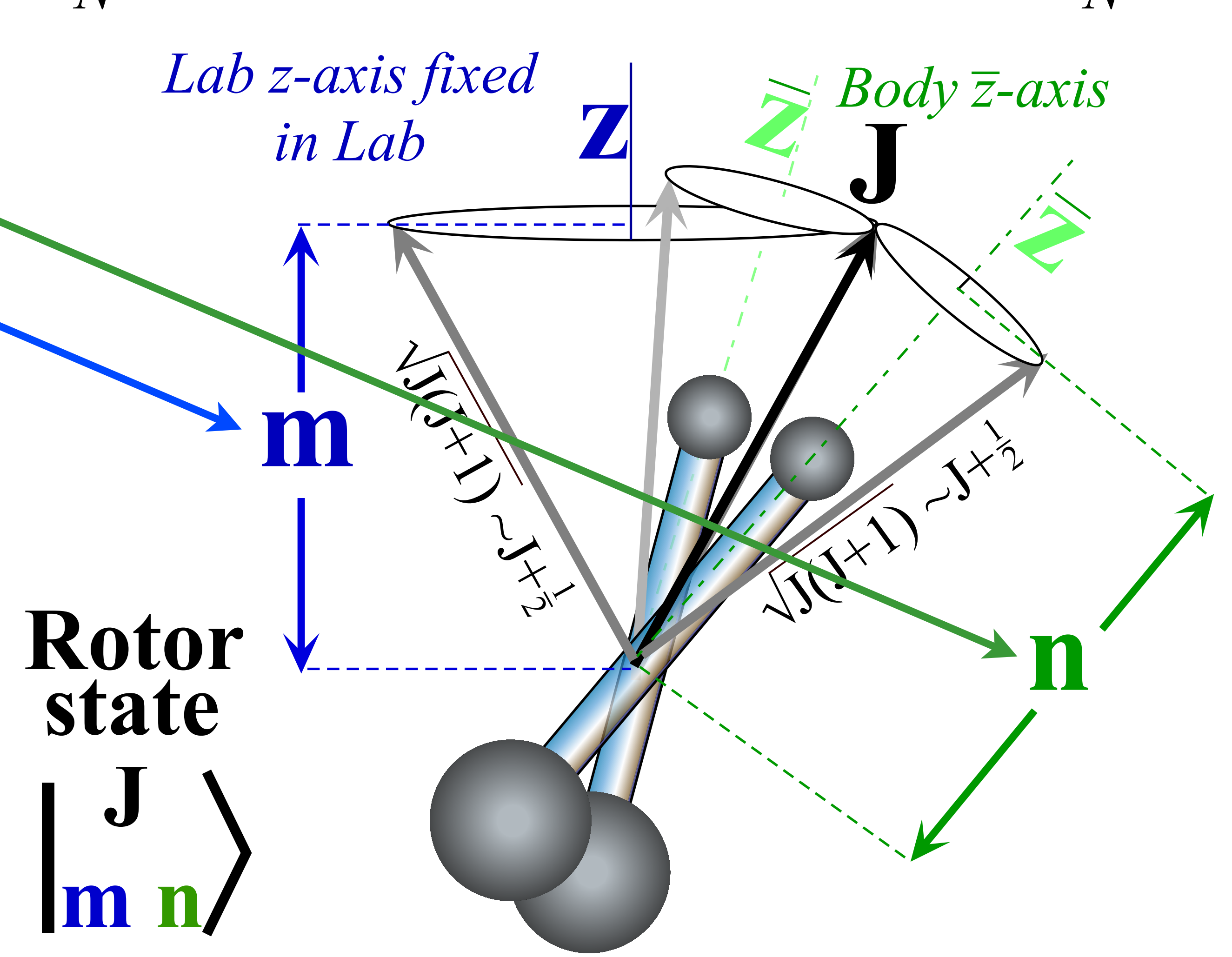

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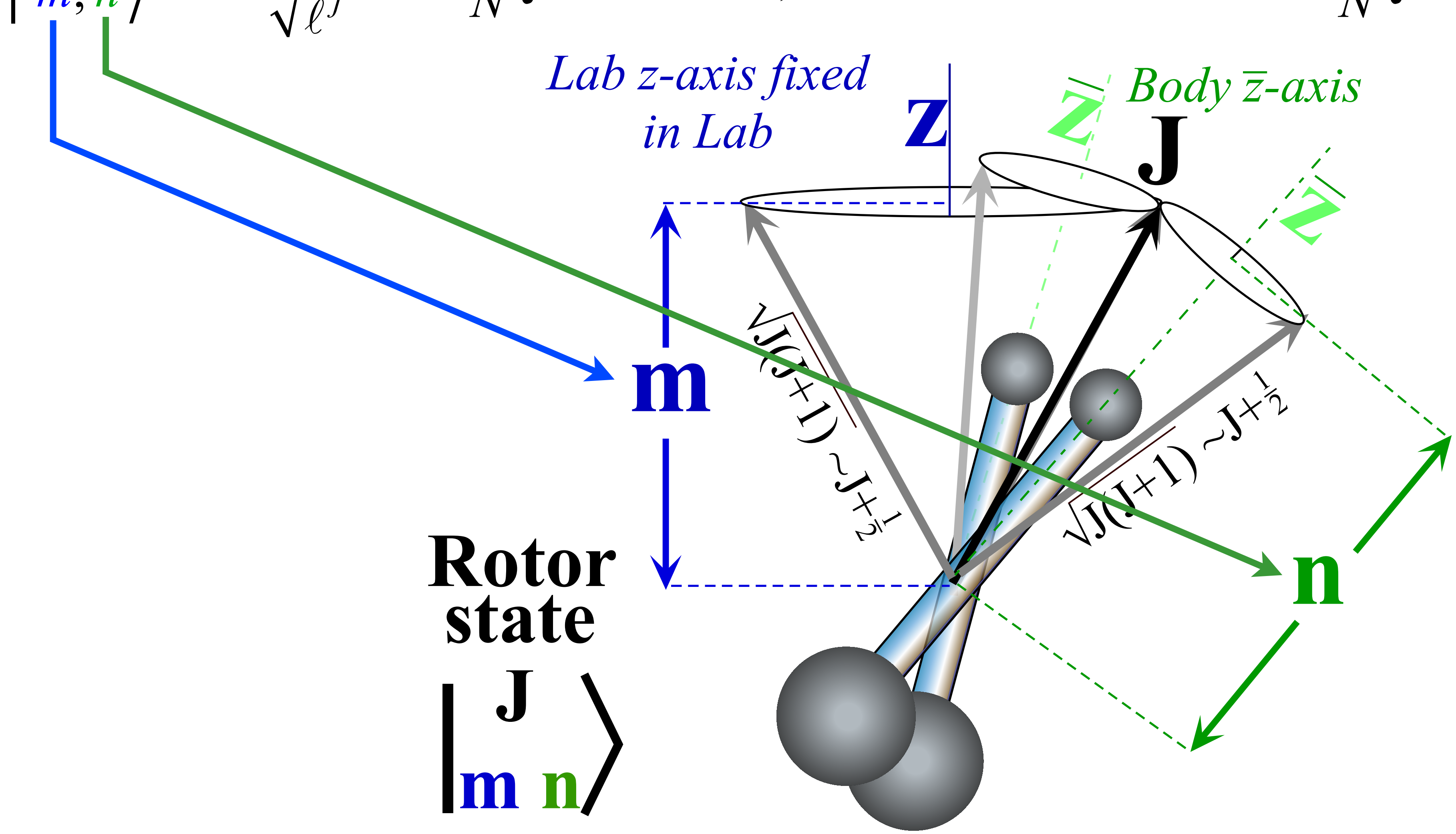

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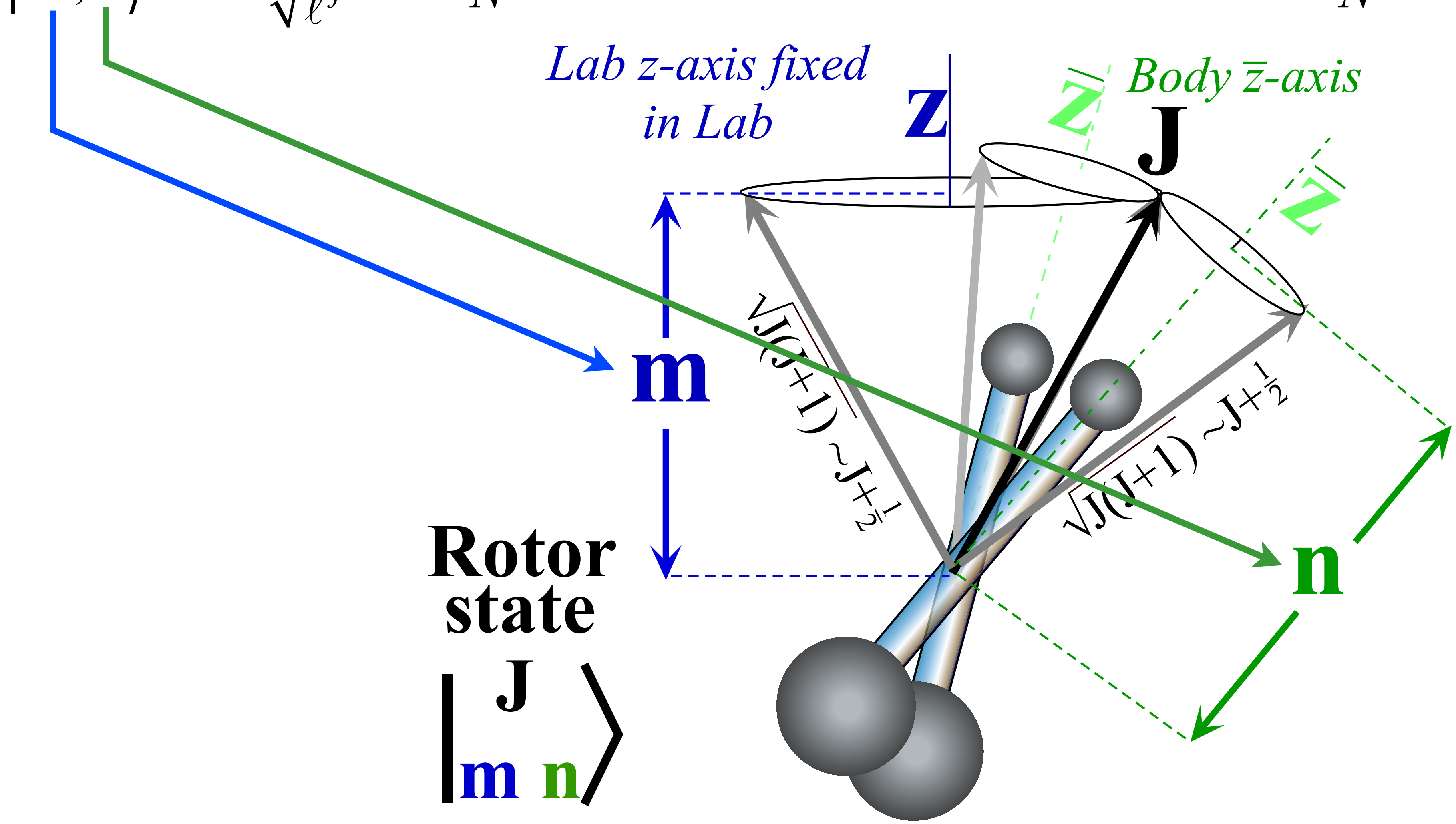

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Θ^J_m-analysis of high J atomic beams

Θ^J_m-properties of high J molecular lab-vs-body states $|{}^J_{mn}\rangle$

Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar* $\mathbf{T}_0^0$ *or tensor* $\mathbf{T}_q^2$ *operators*

Rotational Energy Surfaces (RE or RES) of symmetric rotor and eigensolutions

Rotational Energy Surfaces (RE or RES) of asymmetric rotor (for following class)

Atomic and molecular $D^{J*}_{mn}(\alpha,\beta,\gamma)$-wavefunctions

"Mock-Mach" lab-vs-body-defined states $\left|{}^{J}_{mn}\right\rangle = \mathbf{P}_{mn}{}^{J}\left|(0,0,0)\right\rangle = \int d(\alpha,\beta,\gamma) D^{J*}_{mn}(\alpha,\beta,\gamma)\mathbf{R}(\alpha,\beta,\gamma)\left|(0,0,0)\right\rangle$

For *SU(2)* and *R(3)*, sum over rotations is an integral over Euler angles (α,β,γ).

For integral-$j=0, 1, 2,\ldots$ the *R(3)* integral over polar angle β ranges from 0 to π.

$$\text{for } R(3): \frac{\ell^j}{N}\int d(\alpha\beta\gamma) = \frac{2j+1}{8\pi^2}\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma = 2j+1 = \ell^j$$

For integral-$j=1/2, 3/2,\ldots$ the *U(2)* integral over polar angle β ranges from -π to π.

$$\text{for } SU(2): \frac{\ell^j}{N}\int d(\alpha\beta\gamma) = \frac{2j+1}{16\pi^2}\int_0^{2\pi} d\alpha \int_{-\pi}^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma = 2j+1 = \ell^j$$

Eigenstates of angular momentum are built from projected initial position states $|000\rangle$.

$$\left|\begin{matrix} j \\ m,n\end{matrix}\right\rangle = \frac{\mathbf{P}^j_{m,n}|000\rangle}{\sqrt{\ell^j}} = \frac{1}{N}\int d(\alpha\beta\gamma) D^{j*}_{m,n}(\alpha\beta\gamma)\mathbf{R}(\alpha\beta\gamma)|000\rangle\sqrt{\ell^j} = \frac{1}{N}\int d(\alpha\beta\gamma) D^{j*}_{m,n}(\alpha\beta\gamma)\sqrt{\ell^j}\,|\alpha\beta\gamma\rangle$$

R(3) rotation and U(2) unitary $D^{J}_{mn}(\alpha,\beta,\gamma)$-transformation matrices

General Stern-Gerlach and polarization transformations $\mathbf{R}(\alpha,\beta,\gamma)\left|{}^{J}_{mn}\right\rangle = \Sigma_{m'} D^{J}_{m'm}(\alpha,\beta,\gamma)\left|{}^{J}_{m'n}\right\rangle$

Angular position is defined by a *rotational duality relativity relation* or "Mock-Mach" principle

$$\mathbf{R}(\alpha\beta\gamma)|000\rangle = |\alpha\beta\gamma\rangle = \bar{\mathbf{R}}^\dagger(\alpha\beta\gamma)|000\rangle \quad \text{for all } (\alpha\beta\gamma) \text{ and } (\alpha'\beta'\gamma') \quad \mathbf{R}(\alpha\beta\gamma)\bar{\mathbf{R}}(\alpha'\beta'\gamma') = \bar{\mathbf{R}}(\alpha'\beta'\gamma')\mathbf{R}(\alpha\beta\gamma)$$

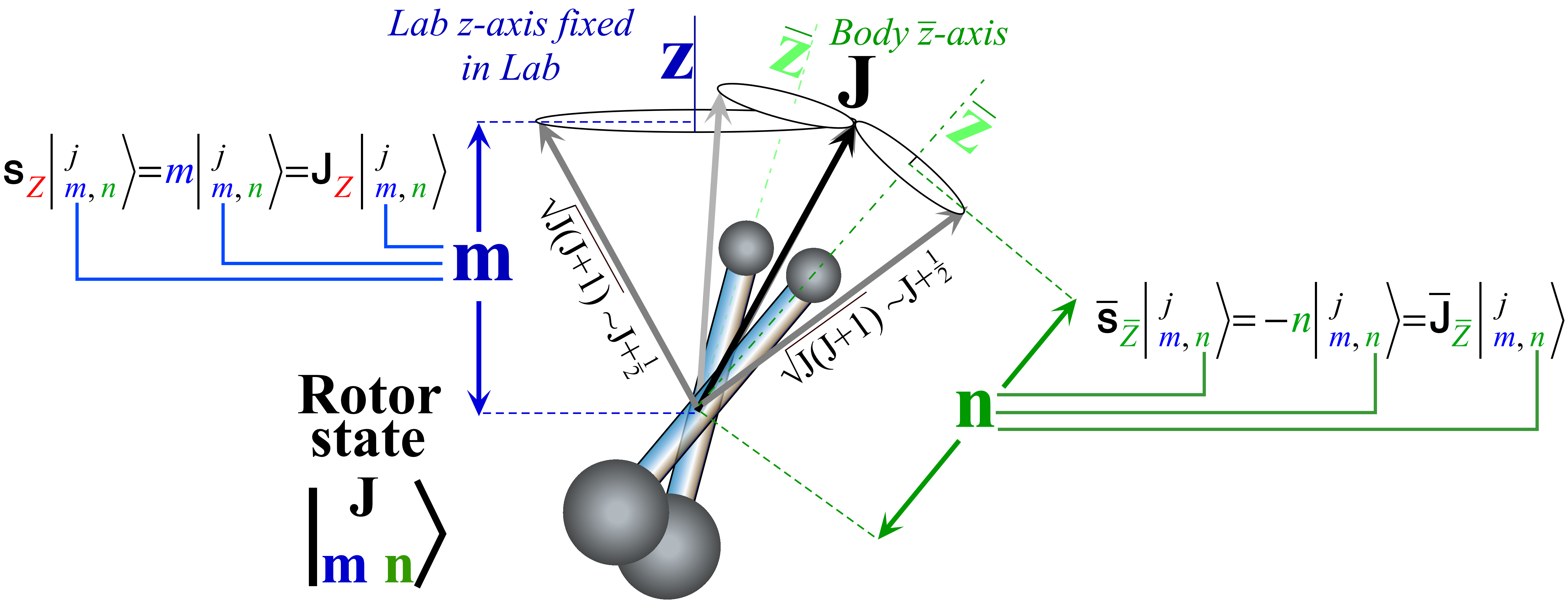
Left hand (LAB-*m*) and right hand (BODY-*n*) quantum *SU(2)* or *R(3)* numbers apply to same state.

LAB $m \leftrightarrow m'$ *transform*
$$\mathbf{R}(\alpha\beta\gamma)\left|\begin{matrix} j \\ m,n\end{matrix}\right\rangle = \sum_{m'=-j}^{j} D^{j}_{m',n}(\alpha\beta\gamma)\left|\begin{matrix} j \\ m',n\end{matrix}\right\rangle$$

BOD $n \leftrightarrow n'$ *transform*
$$\bar{\mathbf{R}}(\alpha\beta\gamma)\left|\begin{matrix} j \\ m,n\end{matrix}\right\rangle = \sum_{n'=-j}^{j} D^{j*}_{n',n}(\alpha\beta\gamma)\left|\begin{matrix} j \\ m,n'\end{matrix}\right\rangle$$

LAB *m* *eigenvalues*
$$\mathbf{s}_Z\left|\begin{matrix} j \\ m,n\end{matrix}\right\rangle = m\left|\begin{matrix} j \\ m,n\end{matrix}\right\rangle$$
LAB *m* *Z-quanta*

BOD *n* *eigenvalues*
$$\bar{\mathbf{s}}_{\bar{Z}}\left|\begin{matrix} j \\ m,n\end{matrix}\right\rangle = -n\left|\begin{matrix} j \\ m,n\end{matrix}\right\rangle$$
BOD -*n* *Z-quanta*



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for all $(\alpha\beta\gamma)$ and $(\alpha'\beta'\gamma')$

$$\mathbf{R}(\alpha\beta\gamma)\bar{\mathbf{R}}(\alpha'\beta'\gamma') = \bar{\mathbf{R}}(\alpha'\beta'\gamma')\mathbf{R}(\alpha\beta\gamma)$$

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$$\bar{\mathbf{R}}(\alpha\beta\gamma)\left|{}^{j}_{m,n}\right\rangle = \sum_{n'=-j}^{j} D^{j*}_{n',n}(\alpha\beta\gamma)\left|{}^{j}_{m,n'}\right\rangle$$

LAB *m* *eigenvalues*

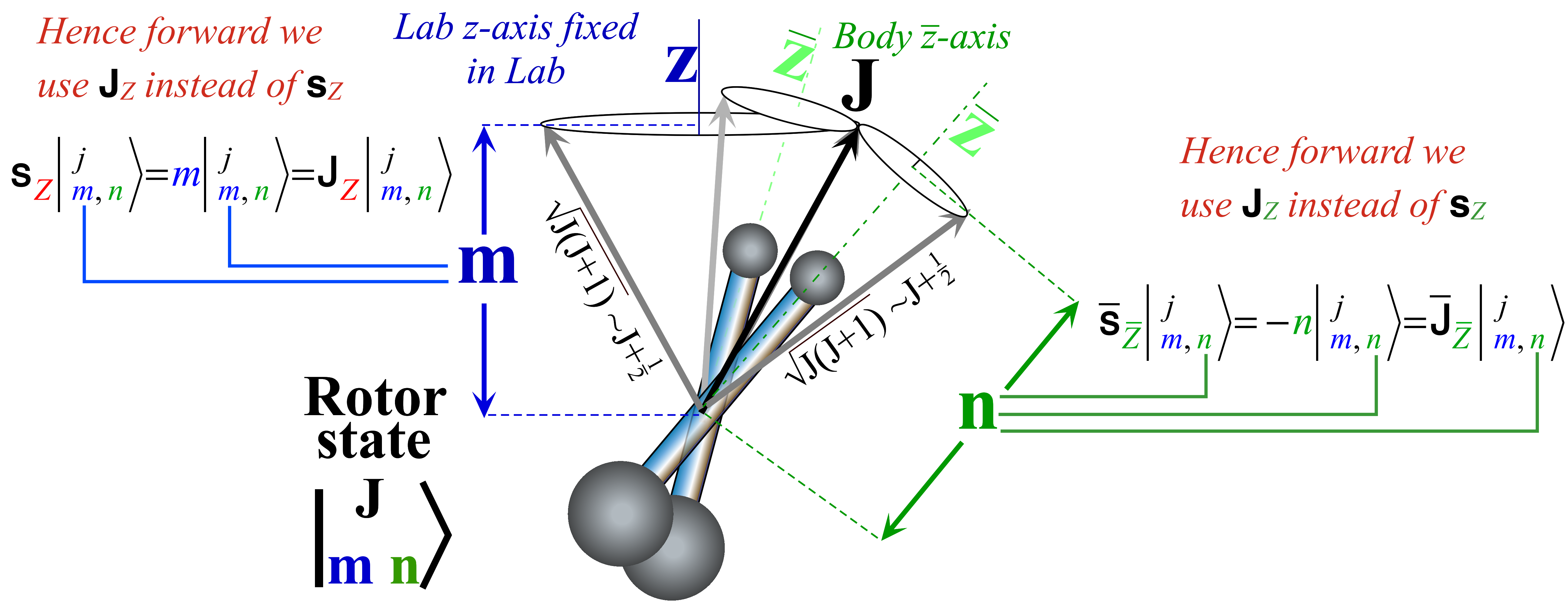
$$\mathbf{S}_Z\left|{}^{j}_{m,n}\right\rangle = m\left|{}^{j}_{m,n}\right\rangle$$

LAB *m* *Z-quanta*

BOD *n* *eigenvalues*

$$\bar{\mathbf{S}}_{\bar{Z}}\left|{}^{j}_{m,n}\right\rangle = -n\left|{}^{j}_{m,n}\right\rangle$$

BOD -*n* *Z-quanta*



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$$\mathbf{R}(\alpha\beta\gamma)\bar{\mathbf{R}}(\alpha'\beta'\gamma') = \bar{\mathbf{R}}(\alpha'\beta'\gamma')\mathbf{R}(\alpha\beta\gamma)$$

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$$\bar{\mathbf{R}}(\alpha\beta\gamma)\left|{}^{j}_{m,n}\right\rangle = \sum_{n'=-j}^{j} D^{j*}_{n',n}(\alpha\beta\gamma)\left|{}^{j}_{m,n'}\right\rangle$$

LAB *m* *eigenvalues*

$$\mathbf{J}_Z\left|{}^{j}_{m,n}\right\rangle = m\left|{}^{j}_{m,n}\right\rangle$$

LAB *m* *Z-quanta*

BOD *n* *eigenvalues*

$$\bar{\mathbf{J}}_{\bar{Z}}\left|{}^{j}_{m,n}\right\rangle = -n\left|{}^{j}_{m,n}\right\rangle$$

BOD -*n* *Z-quanta*

Wigner D^J_{mn} irreps of U(2)~R(3) give atomic and molecular eigenfunctions $\Psi_{m,n}$ of 3D rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ and angular momentum uncertainty effects.

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Review 3. *SU(2)⊂U(2) oscillators vs. R(3)⊂O(3) rotors*

Angular momentum magnitude and Θ^J_m-uncertainty cone polar angles

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Applications of D^j_{mn} representations

Atomic wave functions. $D^L_{m0} \sim Y^L_m$ *Spherical harmonics*

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Molecular D^j_{mn} wave functions in "Mock-Mach" lab-vs-body state space $|^J_{mn}\rangle$

$\mathbf{P}^j_{mn}$ *projector and* $D^j_{mn}(\alpha,\beta,\gamma)$ *wave function*

D^J_{mn} *transform* $\mathbf{R}(\alpha,\beta,\gamma)|^J_{mn}\rangle=\Sigma_{m'} D^J_{m'n}(\alpha,\beta,\gamma)|^J_{m'n}\rangle$ *in lab-space,* $\bar{\mathbf{R}}(\alpha,\beta,\gamma)$ *in body-space.*

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R(3) rotation and U(2) unitary $D^J_{mn}(\alpha,\beta,\gamma)$-transformation matrices

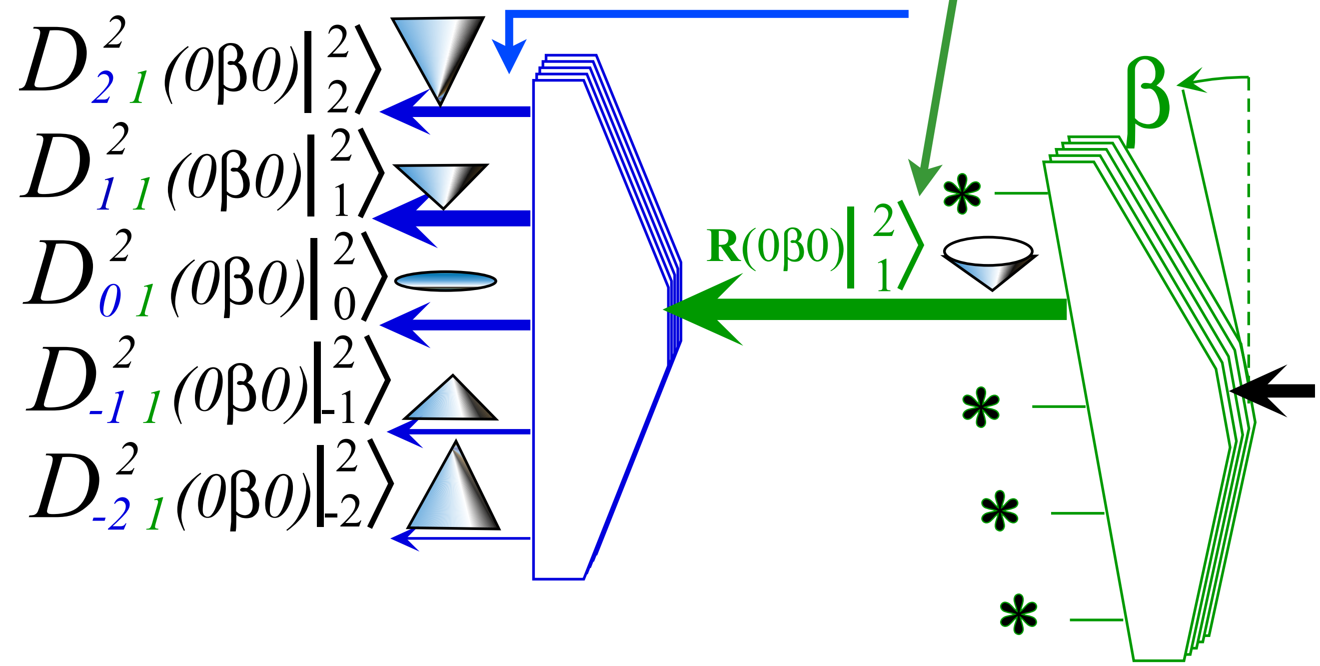
General Stern-Gerlach and polarization transformations $\mathbf{R}(\alpha,\beta,\gamma)|{}^J{}_{mn}\rangle = \Sigma_{m'} D^J{}_{m'm}(\alpha,\beta,\gamma)|{}^J{}_{m'n}\rangle$

Polarization analysis: Suppose a spin-j state $\mathbf{R}(0\beta 0)\,|{}^{j=2}{}_{n=1}\rangle$ exits an analyzer rotated by β

and then enters a vertical ($\beta=0$) analyzer and forced to choose from unrotated states $|{}^{j=2}{}_{m'}\rangle$

$$\mathbf{R}(0\beta 0)\left|{}^{j}_{n}\right\rangle = \sum_{m'=-j}^{j} \left|{}^{j}_{m'}\right\rangle\left\langle{}^{j}_{m'}\right|\mathbf{R}(0\beta 0)\left|{}^{j}_{n}\right\rangle$$

$$= \sum_{m'=-j}^{j} \left|{}^{j}_{m'}\right\rangle D^{j}_{m'n}(0\beta 0)$$



R(3) rotation and U(2) unitary $D^J_{mn}(\alpha,\beta,\gamma)$-transformation matrices

General Stern-Gerlach and polarization transformations $\mathbf{R}(\alpha,\beta,\gamma)\left|{}^J_{mn}\right\rangle = \Sigma_{m'} D^J_{m'm}(\alpha,\beta,\gamma)\left|{}^J_{m'n}\right\rangle$

Polarization analysis: Suppose a spin-j state $\mathbf{R}(0\beta 0)\left|{}^{j=2}_{n=1}\right\rangle$ exits an analyzer rotated by β and then enters a vertical $(\beta=0)$ analyzer and forced to choose from unrotated states $\left|{}^{j=2}_{m'}\right\rangle$

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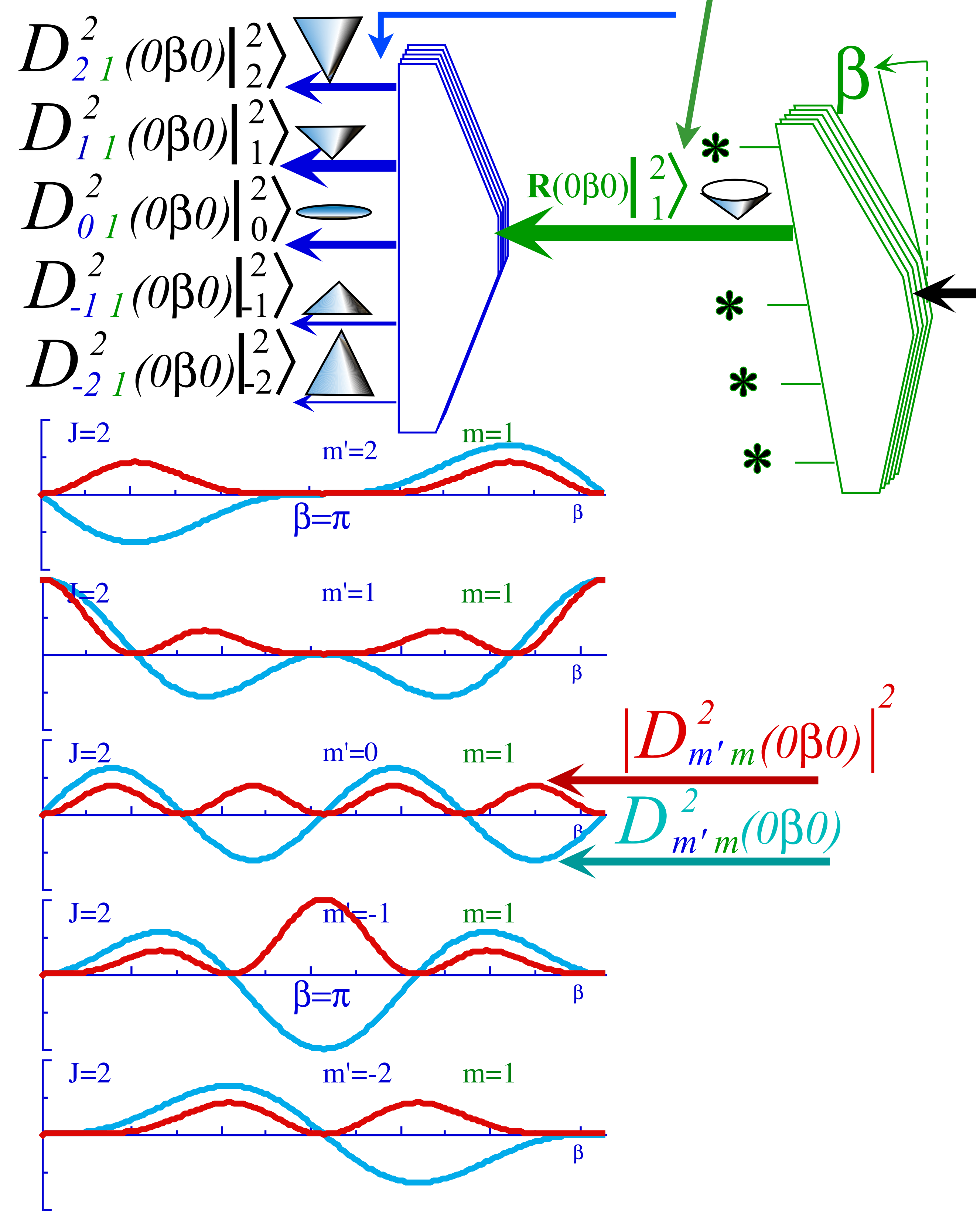
$$= \sum_{m'=-j}^{j}\left|{}^{j}_{m'}\right\rangle D^{j}_{m'n}(0\beta 0)$$



Overlap of state $\mathbf{R}(\alpha\beta\gamma)\left|{}^2_1\right\rangle$ with unrotated $\left|{}^{j=2}_{m'}\right\rangle$ is the corresponding D-matrix element.

$$\left\langle{}^{j'}_{m'}\right|\mathbf{R}(\alpha\beta\gamma)\left|{}^{2}_{1}\right\rangle = \delta^{j'2} D^{2}_{m'1}(\alpha\beta\gamma) = \left\langle{}^{j'}_{m'}\middle|{}^{2}_{1}\right\rangle_R$$

$D^j_{m'n}(0\beta 0)$ plotted vs. β for fixed j,m',n

QTforCA Unit 8. Ch. 23 Fig. 23.2.1

R(3) rotation and U(2) unitary $D^J_{mn}(\alpha,\beta,\gamma)$-transformation matrices

General Stern-Gerlach and polarization transformations $\mathbf{R}(\alpha,\beta,\gamma)\left|{}^J_{mn}\right\rangle=\sum_{m'}D^J_{m'm}(\alpha,\beta,\gamma)\left|{}^J_{m'n}\right\rangle$

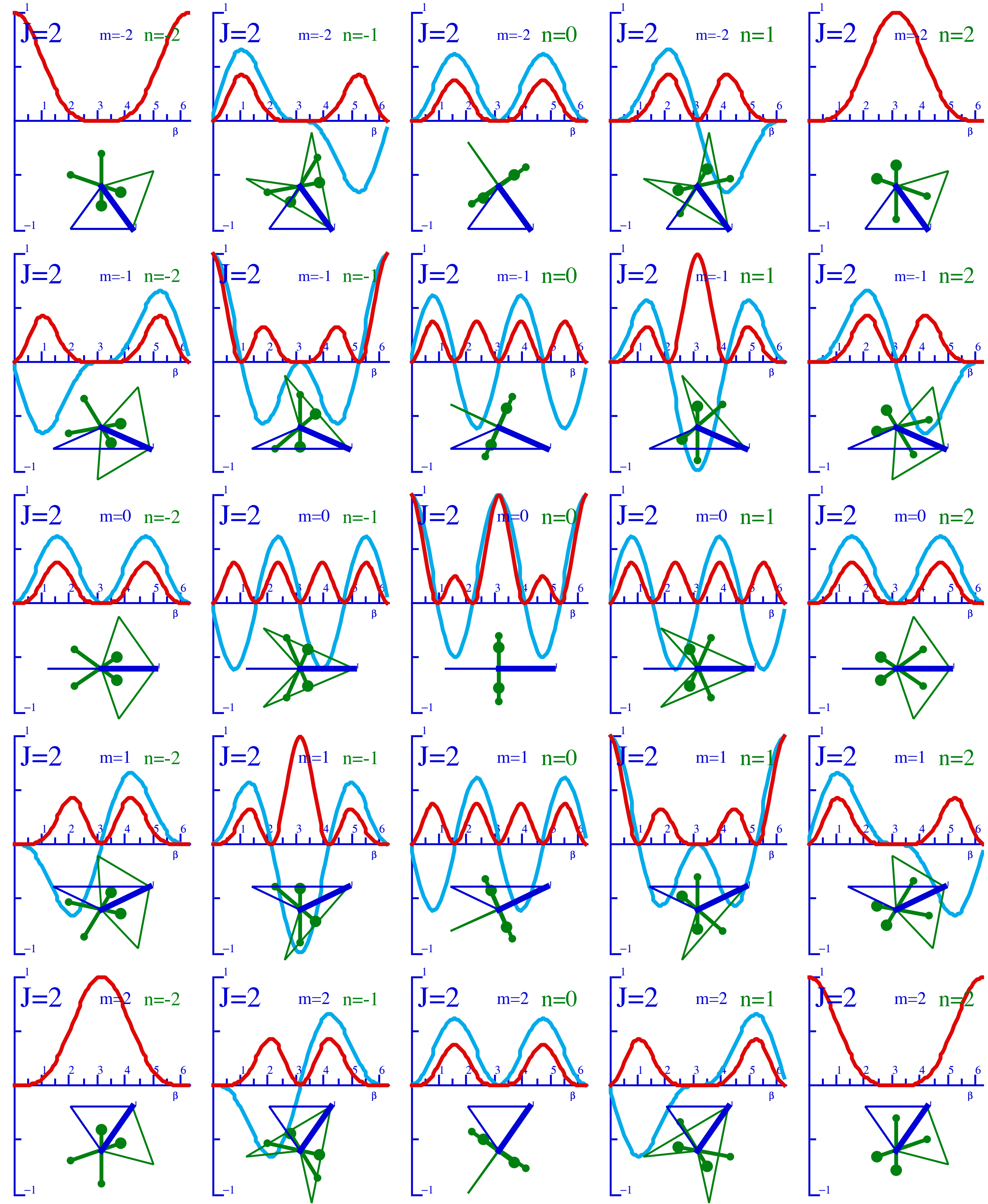
$$D^2(\alpha\beta 0)=\begin{pmatrix} e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)^2 & e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & \sqrt{\frac{3}{8}}e^{-i2\alpha}\sin^2\beta & e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{-i2\alpha}\left(\frac{1-\cos\beta}{2}\right)^2 \\ e^{-i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{-i\alpha}\left(\frac{1+\cos\beta}{2}\right)(2\cos\beta-1) & -\sqrt{\frac{3}{2}}e^{-i\alpha}\sin\beta\cos\beta & e^{-i\alpha}\left(\frac{1-\cos\beta}{2}\right)(2\cos\beta+1) & -e^{-i\alpha}\left(\frac{1-\cos\beta}{2}\right)\sin\beta \\ \sqrt{\frac{3}{8}}\sin^2\beta & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \frac{3\cos^2\beta-1}{2} & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \sqrt{\frac{3}{8}}\sin^2\beta \\ e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{i\alpha}\left(\frac{1-\cos\beta}{2}\right)(2\cos\beta+1) & \sqrt{\frac{3}{2}}e^{i\alpha}\sin\beta\cos\beta & e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)(2\cos\beta-1) & -e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta \\ e^{i2\alpha}\left(\frac{1-\cos\beta}{2}\right)^2 & e^{i2\alpha}\left(\frac{1-\cos\beta}{2}\right)\sin\beta & \sqrt{\frac{3}{8}}e^{i2\alpha}\sin^2\beta & e^{i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{i2\alpha}\left(\frac{1+\cos\beta}{2}\right)^2 \end{pmatrix}$$

$$\mathbf{R}(0\beta 0)\left|{}^j_n\right\rangle=\sum_{m'=-j}^{j}\left|{}^j_{m'}\right\rangle\left\langle{}^j_{m'}\right|\mathbf{R}(0\beta 0)\left|{}^j_n\right\rangle$$

$$=\sum_{m'=-j}^{j}\left|{}^j_{m'}\right\rangle D^j_{m'n}(0\beta 0)$$

Overlap of state $\mathbf{R}(\alpha\beta\gamma)\left|{}^2_1\right\rangle$ on unrotated $\left|{}^{j=2}_{m'}\right\rangle$ is the corresponding D-matrix element.

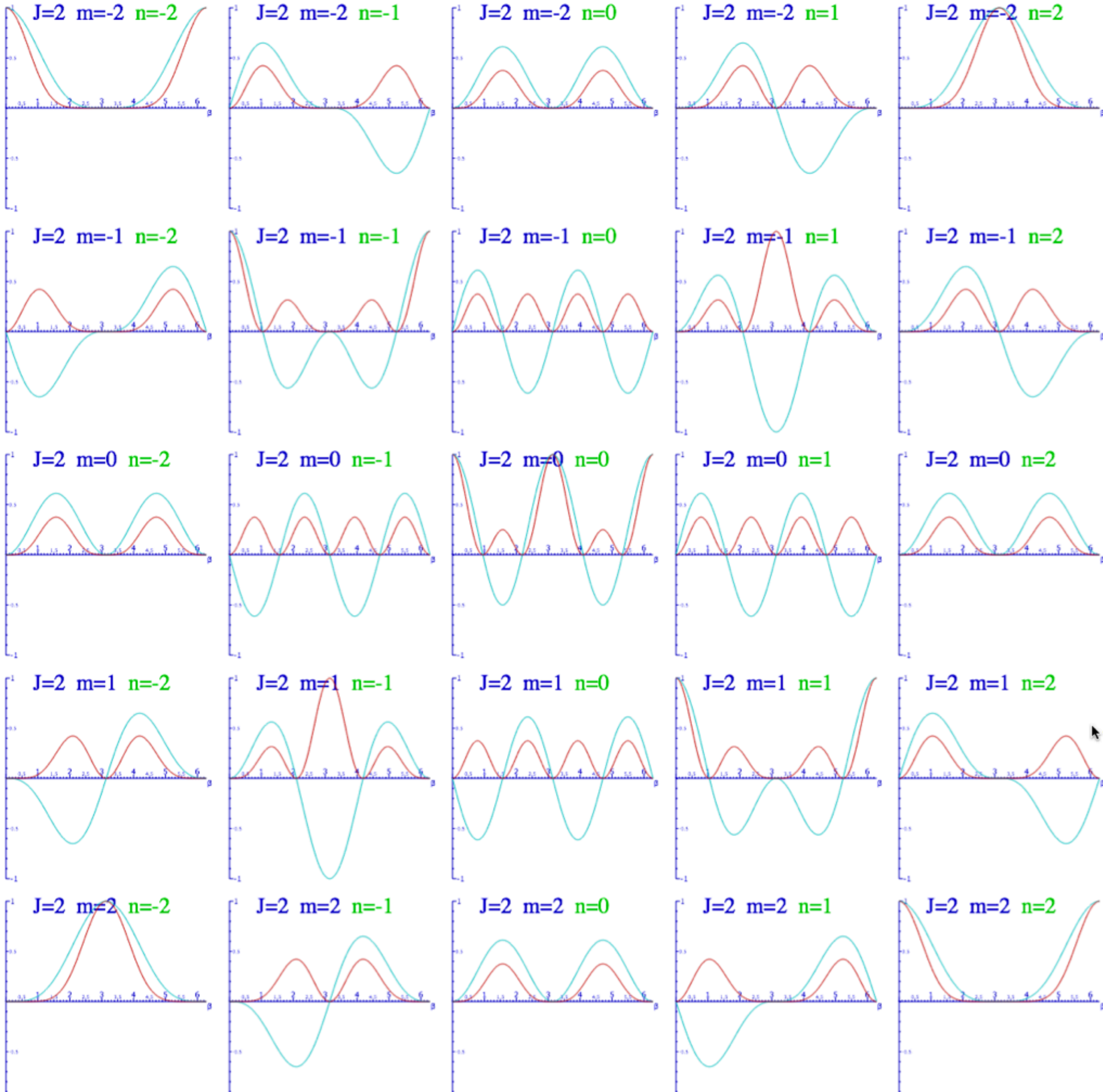
$$\left\langle{}^{j'}_{m'}\right|\mathbf{R}(\alpha\beta\gamma)\left|{}^2_1\right\rangle=\delta^{j'2}D^2_{m'1}(\alpha\beta\gamma)=\left\langle{}^{j'}_{m'}\middle|{}^2_1\right\rangle_R$$



$D^j_{m'n}(0\beta 0)$ plotted vs. β for fixed j,m',n

QTforCA Unit 8. Ch. 23 Fig. 23.2.5

$D^J_{m'n}(0\beta 0)$ plotted vs. β for fixed J,m',n



QuantIt web simulation: Visualizing D representations

Wigner D^J_{mn} irreps of U(2)~R(3) give atomic and molecular eigenfunctions $\Psi_{m,n}$ of 3D rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ and angular momentum uncertainty effects.

Review 1. *Angular momentum raise-n-lower operators* $\mathbf{S}_+$ and $\mathbf{S}_-$ Review 2. Angular momentum commutation

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Rotational Energy Surfaces (RE or RES) of symmetric rotor and eigensolutions

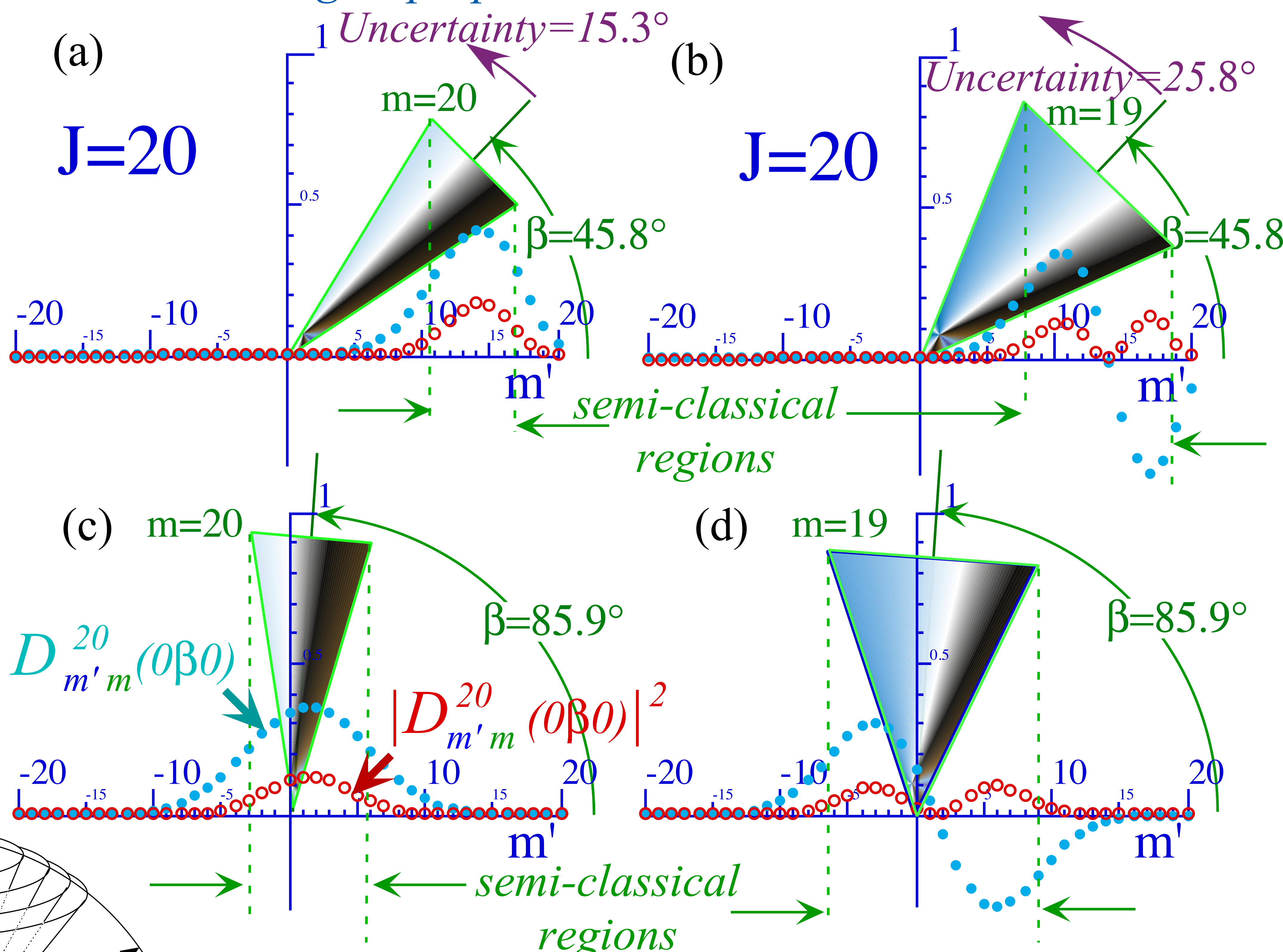
Rotational Energy Surfaces (RE or RES) of asymmetric rotor (for following class)

Angular momentum cones and high J properties

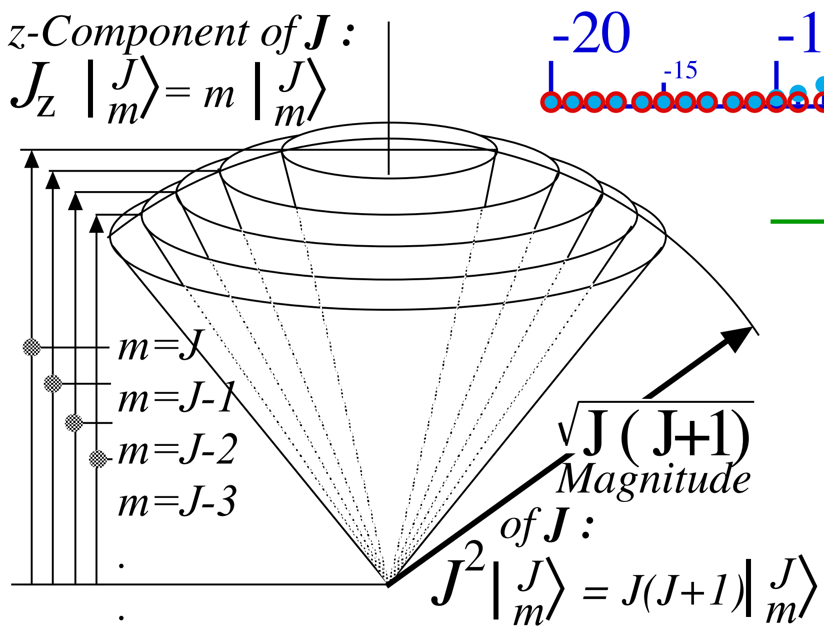
$D^J_{m'm}(0\beta 0)$ plotted vs. m' for fixed J, β, m

J=20

Discrete plots



QTforCA Unit 8. Ch. 23 Fig. 23.1.1



QuantIt web simulation: Visualizing D representations

QTforCA Unit 8. Ch. 23 Fig. 23.2.2

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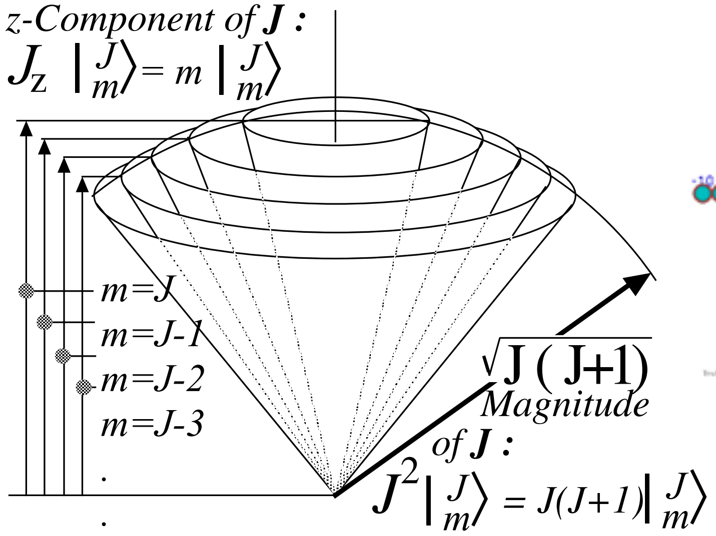
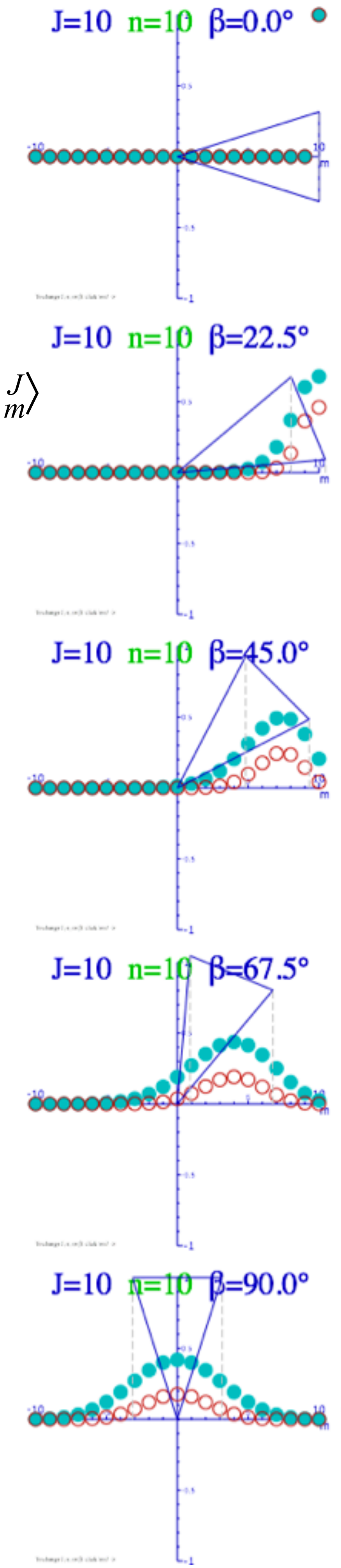
Rotational Energy Surfaces (RE or RES) of asymmetric rotor (for following class)





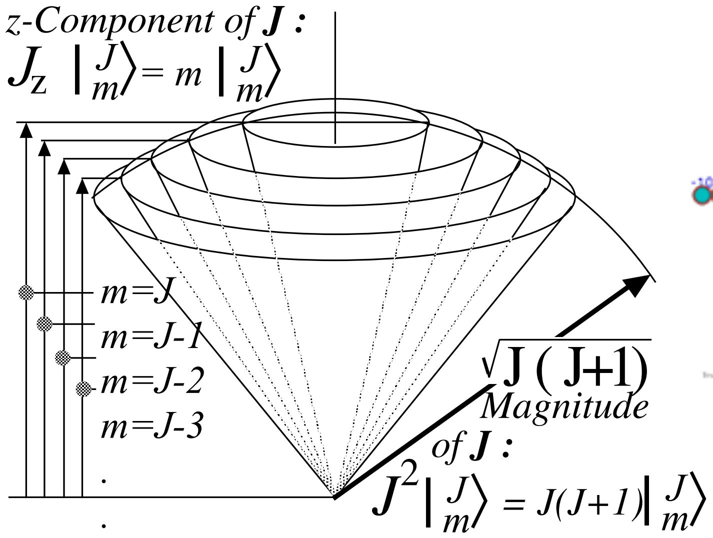
$D^J_{m,n}(0\beta 0)$
plotted
vs. *m*
for fixed
$J=10, \beta, n$

to $n=10$

J=10

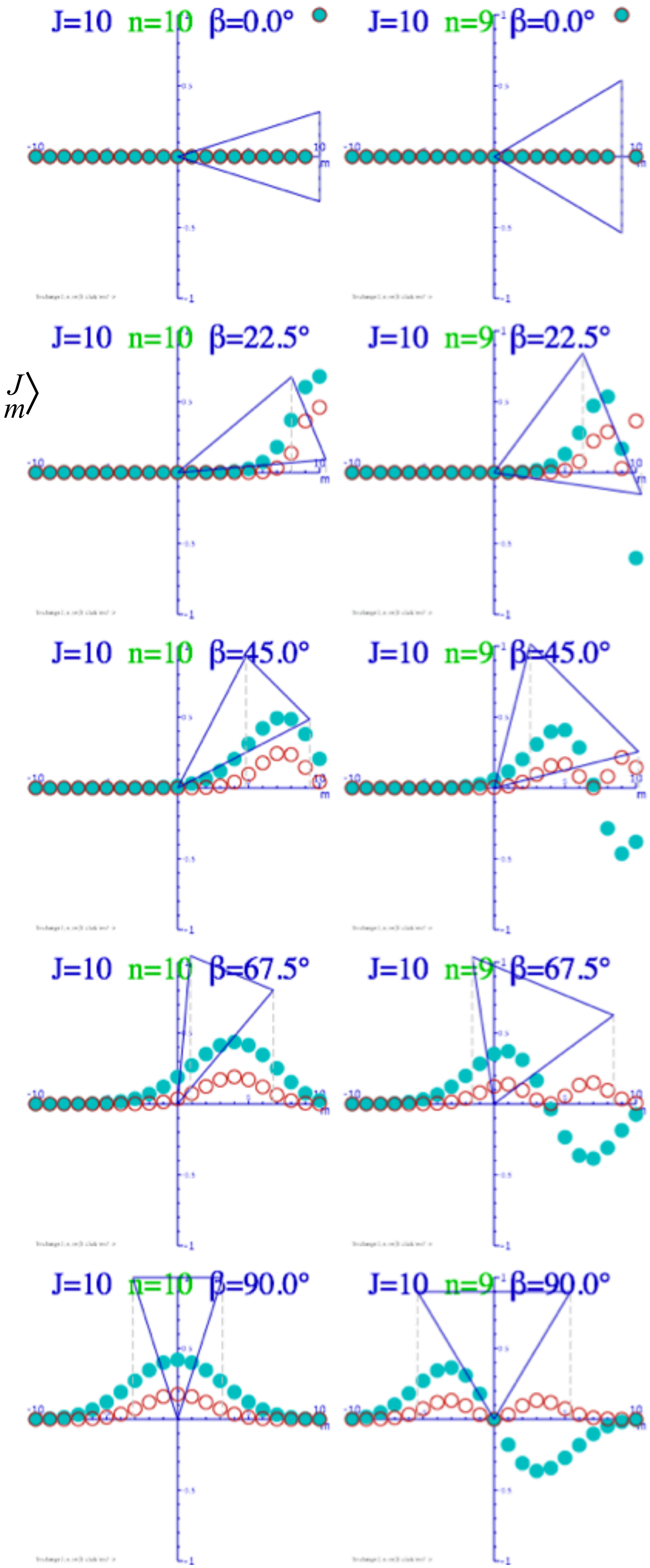
Discrete plots

[QuantIt web simulation: Visualizing D representations]



$D^J_{m,n}(0\beta 0)$
plotted
vs. m
for fixed
$J=10, \beta, n$

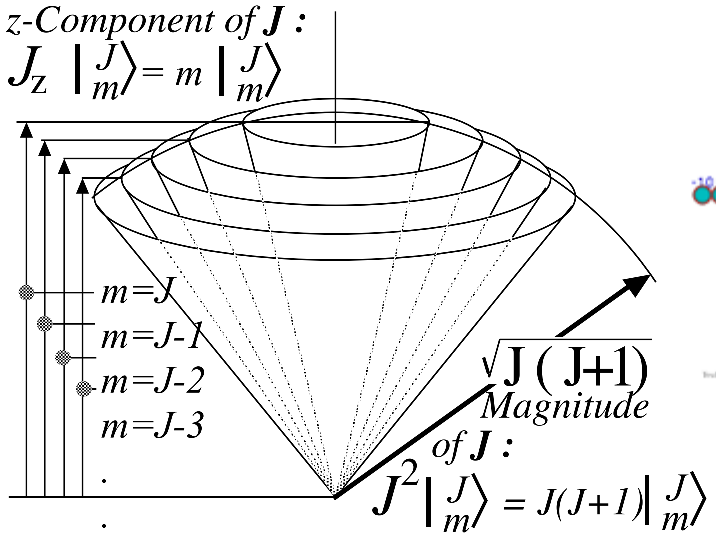
to $n=9$



J=10

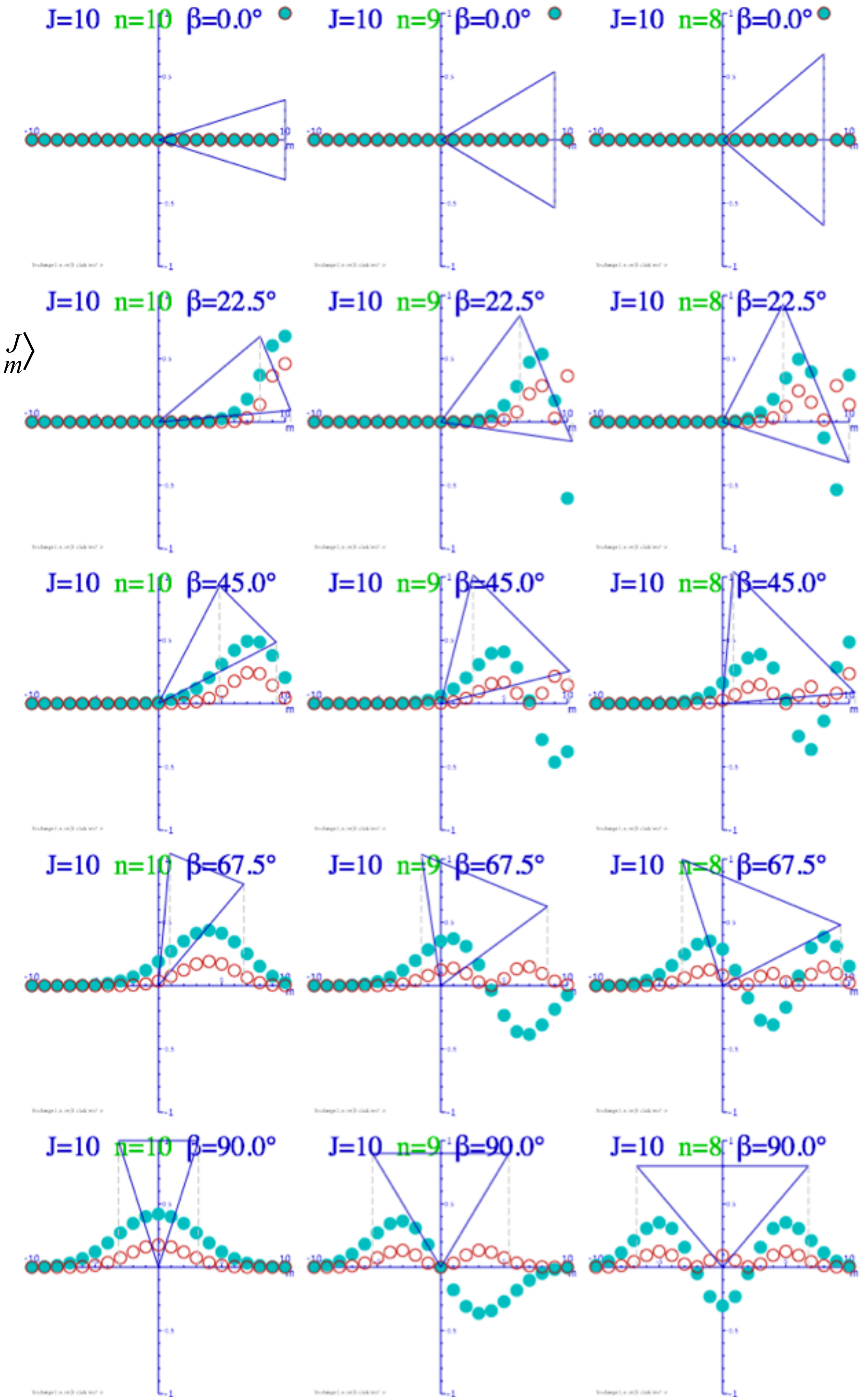
Discrete plots

[*QuantIt web simulation: Visualizing D representations*]



$D^J_{m,n}(0\beta 0)$
plotted
vs. m
for fixed
$J=10, \beta, n$

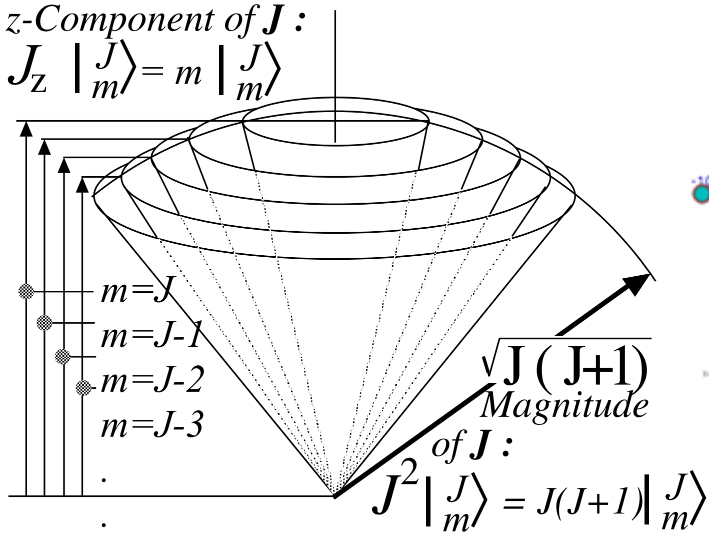
to $n=8$



J=10

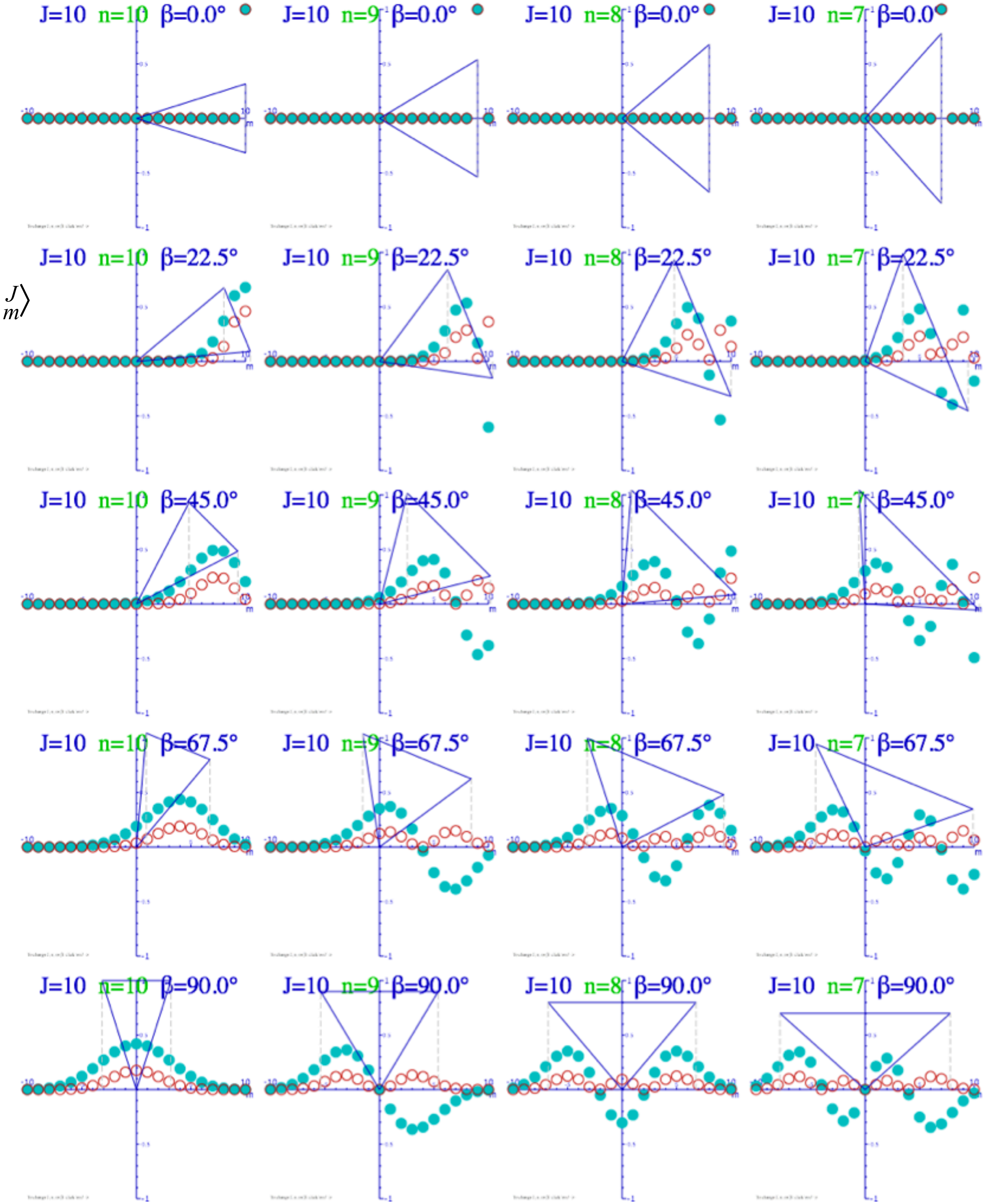
Discrete plots

QuantIt web simulation: Visualizing D representations



$D^J_{m,n}(0\beta 0)$ plotted vs. m for fixed $J=10, \beta, n$

to $n=7$



J=10

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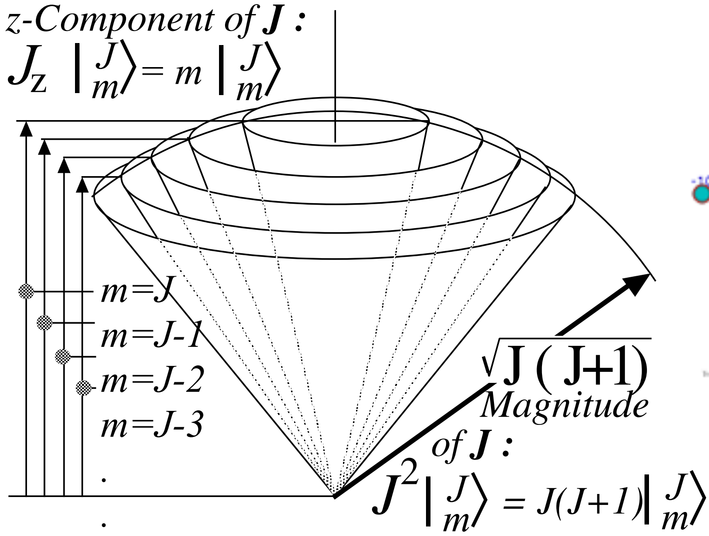

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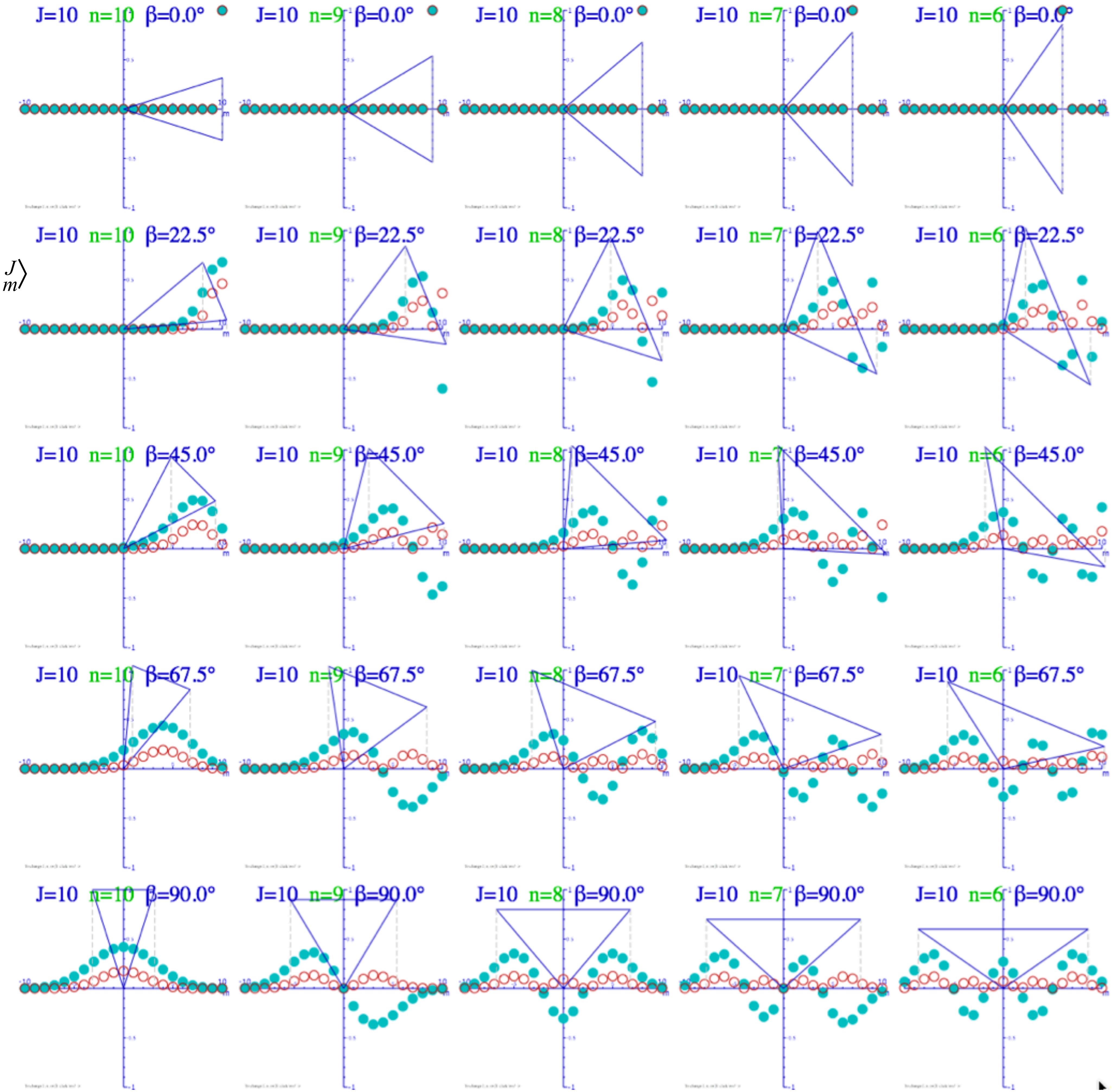

J=10

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Wigner D^J_{mn} irreps of U(2)~R(3) give atomic and molecular eigenfunctions $\Psi_{m,n}$ of 3D rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ and angular momentum uncertainty effects.

Review 1. *Angular momentum raise-n-lower operators* $\mathbf{S}_+$ and $\mathbf{S}_-$ Review 2. Angular momentum commutation

Review 3. *$SU(2)\subset U(2)$ oscillators vs. $R(3)\subset O(3)$ rotors*

Angular momentum magnitude and Θ^J_m-uncertainty cone polar angles

Generating higher-j representations D^j_{mn} of R(3) rotation and U(2) from spinor $D^{1/2}$ irreps

Evaluating D^j_{mn} representations

Applications of D^j_{mn} representations

Atomic wave functions. $D^L_{m0}\sim Y^L_m$ *Spherical harmonics*

$D^{L=1}_{m0}\sim Y^1_m$ *p-waves* $D^{L=2}_{m0}\sim Y^2_m$ *d-waves* $D^L_{00}\sim P^L$ *Legendre waves*

Molecular D^j_{mn} wave functions in "Mock-Mach" lab-vs-body state space $|{}^J_{mn}\rangle$

$\mathbf{P}^j_{mn}$ *projector and* $D^j_{mn}(\alpha,\beta,\gamma)$ *wave function*

D^J_{mn} *transform* $\mathbf{R}(\alpha,\beta,\gamma)|{}^J_{mn}\rangle=\Sigma_{m'}D^J_{m'n}(\alpha,\beta,\gamma)|{}^J_{m'n}\rangle$ *in lab-space,* $\bar{\mathbf{R}}(\alpha,\beta,\gamma)$ *in body-space.*

D^2_{mn} *transform in lab-space (Generalized Stern-Gerlach beam polarization)*

Θ^J_m-cone properties of lab transforms: J=20, J=10, J=30.

Θ^J_m-analysis of high J atomic beams

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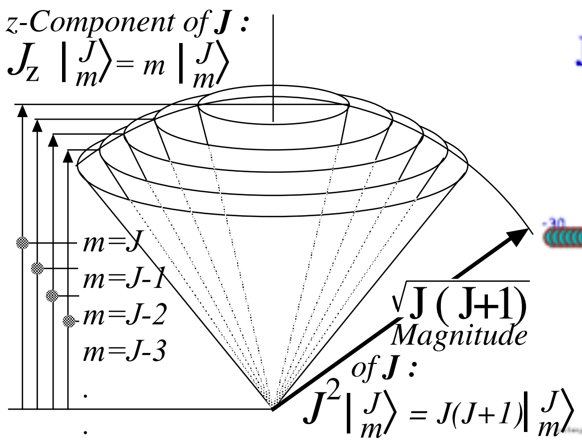
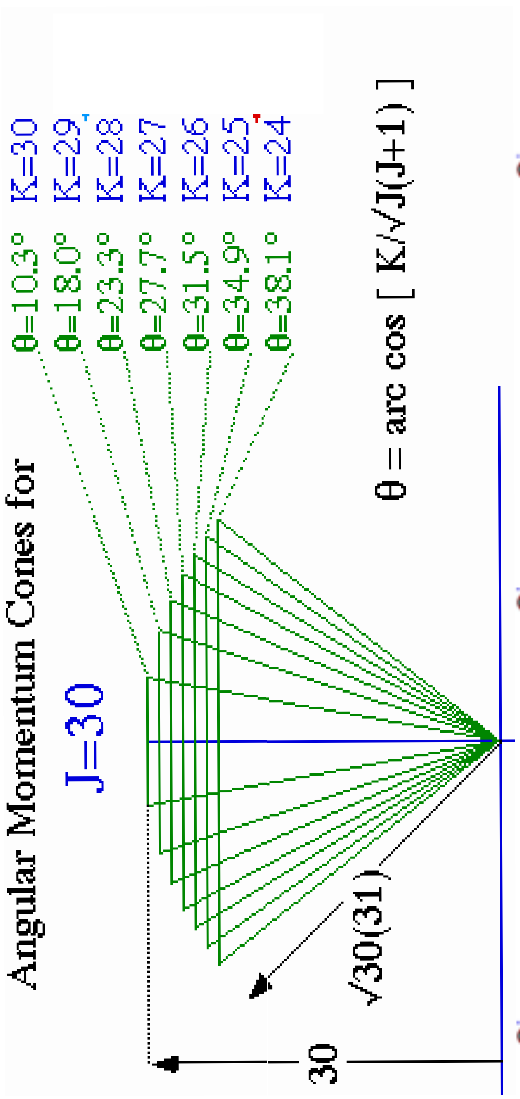
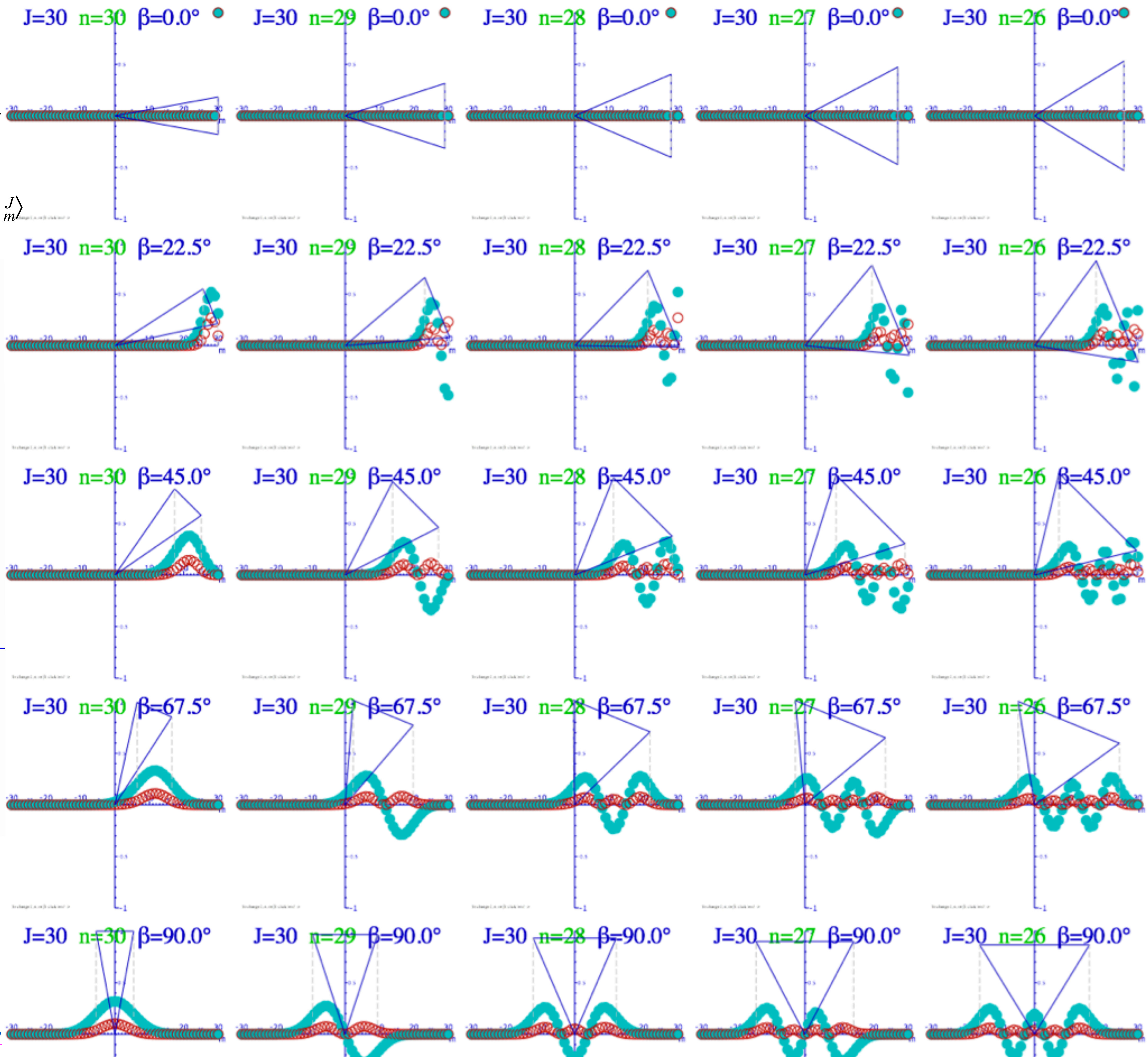
Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar $\mathbf{T}_0^0$ or tensor $\mathbf{T}_q^2$ operators*

Rotational Energy Surfaces (RE or RES) of symmetric rotor and eigensolutions

Rotational Energy Surfaces (RE or RES) of asymmetric rotor (for following class)







J=30

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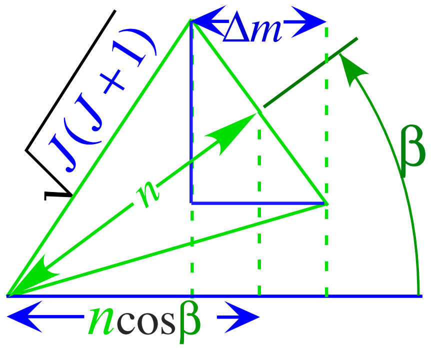
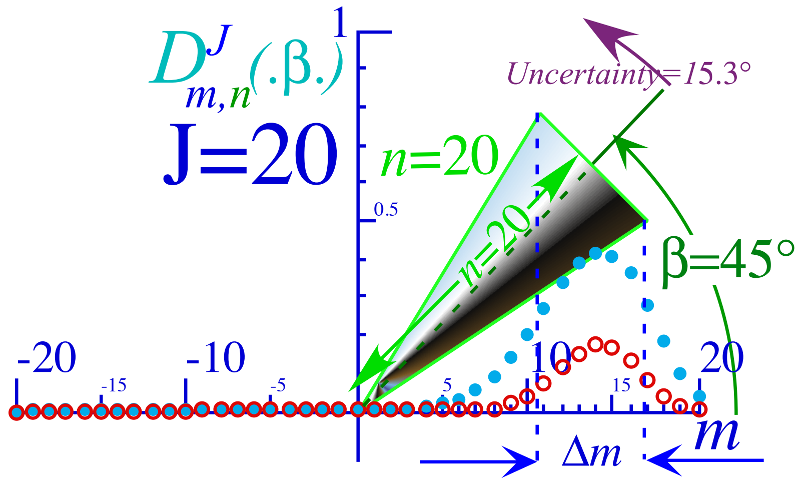
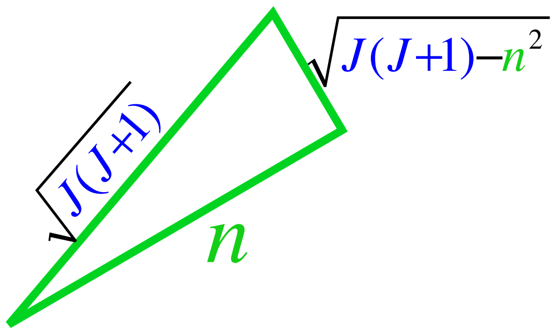
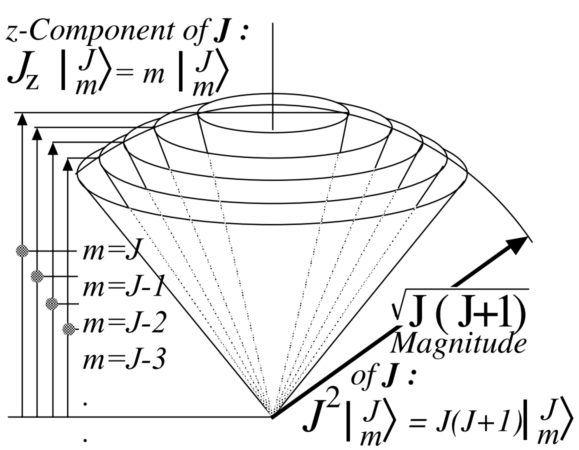
Using literal interpretation of $\left|\begin{matrix} J \\ m \end{matrix}\right\rangle$ to derive approximate number Δm of "most-busy" counters and determine most probable m-values.

$$\Delta m = 2\sqrt{J(J+1)-n^2}\cdot\sin\beta$$









QuantIt web simulation:
Visualizing D representations

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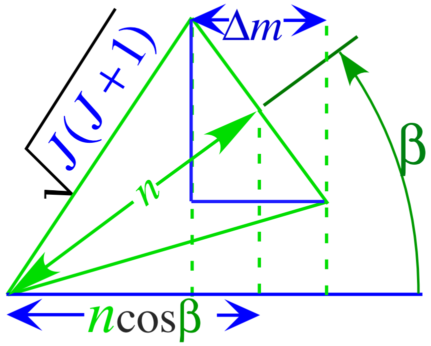
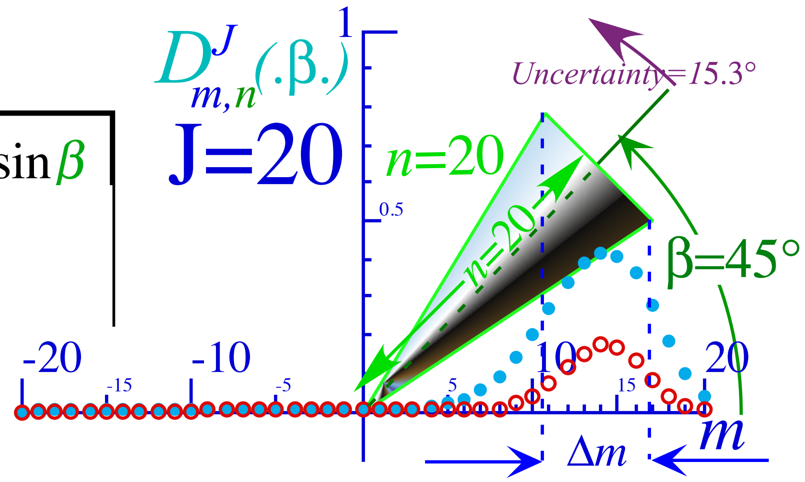


$n=J \quad : \quad \Delta m = 2\sqrt{J} \quad \sin\beta$

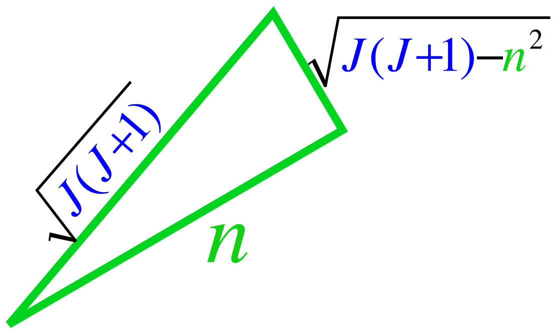
$n=J-1 \quad :$

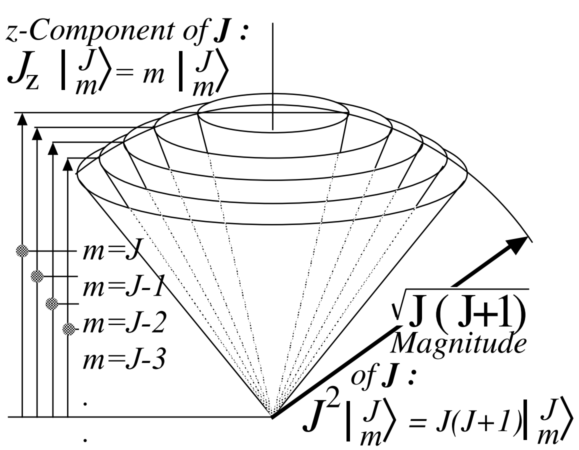
$n=J-2 \quad :$



$\Delta m = 2\sqrt{20}\sin 45° = \sqrt{40} = 6.2$

Testing formula with $J=20$ for $\beta=45°$...





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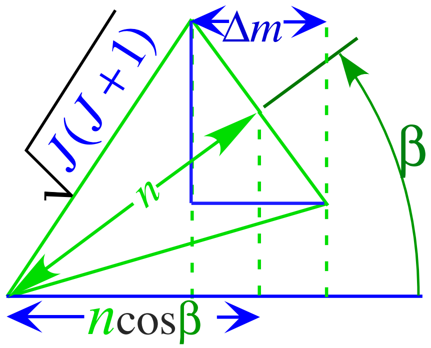

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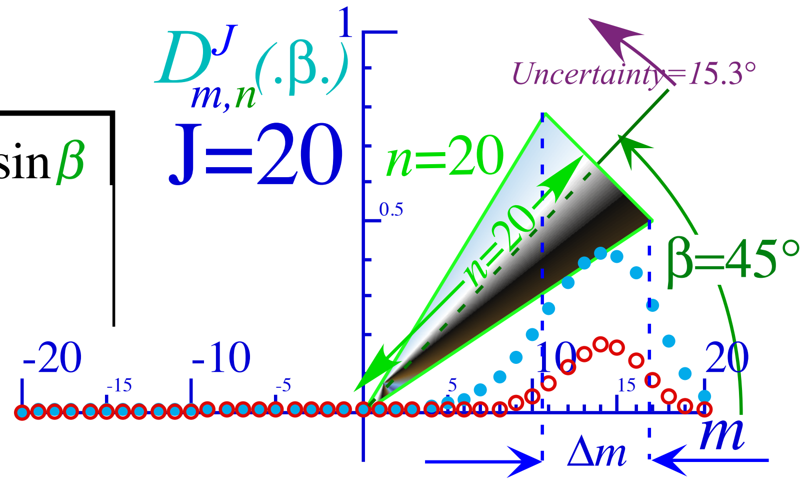

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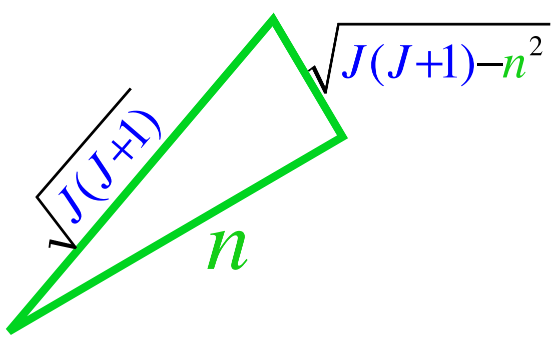

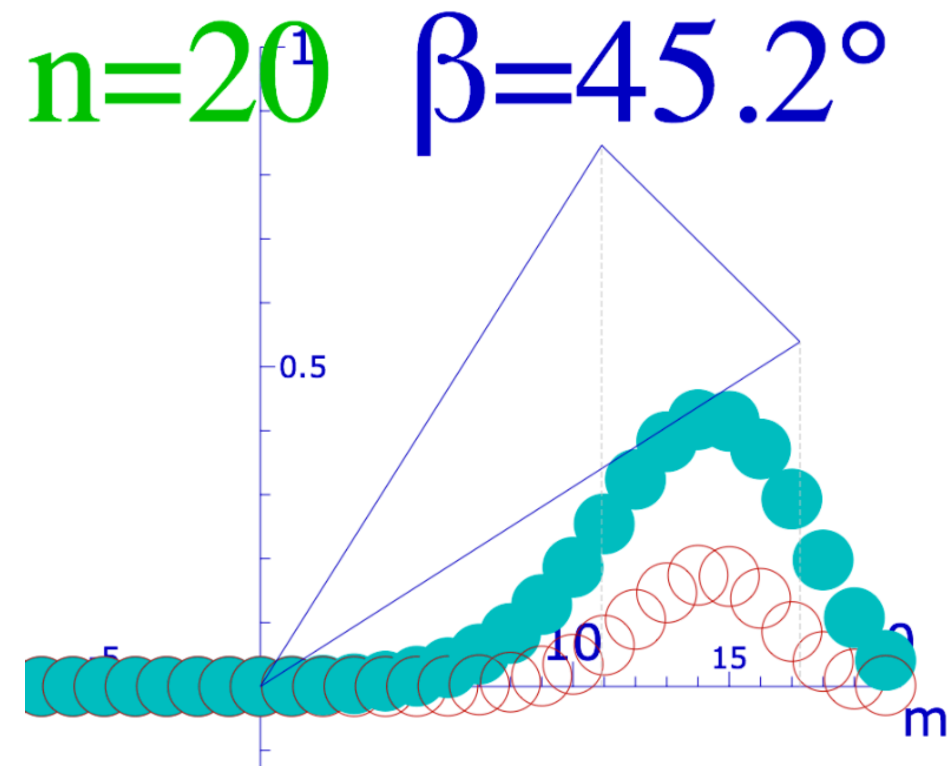

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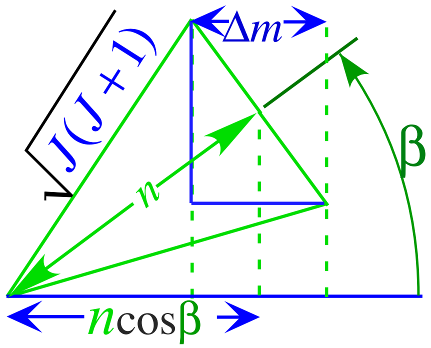

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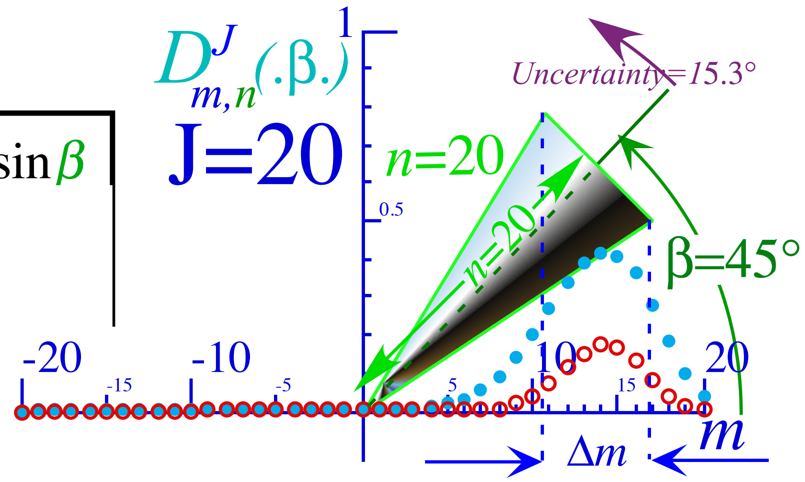

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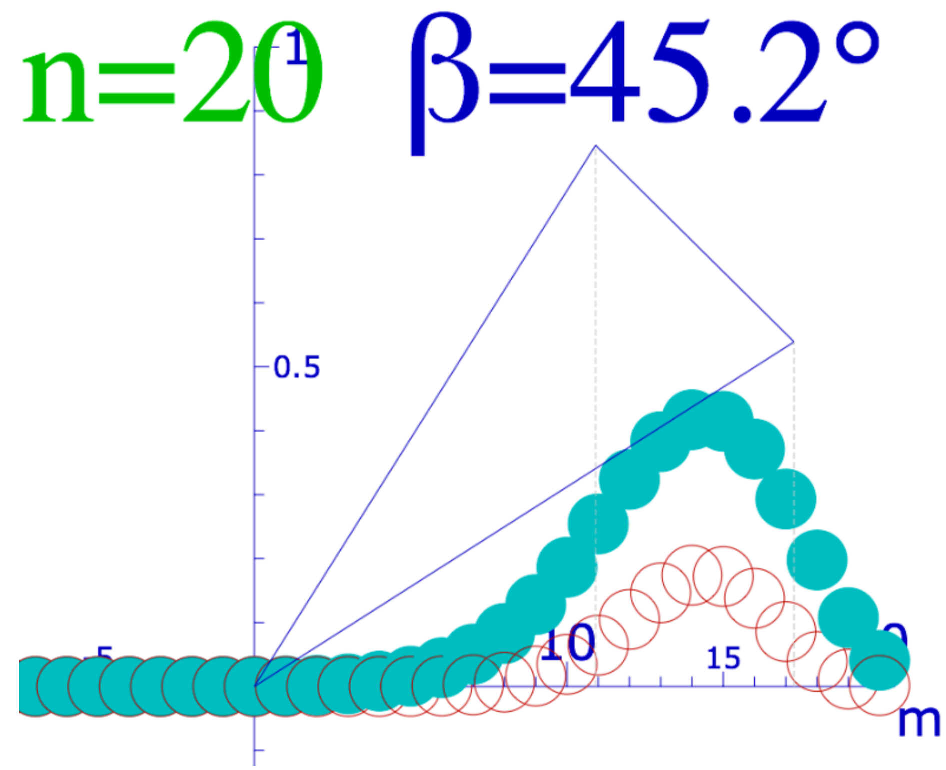
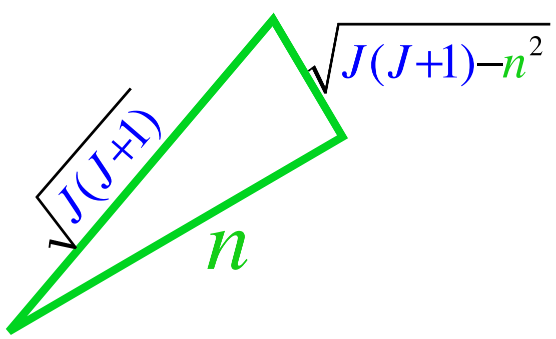
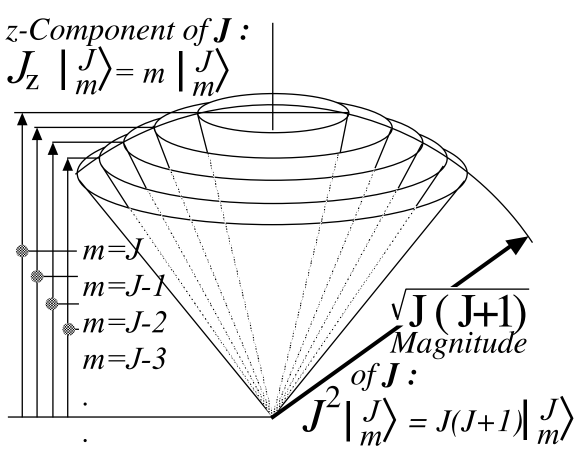
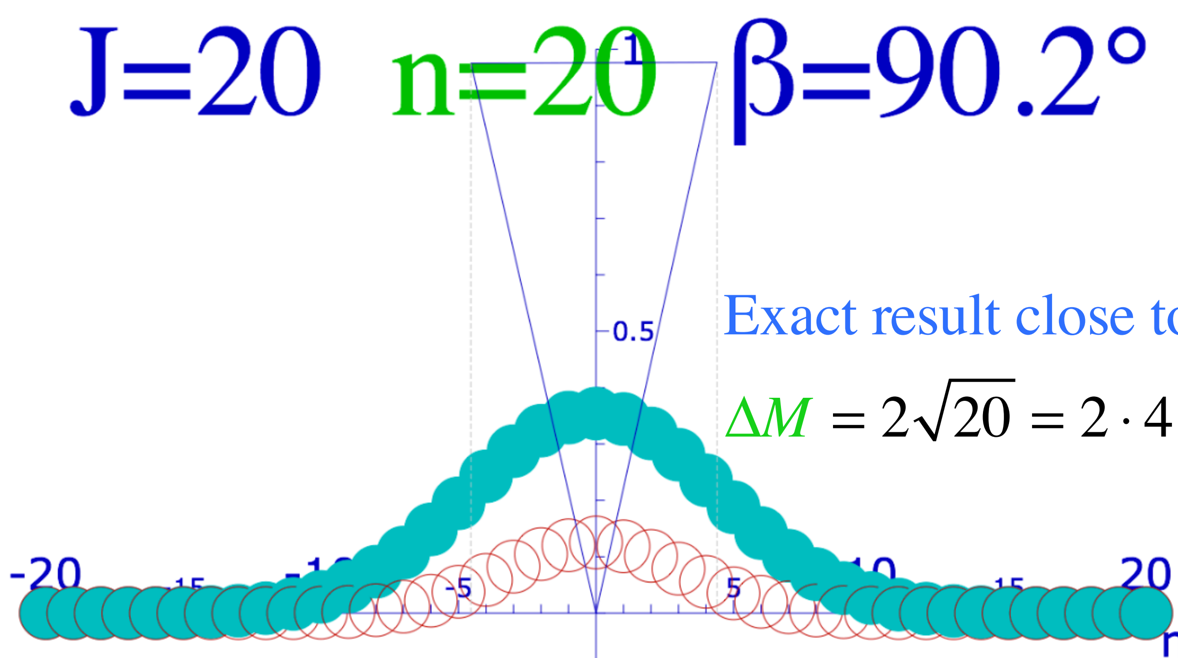






[*QuantIt web simulation: Visualizing D representations*]

...and for $\beta=90°$



Exact result close to:

$$\Delta M = 2\sqrt{20} = 2\cdot 4.47 = 8.94$$

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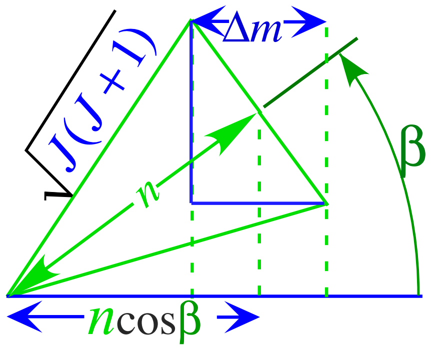

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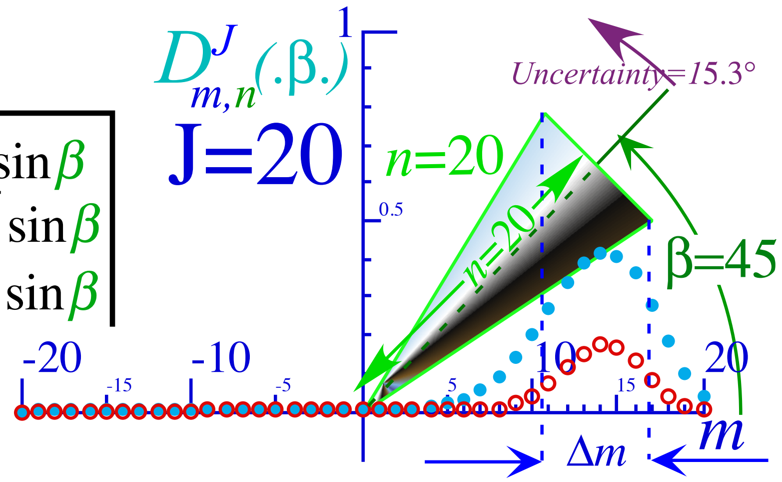

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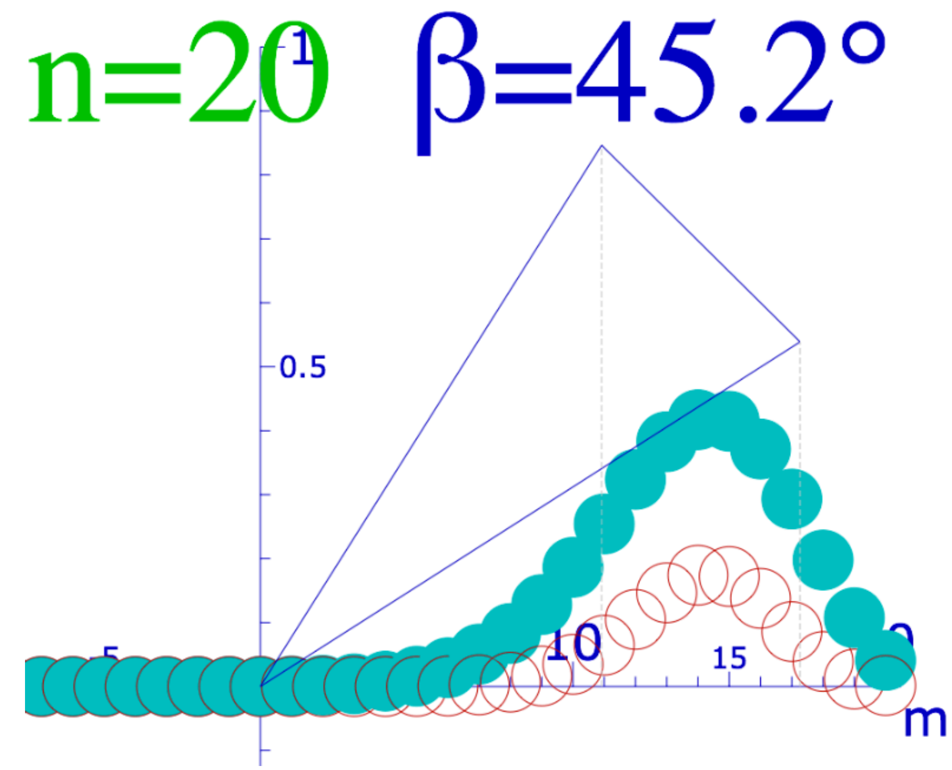

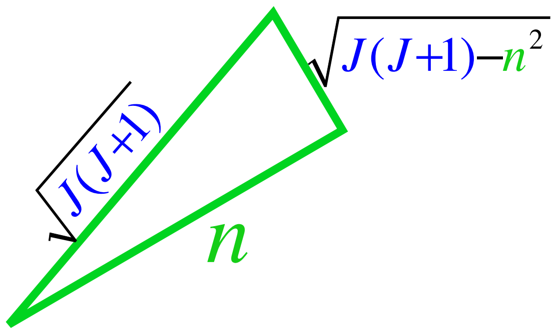

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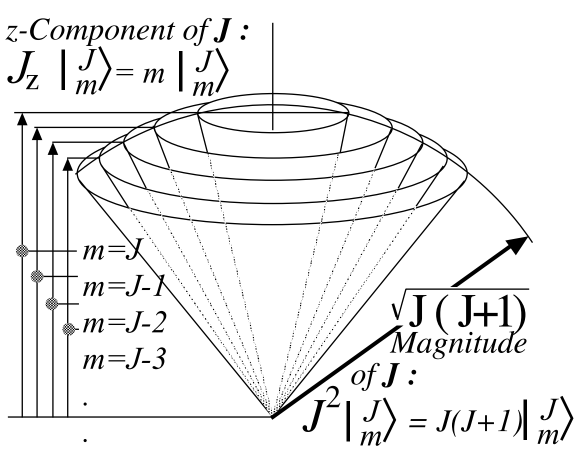
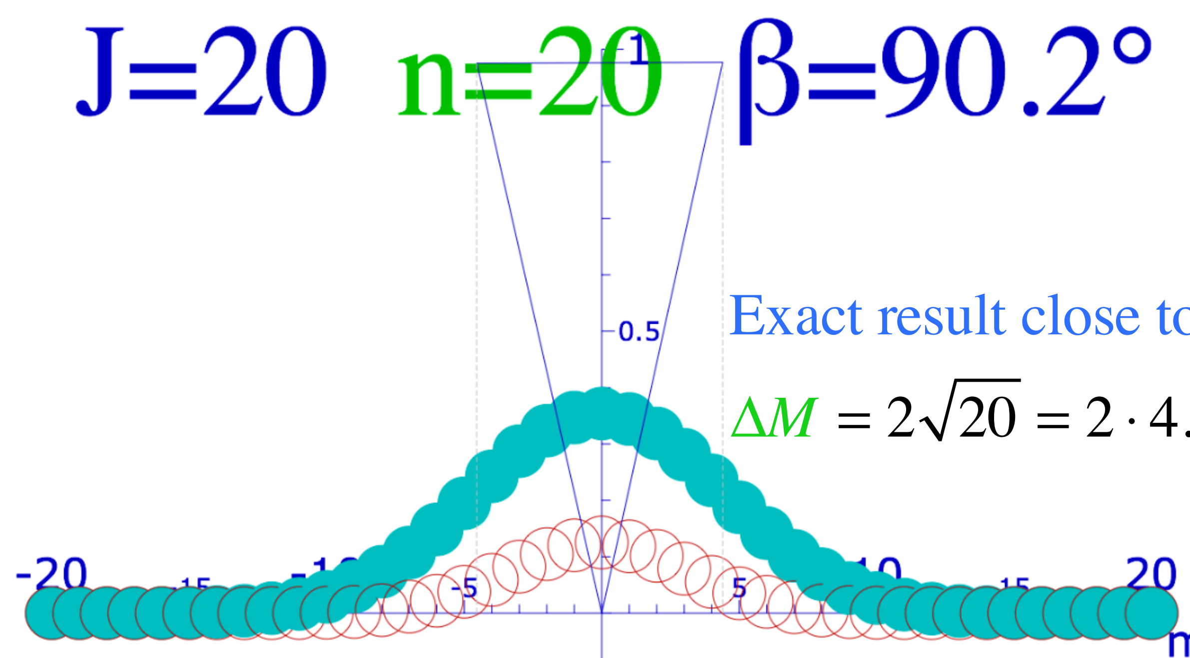


QuantIt web simulation: Visualizing D representations



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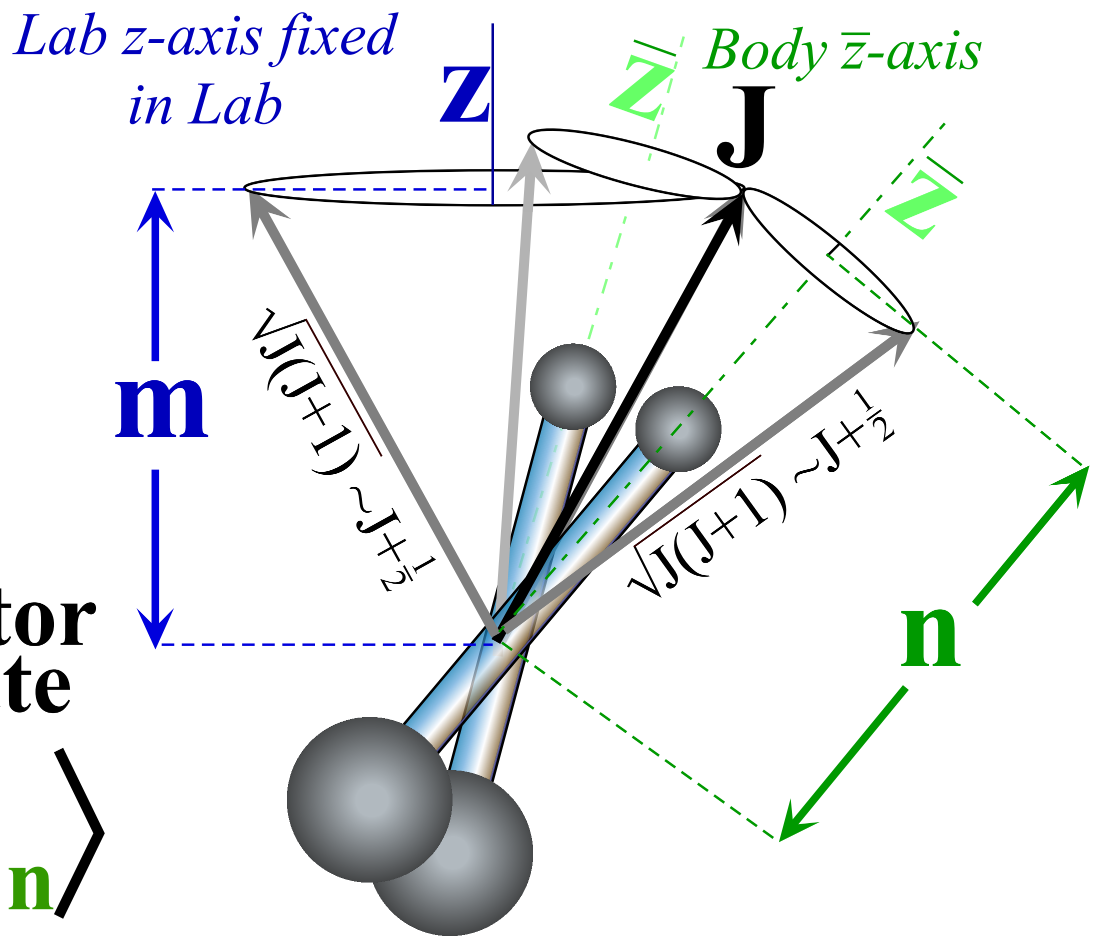
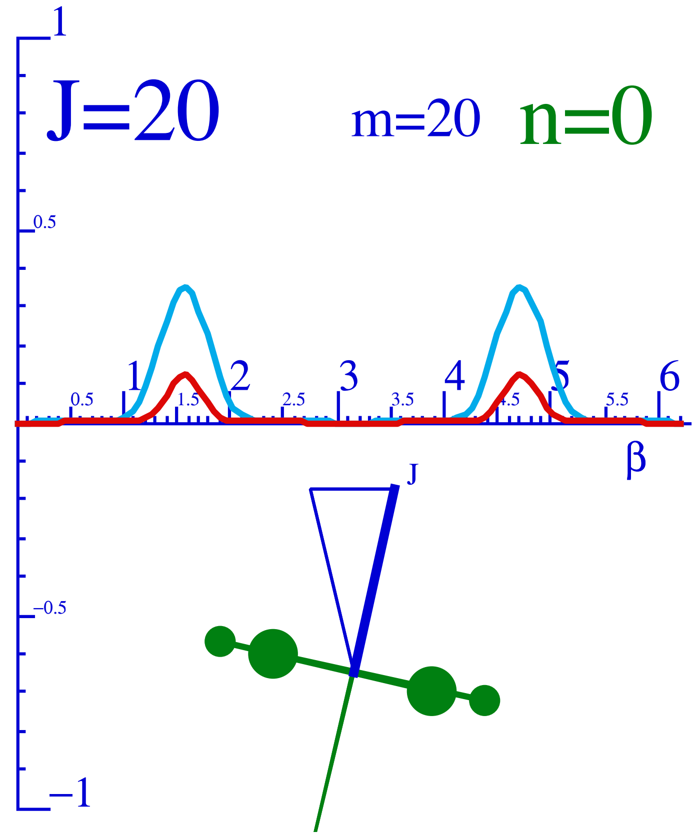
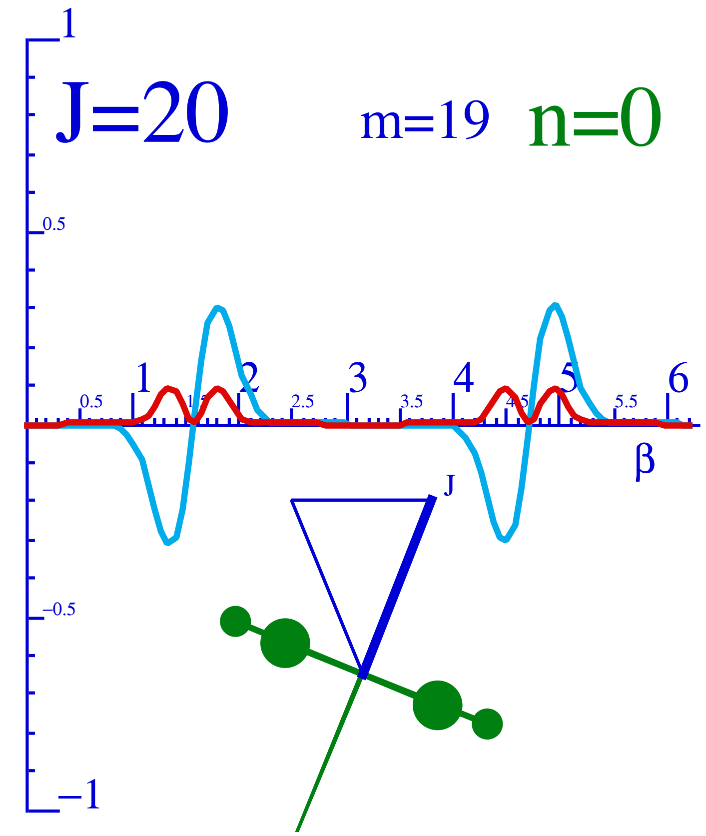
$D^{J=20}_{m,n}(0\beta 0)$ plotted vs. β for fixed J=20,m,n

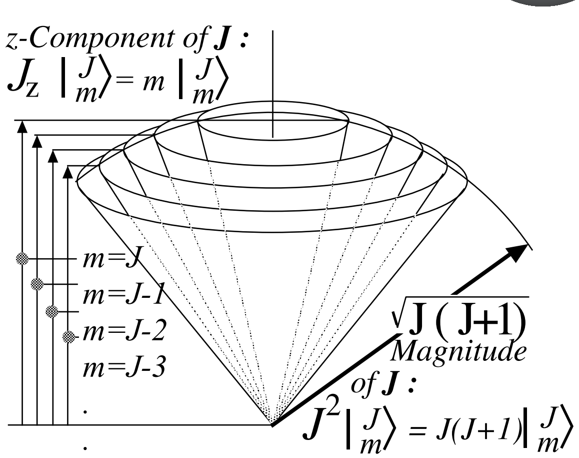
Using literal interpretation of $\left| \begin{matrix} J \\ m\ n \end{matrix} \right\rangle$ to describe approximate rotor wave-functions



Rotor state $\left| \begin{matrix} J \\ m\ n \end{matrix} \right\rangle$







$J_z \left| \begin{matrix} J \\ m \end{matrix} \right\rangle = m \left| \begin{matrix} J \\ m \end{matrix} \right\rangle$

$\sqrt{J(J+1)}$

$J^2 \left| \begin{matrix} J \\ m \end{matrix} \right\rangle = J(J+1) \left| \begin{matrix} J \\ m \end{matrix} \right\rangle$

QuantIt web simulation:
Visualizing D representations

QTforCA Unit 8. Ch. 23 Fig. 23.2.4

QTforCA Unit 8. Ch. 23 Fig. 23.2.7

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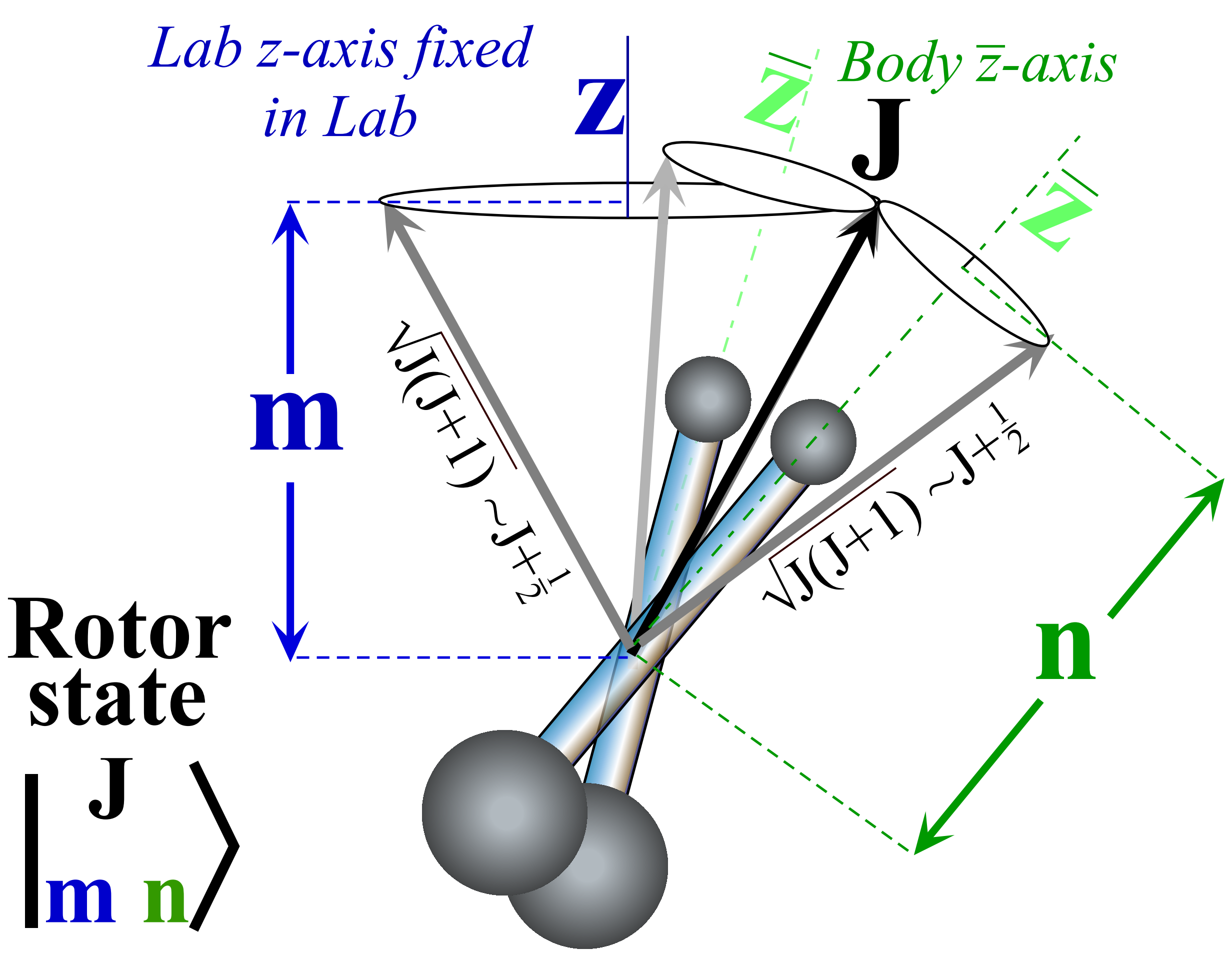
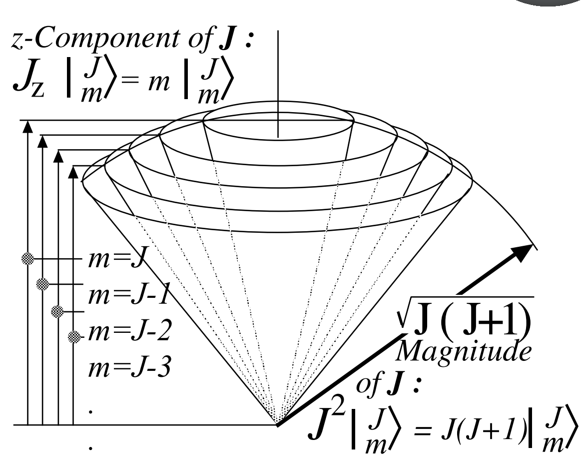
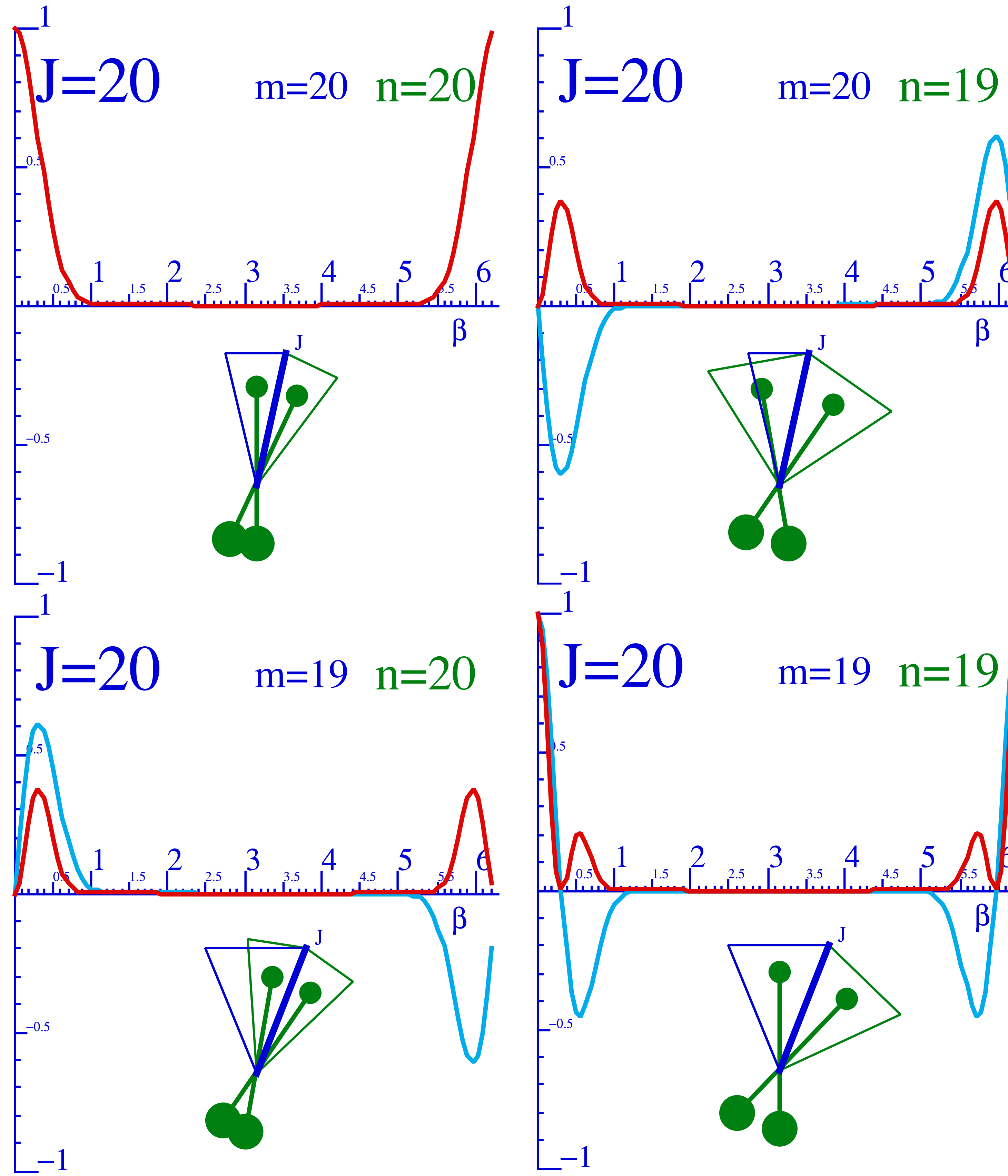
plotted
vs. β
for fixed
J=20,m,n







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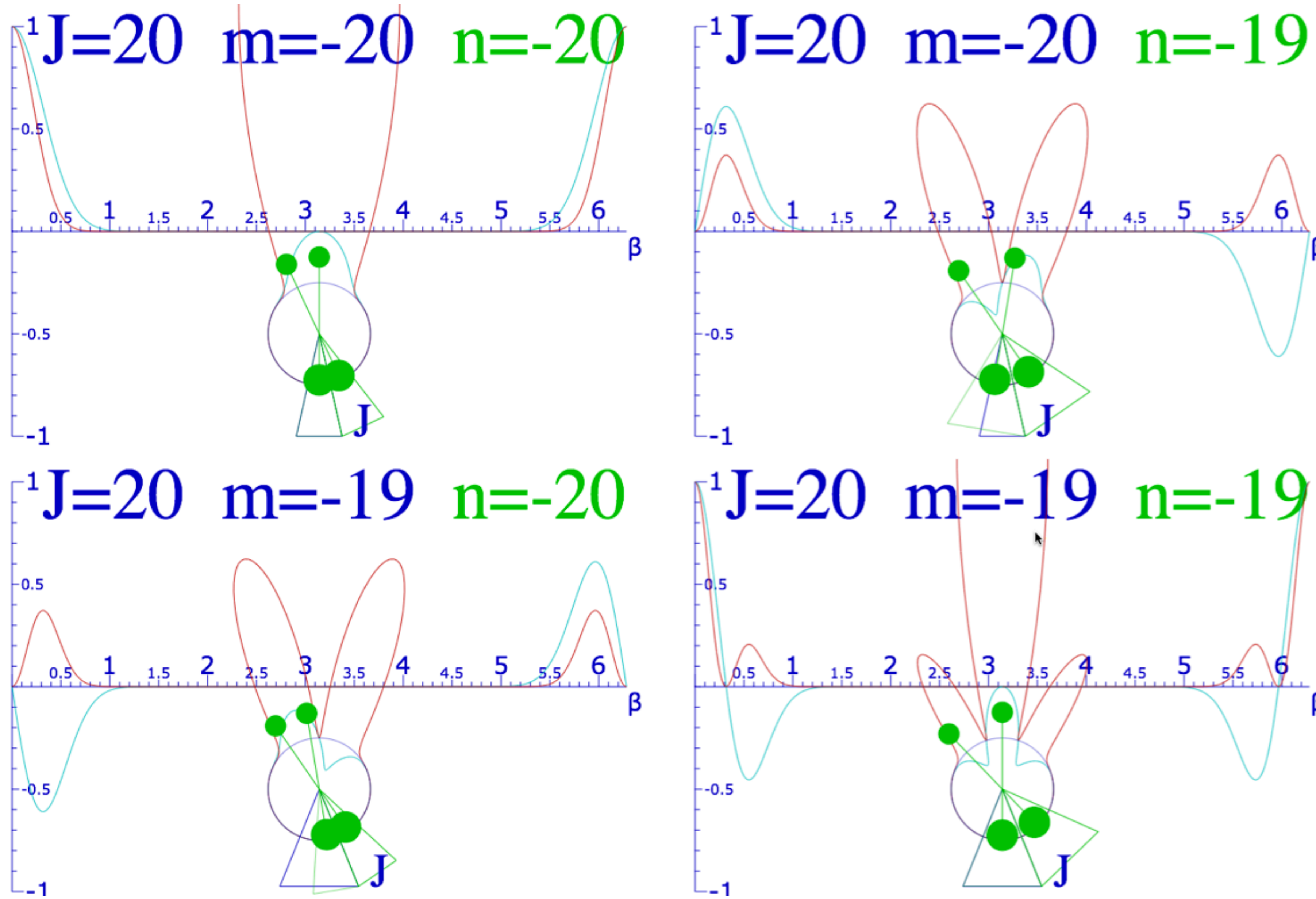

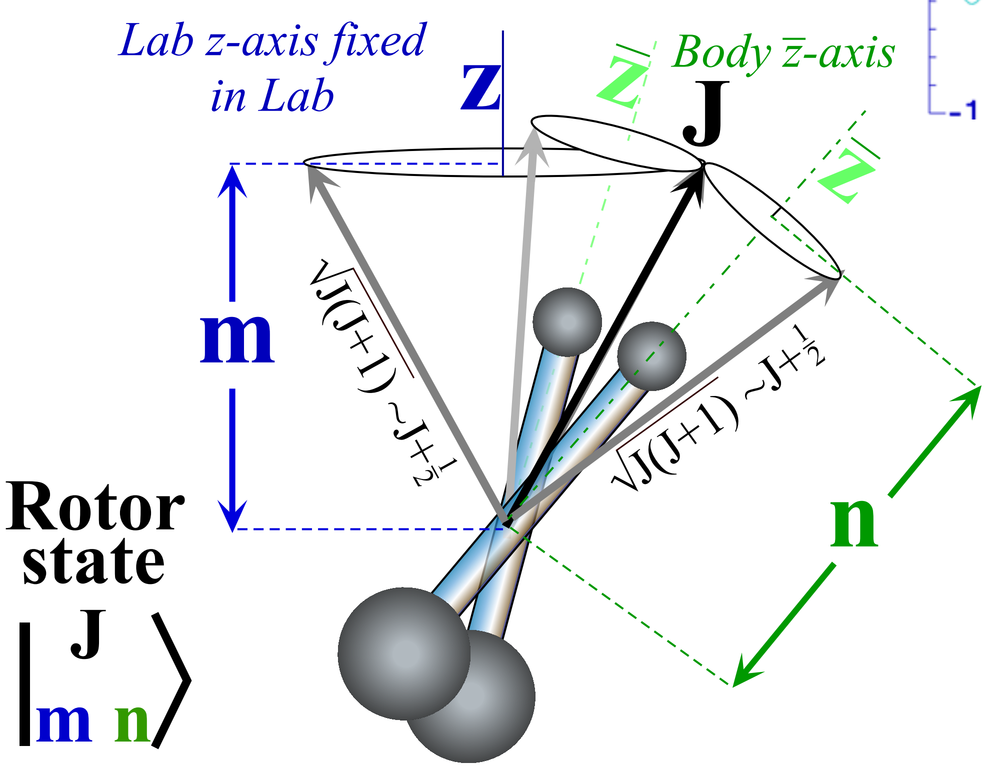

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Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x{}^2+B\mathbf{J}_y{}^2+C\mathbf{J}_z{}^2$ *made of scalar and tensor operators*

Spherical *2^k-multipole functions $X^k{}_q$* or *X-functions* are *D**-functions times the k^{th} power of radius *(r^k)*.

Consider k=2 "quadrupole" functions

$$X^k_q = r^k D^{k*}_{q,0} = \sqrt{\frac{4\pi}{2k+1}} r^k Y^k_q$$

$$\sqrt{4\pi/5}\, Y^{\ell=2}_{m=2}(\phi\theta) = D^{2*}_{2,0}(\phi\theta 0) = \sqrt{\frac{3}{8}} e^{i2\phi} \sin^2\theta = \sqrt{\frac{3}{8}} \frac{(x+iy)^2}{r^2}$$

$$\sqrt{4\pi/5}\, Y^{\ell=2}_{m=1}(\phi\theta) = D^{2*}_{1,0}(\phi\theta 0) = -\sqrt{\frac{3}{2}} e^{i\phi} \sin\theta\cos\theta = -\sqrt{\frac{3}{2}} \frac{(x+iy)z}{r^2}$$

$$\sqrt{4\pi/5}\, Y^{\ell=2}_{m=0}(\phi\theta) = D^{2*}_{0,0}(\phi\theta 0) = \frac{3\cos^2\theta - 1}{2} = \frac{3z^2 - r^2}{2r^2}$$

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Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x{}^2+B\mathbf{J}_y{}^2+C\mathbf{J}_z{}^2$ *made of scalar and tensor operators*

Spherical *2^k-multipole functions* $X^k{}_q$ or *X-functions* are *D**-functions times the k^{th} power of radius (r^k).

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→

$$\sqrt{4\pi/5}\, Y^{\ell=2}_{m=0}(\phi\theta) = X^2_0(\phi\theta 0) = r^2\frac{3\cos^2\theta-1}{2} = \frac{3z^2-r^2}{2} = \frac{2z^2-x^2-y^2}{2}$$

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$$= X_2^2(\phi\theta 0) + X_{-2}^2(\phi\theta 0) = \sqrt{\frac{3}{2}} r^2\frac{e^{i2\phi}+e^{-i2\phi}}{2}\sin^2\theta = \sqrt{\frac{3}{2}}(x^2-y^2) = \sqrt{\frac{3}{2}} r^2\cos 2\phi\sin^2\theta$$

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$$= \quad X_2^2(\phi\theta 0)+X_{-2}^2(\phi\theta 0) = \sqrt{\frac{3}{2}} r^2\frac{e^{i2\phi}+e^{-i2\phi}}{2}\sin^2\theta = \sqrt{\frac{3}{2}}(x^2-y^2) = \sqrt{\frac{3}{2}} r^2\cos 2\phi\sin^2\theta$$

$$\longrightarrow \mathbf{T}_2^2+\mathbf{T}_{-2}^2 = \sqrt{6}\frac{\mathbf{J}_x^2-\mathbf{J}_y^2}{2} = \sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos 2\phi$$

-

$$= \quad X_2^2(\phi\theta 0)-X_{-2}^2(\phi\theta 0) = \sqrt{\frac{3}{2}} r^2\frac{e^{i2\phi}-e^{-i2\phi}}{2}\sin^2\theta = \sqrt{\frac{3}{8}}(i4xy) = i\sqrt{6}xy = i\sqrt{\frac{3}{2}} r^2\sin 2\phi\sin^2\theta$$

$$\longrightarrow \mathbf{T}_2^2-\mathbf{T}_{-2}^2 = i\sqrt{6}\,\mathbf{J}_x\mathbf{J}_y$$

etc.

And, don't forget scalar: $\mathbf{T}_0^0 = \mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2 = \mathbf{J}^2$

Wigner D^J_{mn} irreps of U(2)~R(3) give atomic and molecular eigenfunctions $\Psi_{m,n}$ of 3D rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ and angular momentum uncertainty effects.

Review 1. *Angular momentum raise-n-lower operators* $\mathbf{S}_+$ and $\mathbf{S}_-$ Review 2. Angular momentum commutation

Review 3. *SU(2)⊂U(2) oscillators vs. R(3)⊂O(3) rotors*

Angular momentum magnitude and Θ^J_m-uncertainty cone polar angles

Generating higher-j representations D^j_{mn} of R(3) rotation and U(2) from spinor $D^{1/2}$ irreps

Evaluating D^j_{mn} representations

Applications of D^j_{mn} representations

Atomic wave functions. $D^L_{m0} \sim Y^L_m$ *Spherical harmonics*

$D^{L=1}_{m0} \sim Y^1_m$ *p-waves* $D^{L=2}_{m0} \sim Y^2_m$ *d-waves* $D^L_{00} \sim P^L$ *Legendre waves*

Molecular D^j_{mn} wave functions in "Mock-Mach" lab-vs-body state space $|^J_{mn}\rangle$

$\mathbf{P}^j_{mn}$ *projector and* $D^j_{mn}(\alpha,\beta,\gamma)$ *wave function*

D^J_{mn} *transform* $\mathbf{R}(\alpha,\beta,\gamma)|^J_{mn}\rangle=\Sigma_{m'}D^J_{m'n}(\alpha,\beta,\gamma)|^J_{m'n}\rangle$ *in lab-space,* $\bar{\mathbf{R}}(\alpha,\beta,\gamma)$ *in body-space.*

D^2_{mn} *transform in lab-space (Generalized Stern-Gerlach beam polarization)*

Θ^J_m*-cone properties of lab transforms: J=20, J=10, J=30.*

Θ^J_m*-analysis of high J atomic beams*

Θ^J_m*-properties of high J molecular lab-vs-body states* $|^J_{mn}\rangle$

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Rotational Energy Surfaces (RE or RES) of symmetric rotor and eigensolutions

Rotational Energy Surfaces (RE or RES) of asymmetric rotor (for following class)

Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar and tensor operators*

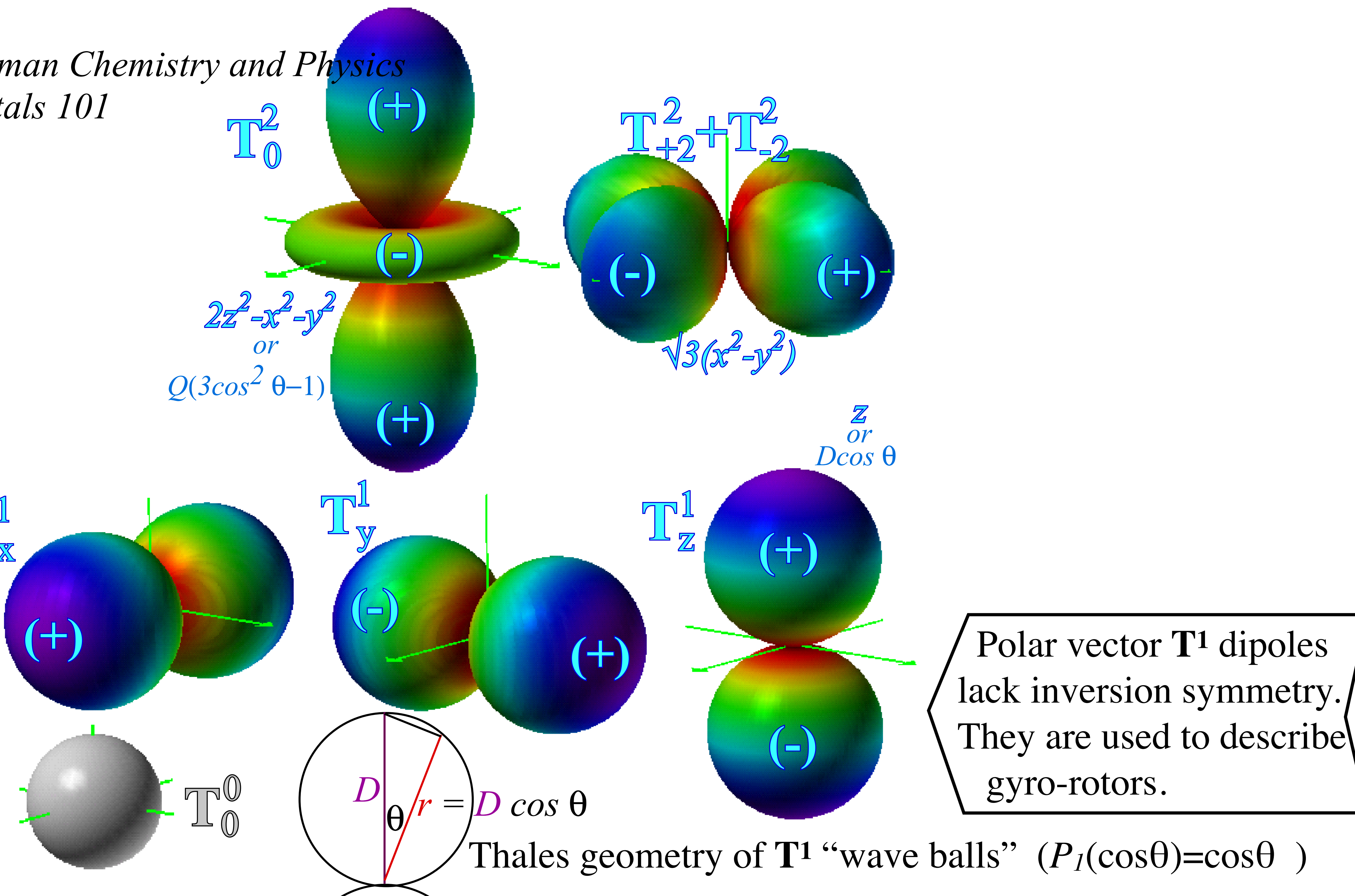
$\mathbf{T}_0^0=\mathbf{J}_x{}^2+\mathbf{J}_y{}^2+\mathbf{J}_z{}^2=\mathbf{J}^2$	$\mathbf{T}_0^2=\frac{2\mathbf{J}_z{}^2-\mathbf{J}_x{}^2-\mathbf{J}_y{}^2}{2}=\mathbf{J}^2\frac{3\cos^2\theta-1}{2}=\mathbf{J}^2P_2(\cos\theta)$	$\mathbf{T}_2^2+\mathbf{T}_{-2}^2=\sqrt{6}\frac{\mathbf{J}_x{}^2-\mathbf{J}_y{}^2}{2}=\sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos 2\phi$

Review of freshman Chemistry and Physics
Electronic orbitals 101

Quadrupoles
(d-orbitals)

Dipoles
(p-orbitals)

Monopole
(s-orbital)



Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar and tensor operators*

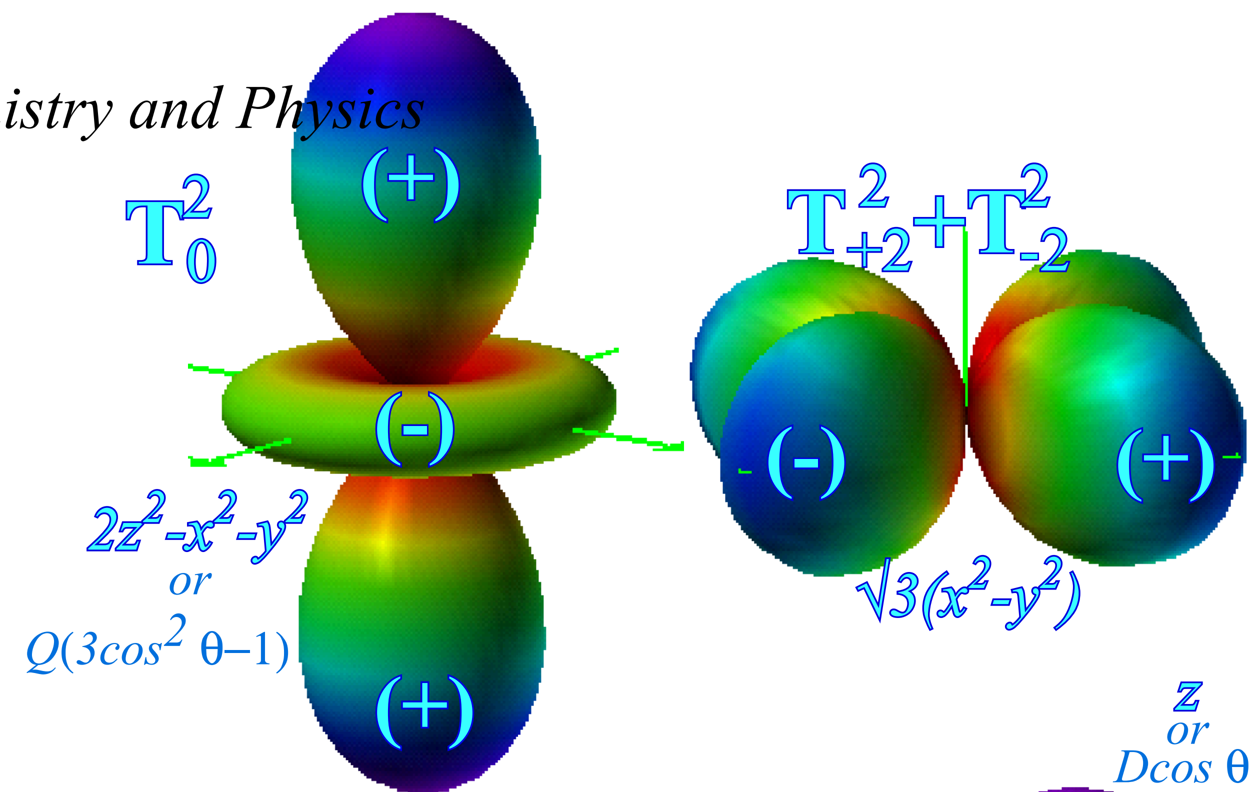
$$\mathbf{T}^0_0=\mathbf{J}_x{}^2+\mathbf{J}_y{}^2+\mathbf{J}_z{}^2=\mathbf{J}^2$$

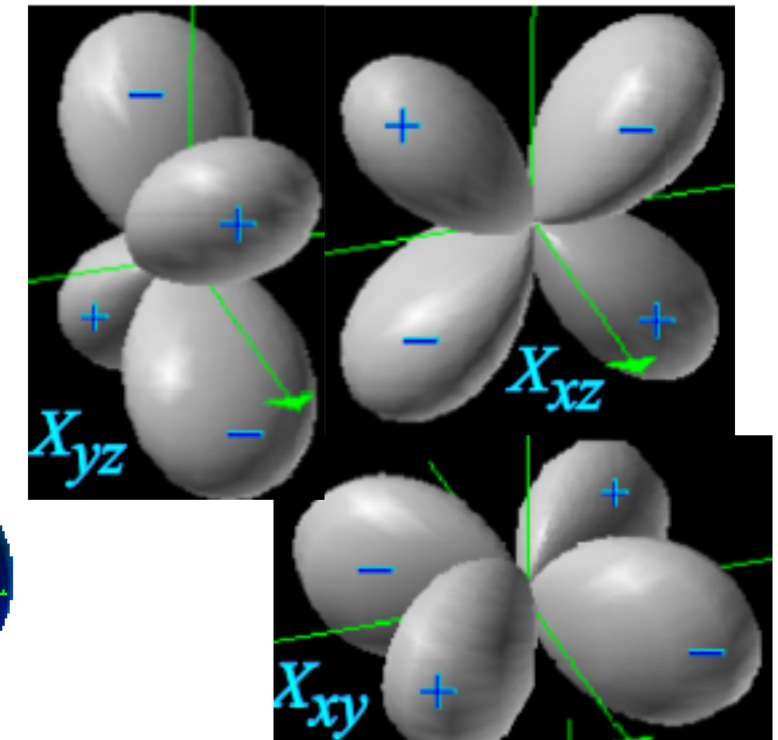
$$\mathbf{T}^2_0=\frac{2\mathbf{J}_z{}^2-\mathbf{J}_x{}^2-\mathbf{J}_y{}^2}{2}=\mathbf{J}^2\frac{3\cos^2\theta-1}{2}=\mathbf{J}^2P_2(\cos\theta)$$

$$\mathbf{T}^2_2+\mathbf{T}^2_{-2}=\sqrt{6}\frac{\mathbf{J}_x{}^2-\mathbf{J}_y{}^2}{2}=\sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos 2\phi$$

Review of freshman Chemistry and Physics
Electronic orbitals 101

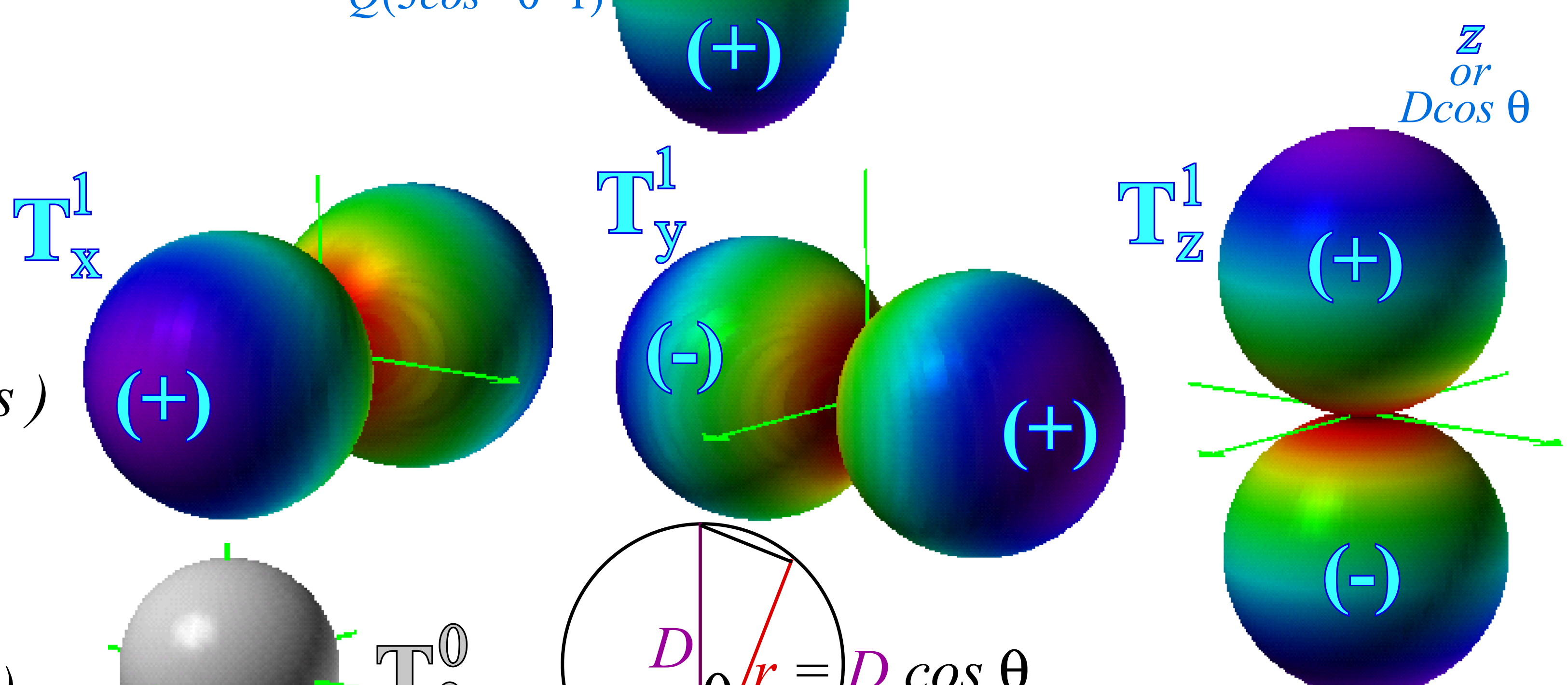
Quadrupoles
(d-orbitals)





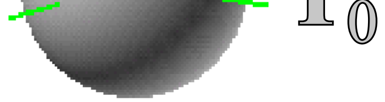
Axial $\mathbf{T}^2$ *tensor-poles not needed in a diagonal rotor Hamiltonian that has no* $\mathbf{J}_x\mathbf{J}_y$, $\mathbf{J}_x\mathbf{J}_z$, *or* $\mathbf{J}_y\mathbf{J}_z$

Dipoles
(p-orbitals)



Polar vector $\mathbf{T}^1$ dipoles lack inversion symmetry. They are used to describe gyro-rotors.

Monopole
(s-orbital)



Thales geometry of $\mathbf{T}^1$ "wave balls" ($P_1(\cos\theta)=\cos\theta$)

Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar and tensor operators*

$$\mathbf{T}_0^0=\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2=\mathbf{J}^2$$

$$\mathbf{T}_0^2=\frac{2\mathbf{J}_z^2-\mathbf{J}_x^2-\mathbf{J}_y^2}{2}=\mathbf{J}^2\frac{3\cos^2\theta-1}{2}=\mathbf{J}^2P_2(\cos\theta)$$

$$\mathbf{T}_2^2+\mathbf{T}_{-2}^2=\sqrt{6}\frac{\mathbf{J}_x^2-\mathbf{J}_y^2}{2}=\sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos 2\phi$$

Kinetic energy inertial coefficients: $A=\frac{1}{2I_x},\ B=\frac{1}{2I_y},\ C=\frac{1}{2I_z}$

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$$

$$=\left(\frac{1}{3}A+\frac{1}{3}B+\frac{1}{3}C\right)\left(\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2\right)$$

$$+\left(\frac{-1}{6}A+\frac{-1}{6}B+\frac{2}{6}C\right)\left(-\mathbf{J}_x^2-\mathbf{J}_y^2+2\mathbf{J}_z^2\right)$$

$$+\left(\frac{1}{2}A+\frac{-1}{2}B+0\cdot C\right)\left(\mathbf{J}_x^2-\mathbf{J}_y^2+0\right)$$

Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar and tensor operators*

$$\mathbf{T}_0^0=\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2=\mathbf{J}^2$$

$$\mathbf{T}_0^2=\frac{2\mathbf{J}_z^2-\mathbf{J}_x^2-\mathbf{J}_y^2}{2}=\mathbf{J}^2\frac{3\cos^2\theta-1}{2}=\mathbf{J}^2P_2(\cos\theta)$$

$$\mathbf{T}_2^2+\mathbf{T}_{-2}^2=\sqrt{6}\frac{\mathbf{J}_x^2-\mathbf{J}_y^2}{2}=\sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos 2\phi$$

Kinetic energy inertial coefficients : $A=\frac{1}{2I_x}, B=\frac{1}{2I_y}, C=\frac{1}{2I_z}$

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$$

$$=(\frac{1}{3}A+\frac{1}{3}B+\frac{1}{3}C)(\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2)$$
$$+(\frac{-1}{6}A+\frac{-1}{6}B+\frac{2}{6}C)(-\mathbf{J}_x^2-\mathbf{J}_y^2+2\mathbf{J}_z^2)$$
$$+(\frac{1}{2}A+\frac{-1}{2}B+0\cdot C)(\mathbf{J}_x^2-\mathbf{J}_y^2+0)$$

$$=(\frac{1}{3}A+\frac{1}{3}B+\frac{1}{3}C)(\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2)$$
$$+(\frac{-1}{3}A+\frac{-1}{3}B+\frac{2}{3}C)(\frac{2\mathbf{J}_z^2-\mathbf{J}_x^2-\mathbf{J}_y^2}{2})$$
$$+(\frac{1}{\sqrt{6}}A+\frac{-1}{\sqrt{6}}B+0\cdot C)(\sqrt{6}\frac{\mathbf{J}_x^2-\mathbf{J}_y^2}{2})$$

Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x{}^2+B\mathbf{J}_y{}^2+C\mathbf{J}_z{}^2$ *made of scalar and tensor operators*

$\mathbf{T}^0_0=\mathbf{J}_x{}^2+\mathbf{J}_y{}^2+\mathbf{J}_z{}^2=\mathbf{J}^2$	$\mathbf{T}^2_0=\frac{2\mathbf{J}_z{}^2-\mathbf{J}_x{}^2-\mathbf{J}_y{}^2}{2}=\mathbf{J}^2\frac{3\cos^2\theta-1}{2}=\mathbf{J}^2P_2(\cos\theta)$	$\mathbf{T}^2_2+\mathbf{T}^2_{-2}=\sqrt{6}\frac{\mathbf{J}_x{}^2-\mathbf{J}_y{}^2}{2}=\sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos2\phi$

Kinetic energy inertial coefficients : $A=\frac{1}{2I_x},B=\frac{1}{2I_y},C=\frac{1}{2I_z}$

$$\mathbf{H}=A\mathbf{J}_x{}^2+B\mathbf{J}_y{}^2+C\mathbf{J}_z{}^2$$

$$=(\tfrac{1}{3}A+\tfrac{1}{3}B+\tfrac{1}{3}C)(\mathbf{J}_x{}^2+\mathbf{J}_y{}^2+\mathbf{J}_z{}^2)$$
$$+(\tfrac{-1}{6}A+\tfrac{-1}{6}B+\tfrac{2}{6}C)(-\mathbf{J}_x{}^2-\mathbf{J}_y{}^2+2\mathbf{J}_z{}^2)$$
$$+(\tfrac{1}{2}A+\tfrac{-1}{2}B+0\cdot C)(\mathbf{J}_x{}^2-\mathbf{J}_y{}^2+0)$$

$$=(\tfrac{1}{3}A+\tfrac{1}{3}B+\tfrac{1}{3}C)(\mathbf{J}_x{}^2+\mathbf{J}_y{}^2+\mathbf{J}_z{}^2)$$
$$+(\tfrac{-1}{3}A+\tfrac{-1}{3}B+\tfrac{2}{3}C)(\frac{2\mathbf{J}_z{}^2-\mathbf{J}_x{}^2-\mathbf{J}_y{}^2}{2})$$
$$+(\tfrac{1}{\sqrt{6}}A+\tfrac{-1}{\sqrt{6}}B+0\cdot C)(\sqrt{6}\frac{\mathbf{J}_x{}^2-\mathbf{J}_y{}^2}{2})$$

$$=\tfrac{1}{3}(A+B+C)(\mathbf{T}^0_0)$$
$$+\tfrac{1}{3}(-A-B+2C)(\mathbf{T}^2_0)$$
$$+\tfrac{1}{\sqrt{6}}(A-B)(\mathbf{T}^2_2+\mathbf{T}^2_{-2})$$

Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar and tensor operators*

$\mathbf{T}_0^0=\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2=\mathbf{J}^2$	$\mathbf{T}_0^2=\frac{2\mathbf{J}_z^2-\mathbf{J}_x^2-\mathbf{J}_y^2}{2}=\mathbf{J}^2\frac{3\cos^2\theta-1}{2}=\mathbf{J}^2P_2(\cos\theta)$	$\mathbf{T}_2^2+\mathbf{T}_{-2}^2=\sqrt{6}\frac{\mathbf{J}_x^2-\mathbf{J}_y^2}{2}=\sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos 2\phi$

Kinetic energy inertial coefficients: $A=\frac{1}{2I_x}, B=\frac{1}{2I_y}, C=\frac{1}{2I_z}$

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$$

$$=(\tfrac{1}{3}A+\tfrac{1}{3}B+\tfrac{1}{3}C)(\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2) \quad =(\tfrac{1}{3}A+\tfrac{1}{3}B+\tfrac{1}{3}C)(\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2) \quad =\tfrac{1}{3}(A+B+C)(\mathbf{T}_0^0)$$

$$+(\tfrac{-1}{6}A+\tfrac{-1}{6}B+\tfrac{2}{6}C)(-\mathbf{J}_x^2-\mathbf{J}_y^2+2\mathbf{J}_z^2) \quad +(\tfrac{-1}{3}A+\tfrac{-1}{3}B+\tfrac{2}{3}C)(\tfrac{2\mathbf{J}_z^2-\mathbf{J}_x^2-\mathbf{J}_y^2}{2}) \quad +\tfrac{1}{3}(-A-B+2C)(\mathbf{T}_0^2)$$

$$+(\tfrac{1}{2}A+\tfrac{-1}{2}B+0\cdot C)(\mathbf{J}_x^2-\mathbf{J}_y^2+0) \quad +(\tfrac{1}{\sqrt{6}}A+\tfrac{-1}{\sqrt{6}}B+0\cdot C)(\sqrt{6}\tfrac{\mathbf{J}_x^2-\mathbf{J}_y^2}{2}) \quad +\tfrac{1}{\sqrt{6}}(A-B)(\mathbf{T}_2^2+\mathbf{T}_{-2}^2)$$

Resulting asymmetric top Hamiltonian expansion:

asymmetry term

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2=\frac{1}{3}(A+B+C)(\mathbf{T}_0^0)+\frac{1}{3}(2C-A-B)(\mathbf{T}_0^2)+\frac{A-B}{\sqrt{6}}(\mathbf{T}_2^2+\mathbf{T}_{-2}^2)$$

Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x{}^2+B\mathbf{J}_y{}^2+C\mathbf{J}_z{}^2$ *made of scalar and tensor operators*

$\mathbf{T}_0^0=\mathbf{J}_x{}^2+\mathbf{J}_y{}^2+\mathbf{J}_z{}^2=\mathbf{J}^2$ | $\mathbf{T}_0^2=\dfrac{2\mathbf{J}_z{}^2-\mathbf{J}_x{}^2-\mathbf{J}_y{}^2}{2}=\mathbf{J}^2\dfrac{3\cos^2\theta-1}{2}=\mathbf{J}^2P_2(\cos\theta)$ | $\mathbf{T}_2^2+\mathbf{T}_{-2}^2=\sqrt{6}\dfrac{\mathbf{J}_x{}^2-\mathbf{J}_y{}^2}{2}=\sqrt{\dfrac{3}{2}}\mathbf{J}^2\sin^2\theta\cos 2\phi$

Kinetic energy inertial coefficients: $A=\dfrac{1}{2I_x}, B=\dfrac{1}{2I_y}, C=\dfrac{1}{2I_z}$

$$\mathbf{H}=A\mathbf{J}_x{}^2+B\mathbf{J}_y{}^2+C\mathbf{J}_z{}^2$$

$$=(\tfrac{1}{3}A+\tfrac{1}{3}B+\tfrac{1}{3}C)(\mathbf{J}_x{}^2+\mathbf{J}_y{}^2+\mathbf{J}_z{}^2)$$
$$+(\tfrac{-1}{6}A+\tfrac{-1}{6}B+\tfrac{2}{6}C)(-\mathbf{J}_x{}^2-\mathbf{J}_y{}^2+2\mathbf{J}_z{}^2)$$
$$+(\tfrac{1}{2}A+\tfrac{-1}{2}B+0\cdot C)(\mathbf{J}_x{}^2-\mathbf{J}_y{}^2+0)$$

$$=(\tfrac{1}{3}A+\tfrac{1}{3}B+\tfrac{1}{3}C)(\mathbf{J}_x{}^2+\mathbf{J}_y{}^2+\mathbf{J}_z{}^2)$$
$$+(\tfrac{-1}{3}A+\tfrac{-1}{3}B+\tfrac{2}{3}C)(\frac{2\mathbf{J}_z{}^2-\mathbf{J}_x{}^2-\mathbf{J}_y{}^2}{2})$$
$$+(\tfrac{1}{\sqrt{6}}A+\tfrac{-1}{\sqrt{6}}B+0\cdot C)(\sqrt{6}\frac{\mathbf{J}_x{}^2-\mathbf{J}_y{}^2}{2})$$

$$=\tfrac{1}{3}(A+B+C)(\mathbf{T}_0^0)$$
$$+\tfrac{1}{3}(-A-B+2C)(\mathbf{T}_0^2)$$
$$+\tfrac{1}{\sqrt{6}}(A-B)(\mathbf{T}_2^2+\mathbf{T}_{-2}^2)$$

Resulting asymmetric top Hamiltonian expansion:

asymmetry term

$$\mathbf{H}=A\mathbf{J}_x{}^2+B\mathbf{J}_y{}^2+C\mathbf{J}_z{}^2=\frac{1}{3}(A+B+C)(\mathbf{T}_0^0)+\frac{1}{3}(2C-A-B)(\mathbf{T}_0^2)+\frac{A-B}{\sqrt{6}}(\mathbf{T}_2^2+\mathbf{T}_{-2}^2)$$

Resulting semi-classical asymmetric top Hamiltonian expansion:

asymmetry term

$$\mathbf{H}=A\mathbf{J}_x{}^2+B\mathbf{J}_y{}^2+C\mathbf{J}_z{}^2=\frac{1}{3}(A+B+C)(\mathbf{J}^2)+\frac{1}{3}(2C-A-B)(\mathbf{J}^2\frac{3\cos^2\theta-1}{2})+\frac{A-B}{\sqrt{6}}(\sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos 2\phi)$$

Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar and tensor operators*

$$\mathbf{T}^0_0=\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2=\mathbf{J}^2$$

$$\mathbf{T}^2_0=\frac{2\mathbf{J}_z^2-\mathbf{J}_x^2-\mathbf{J}_y^2}{2}=\mathbf{J}^2\frac{3\cos^2\theta-1}{2}=\mathbf{J}^2P_2(\cos\theta)$$

$$\mathbf{T}^2_2+\mathbf{T}^2_{-2}=\sqrt{6}\frac{\mathbf{J}_x^2-\mathbf{J}_y^2}{2}=\sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos 2\phi$$

Kinetic energy inertial coefficients: $A=\frac{1}{2I_x}, B=\frac{1}{2I_y}, C=\frac{1}{2I_z}$

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$$

$$=(\tfrac{1}{3}A+\tfrac{1}{3}B+\tfrac{1}{3}C)(\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2)+(\tfrac{-1}{6}A+\tfrac{-1}{6}B+\tfrac{2}{6}C)(-\mathbf{J}_x^2-\mathbf{J}_y^2+2\mathbf{J}_z^2)+(\tfrac{1}{2}A+\tfrac{-1}{2}B+0\cdot C)(\mathbf{J}_x^2-\mathbf{J}_y^2+0)$$

$$=(\tfrac{1}{3}A+\tfrac{1}{3}B+\tfrac{1}{3}C)(\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2)+(\tfrac{-1}{3}A+\tfrac{-1}{3}B+\tfrac{2}{3}C)(\frac{2\mathbf{J}_z^2-\mathbf{J}_x^2-\mathbf{J}_y^2}{2})+(\tfrac{1}{\sqrt{6}}A+\tfrac{-1}{\sqrt{6}}B+0\cdot C)(\sqrt{6}\frac{\mathbf{J}_x^2-\mathbf{J}_y^2}{2})$$

$$=\tfrac{1}{3}(A+B+C)(\mathbf{T}^0_0)+\tfrac{1}{3}(-A-B+2C)(\mathbf{T}^2_0)+\tfrac{1}{\sqrt{6}}(A-B)(\mathbf{T}^2_2+\mathbf{T}^2_{-2})$$

Resulting asymmetric top Hamiltonian expansion:

asymmetry term

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2=\frac{1}{3}(A+B+C)(\mathbf{T}^0_0)+\frac{1}{3}(2C-A-B)(\mathbf{T}^2_0)+\frac{A-B}{\sqrt{6}}(\mathbf{T}^2_2+\mathbf{T}^2_{-2})$$

Resulting semi-classical asymmetric top Hamiltonian expansion:

asymmetry term

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2=\frac{1}{3}(A+B+C)(\mathbf{J}^2)+\frac{1}{3}(2C-A-B)(\mathbf{J}^2\frac{3\cos^2\theta-1}{2})+\frac{A-B}{\sqrt{6}}(\sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos 2\phi)$$

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2=\mathbf{J}^2\left[\frac{A+B+C}{3}+\frac{2C-A-B}{6}(3\cos^2\theta-1)+\frac{A-B}{2}\sin^2\theta\cos 2\phi\right]$$

Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar and tensor operators*

$\mathbf{T}_0^0=\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2=\mathbf{J}^2$	$\mathbf{T}_0^2=\frac{2\mathbf{J}_z^2-\mathbf{J}_x^2-\mathbf{J}_y^2}{2}=\mathbf{J}^2\frac{3\cos^2\theta-1}{2}=\mathbf{J}^2P_2(\cos\theta)$	$\mathbf{T}_2^2+\mathbf{T}_{-2}^2=\sqrt{6}\frac{\mathbf{J}_x^2-\mathbf{J}_y^2}{2}=\sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos2\phi$

Kinetic energy inertial coefficients: $A=\frac{1}{2I_x}, B=\frac{1}{2I_y}, C=\frac{1}{2I_z}$

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$$

$$=(\tfrac{1}{3}A+\tfrac{1}{3}B+\tfrac{1}{3}C)(\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2) \quad =(\tfrac{1}{3}A+\tfrac{1}{3}B+\tfrac{1}{3}C)(\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2) \quad =\tfrac{1}{3}(A+B+C)(\mathbf{T}_0^0)$$

$$+(\tfrac{-1}{6}A+\tfrac{-1}{6}B+\tfrac{2}{6}C)(-\mathbf{J}_x^2-\mathbf{J}_y^2+2\mathbf{J}_z^2) \quad +(\tfrac{-1}{3}A+\tfrac{-1}{3}B+\tfrac{2}{3}C)(\tfrac{2\mathbf{J}_z^2-\mathbf{J}_x^2-\mathbf{J}_y^2}{2}) \quad +\tfrac{1}{3}(-A-B+2C)(\mathbf{T}_0^2)$$

$$+(\tfrac{1}{2}A+\tfrac{-1}{2}B+0\cdot C)(\mathbf{J}_x^2-\mathbf{J}_y^2+0) \quad +(\tfrac{1}{\sqrt{6}}A+\tfrac{-1}{\sqrt{6}}B+0\cdot C)(\sqrt{6}\tfrac{\mathbf{J}_x^2-\mathbf{J}_y^2}{2}) \quad +\tfrac{1}{\sqrt{6}}(A-B)(\mathbf{T}_2^2+\mathbf{T}_{-2}^2)$$

Resulting asymmetric top Hamiltonian expansion: *asymmetry term*

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2=\frac{1}{3}(A+B+C)(\mathbf{T}_0^0)+\frac{1}{3}(2C-A-B)(\mathbf{T}_0^2)+\frac{A-B}{\sqrt{6}}(\mathbf{T}_2^2+\mathbf{T}_{-2}^2)$$

Resulting semi-classical asymmetric top Hamiltonian expansion: *asymmetry term*

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2=\frac{1}{3}(A+B+C)(\mathbf{J}^2)+\frac{1}{3}(2C-A-B)(\mathbf{J}^2\frac{3\cos^2\theta-1}{2})+\frac{A-B}{\sqrt{6}}(\sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos2\phi)$$

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2=\mathbf{J}^2\left[\frac{A+B+C}{3}+\frac{2C-A-B}{6}(3\cos^2\theta-1)+\frac{A-B}{2}\sin^2\theta\cos2\phi\right]$$

Resulting semi-classical symmetric top Hamiltonian expansion: $(A=B)$ *(asymmetry term not present)*

$$\mathbf{H}=B\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2=\mathbf{J}^2\left[\frac{B+B+C}{3}+\frac{2C-B-B}{6}(3\cos^2\theta-1)+\frac{B-B}{2}\sin^2\theta\cos2\phi\right]=\mathbf{J}^2\left[B+\frac{C-B}{3}3\cos^2\theta\right]$$

Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar and tensor operators*

$\mathbf{T}_0^0=\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2=\mathbf{J}^2$	$\mathbf{T}_0^2=\frac{2\mathbf{J}_z^2-\mathbf{J}_x^2-\mathbf{J}_y^2}{2}=\mathbf{J}^2\frac{3\cos^2\theta-1}{2}=\mathbf{J}^2P_2(\cos\theta)$	$\mathbf{T}_2^2+\mathbf{T}_{-2}^2=\sqrt{6}\frac{\mathbf{J}_x^2-\mathbf{J}_y^2}{2}=\sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos 2\phi$

Kinetic energy inertial coefficients : $A=\frac{1}{2I_x}, B=\frac{1}{2I_y}, C=\frac{1}{2I_z}$

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$$

$$=(\tfrac{1}{3}A+\tfrac{1}{3}B+\tfrac{1}{3}C)(\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2) \quad =(\tfrac{1}{3}A+\tfrac{1}{3}B+\tfrac{1}{3}C)(\mathbf{J}_x^2+\mathbf{J}_y^2+\mathbf{J}_z^2) \quad =\tfrac{1}{3}(A+B+C)(\mathbf{T}_0^0)$$

$$+(\tfrac{-1}{6}A+\tfrac{-1}{6}B+\tfrac{2}{6}C)(-\mathbf{J}_x^2-\mathbf{J}_y^2+2\mathbf{J}_z^2) \quad +(\tfrac{-1}{3}A+\tfrac{-1}{3}B+\tfrac{2}{3}C)\left(\frac{2\mathbf{J}_z^2-\mathbf{J}_x^2-\mathbf{J}_y^2}{2}\right) \quad +\tfrac{1}{3}(-A-B+2C)(\mathbf{T}_0^2)$$

$$+(\tfrac{1}{2}A+\tfrac{-1}{2}B+0\cdot C)(\mathbf{J}_x^2-\mathbf{J}_y^2+0) \quad +(\tfrac{1}{\sqrt{6}}A+\tfrac{-1}{\sqrt{6}}B+0\cdot C)\left(\sqrt{6}\frac{\mathbf{J}_x^2-\mathbf{J}_y^2}{2}\right) \quad +\tfrac{1}{\sqrt{6}}(A-B)(\mathbf{T}_2^2+\mathbf{T}_{-2}^2)$$

Resulting asymmetric top Hamiltonian expansion:

asymmetry term

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2=\frac{1}{3}(A+B+C)(\mathbf{T}_0^0)+\frac{1}{3}(2C-A-B)(\mathbf{T}_0^2)+\frac{A-B}{\sqrt{6}}(\mathbf{T}_2^2+\mathbf{T}_{-2}^2)$$

Resulting semi-classical asymmetric top Hamiltonian expansion:

asymmetry term

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2=\frac{1}{3}(A+B+C)(\mathbf{J}^2)+\frac{1}{3}(2C-A-B)\left(\mathbf{J}^2\frac{3\cos^2\theta-1}{2}\right)+\frac{A-B}{\sqrt{6}}\left(\sqrt{\frac{3}{2}}\mathbf{J}^2\sin^2\theta\cos 2\phi\right)$$

$$\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2=\mathbf{J}^2\left[\frac{A+B+C}{3}+\frac{2C-A-B}{6}(3\cos^2\theta-1)+\frac{A-B}{2}\sin^2\theta\cos 2\phi\right]$$

Resulting semi-classical symmetric top Hamiltonian expansion: $(A=B)$ *(asymmetry term not present)*

$$\mathbf{H}=B\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2=\mathbf{J}^2\left[\frac{B+B+C}{3}+\frac{2C-B-B}{6}(3\cos^2\theta-1)+\frac{B-B}{2}\sin^2\theta\cos 2\phi\right]=\mathbf{J}^2\left[B+(C-B)\cos^2\theta\right]$$

$$=B\mathbf{J}^2+(C-B)\mathbf{J}_z^2=B\mathbf{J}^2+(C-B)\mathbf{J}^2\cos^2\theta$$

Wigner D^J_{mn} irreps of U(2)~R(3) give atomic and molecular eigenfunctions $\Psi_{m,n}$ of 3D rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ and angular momentum uncertainty effects.

Review 1. *Angular momentum raise-n-lower operators* $\mathbf{S}_+$ and $\mathbf{S}_-$ Review 2. Angular momentum commutation

Review 3. *SU(2)⊂U(2) oscillators vs. R(3)⊂O(3) rotors*

Angular momentum magnitude and Θ^J_m-uncertainty cone polar angles

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Atomic wave functions. $D^L_{m0}\sim Y^L_m$ *Spherical harmonics*

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Molecular D^j_{mn} wave functions in "Mock-Mach" lab-vs-body state space $|^J_{mn}\rangle$

$\mathbf{P}^j_{mn}$ *projector and* $D^j_{mn}(\alpha,\beta,\gamma)$ *wave function*

D^J_{mn} *transform* $\mathbf{R}(\alpha,\beta,\gamma)|^J_{mn}\rangle=\Sigma_{m'}D^J_{m'n}(\alpha,\beta,\gamma)|^J_{m'n}\rangle$ *in lab-space,* $\overline{\mathbf{R}}(\alpha,\beta,\gamma)$ *in body-space.*

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Θ^J_m-cone properties of lab transforms: J=20, J=10, J=30.

Θ^J_m-analysis of high J atomic beams

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Rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ *made of scalar* $\mathbf{T}_0^0$ *or tensor* $\mathbf{T}_q^2$ *operators*

➡ *Rotational Energy Surfaces (RE or RES) of symmetric rotor and eigensolutions* ⬅

Rotational Energy Surfaces (RE or RES) of asymmetric rotor (for following class)

Rotational Energy Surfaces (RE or RES) of symmetric rotor and eigensolutions

Plot Hamiltonian $\mathbf{H}=B\mathbf{J}^2+(C-B)\mathbf{J}_z^{\ 2}$ radially as $H(\Theta)=BJ(J+1)+(C-B)J(J+1)\cos^2\Theta$

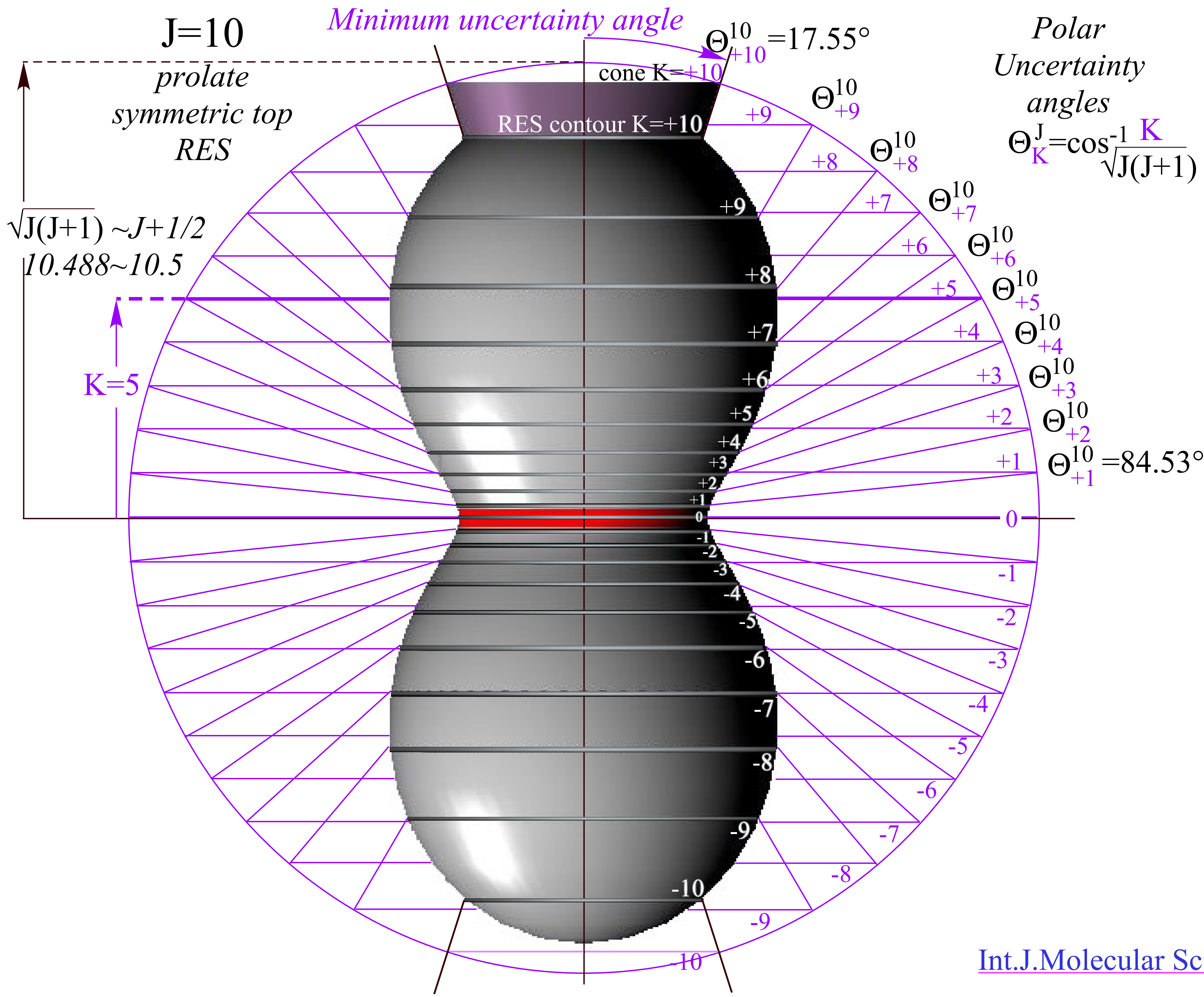
where: $\mathbf{J}_z = |\mathbf{J}|\cos\Theta = \sqrt{J(J+1)}\cos\Theta$

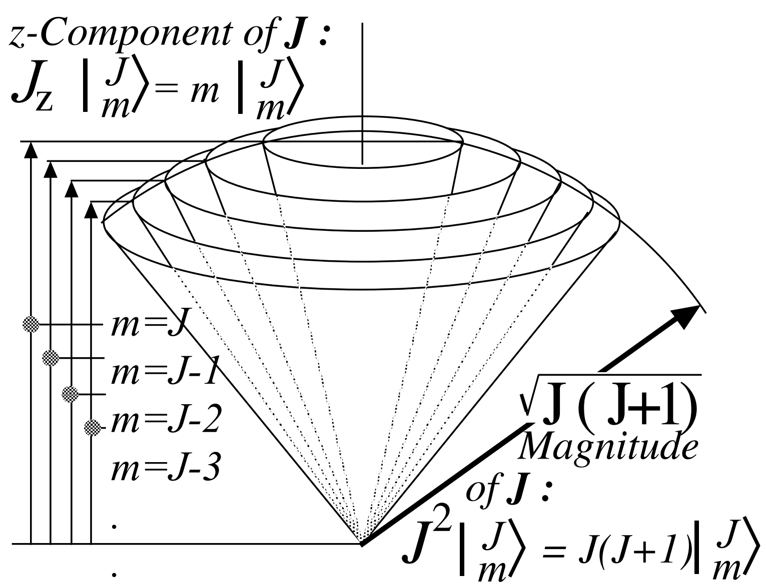
$\left|\begin{matrix} j \\ m,n \end{matrix}\right\rangle$

LAB $m=M$ BOD $n=K$

Conventional notation:

$$n=K=\mathbf{J}_z=\sqrt{J(J+1)}\cos\Theta$$





Int.J.Molecular Science 14.(2013) Fig.1 p. 730

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Plot Hamiltonian $\mathbf{H}=B\mathbf{J}^2+(C-B)\mathbf{J}_z^{\ 2}$ radially as $H(\Theta)=BJ(J+1)+(C-B)J(J+1)\cos^2\Theta$

$$H(\Theta_K^J)=BJ(J+1)+(C-B)J(J+1)\cos^2\Theta_K^J$$

$$=BJ(J+1)+(C-B)K^2$$

where: $\mathbf{J}_z = |\mathbf{J}|\cos\Theta = \sqrt{J(J+1)}\cos\Theta$

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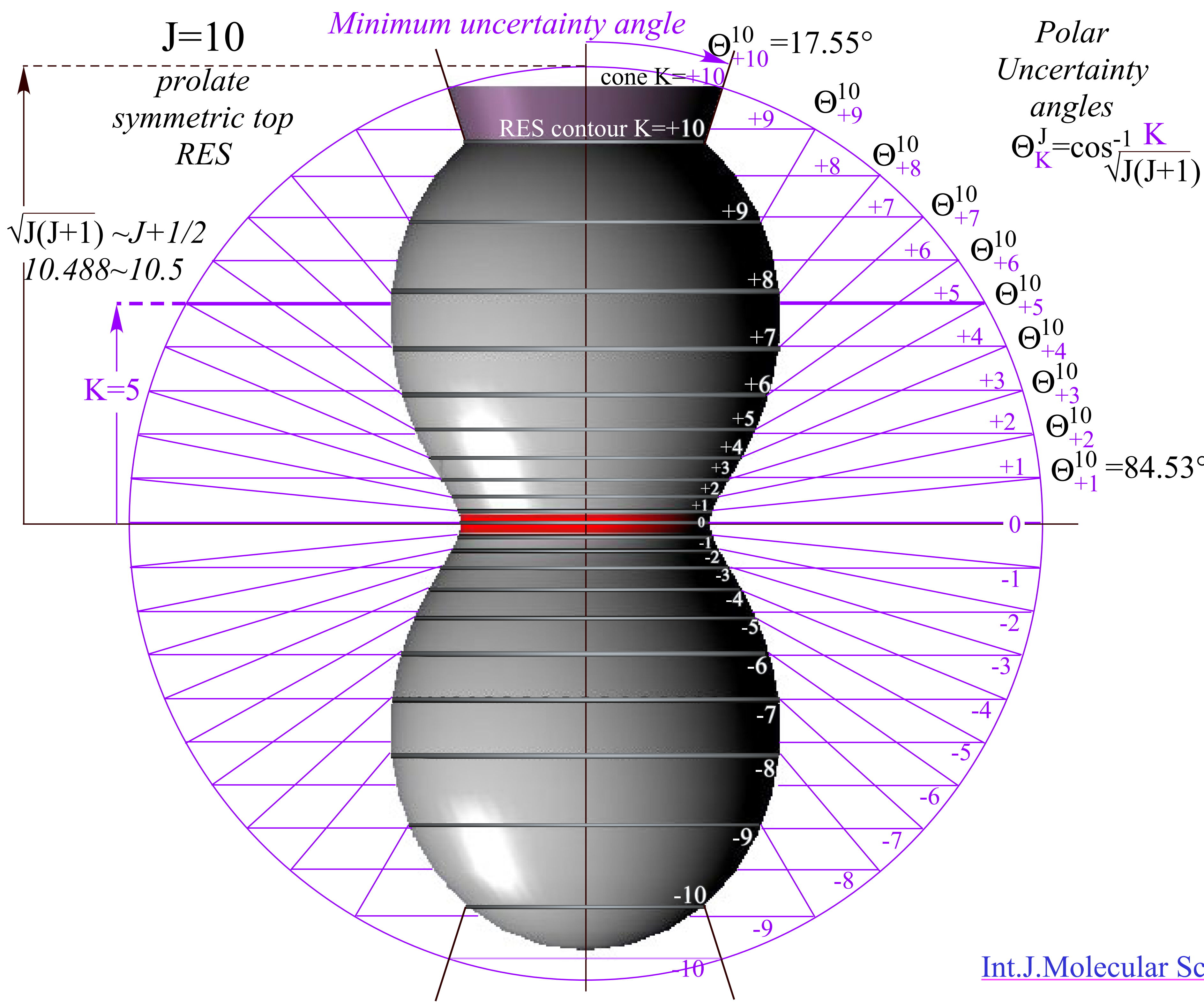

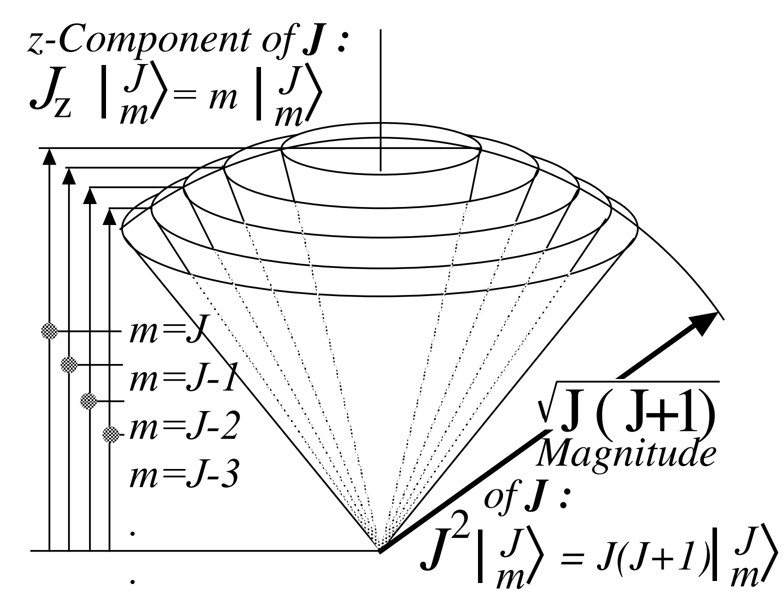

Int.J.Molecular Science 14.(2013) Fig.1 p. 730

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$H(\Theta^J_K) = BJ(J+1) + (C-B)J(J+1)\cos^2\Theta^J_K$

$= BJ(J+1) + (C-B)K^2$

where: $\mathbf{J}_z = |\mathbf{J}|\cos\Theta = \sqrt{J(J+1)}\cos\Theta$

$\left|\begin{matrix} j \\ m,n \end{matrix}\right\rangle$

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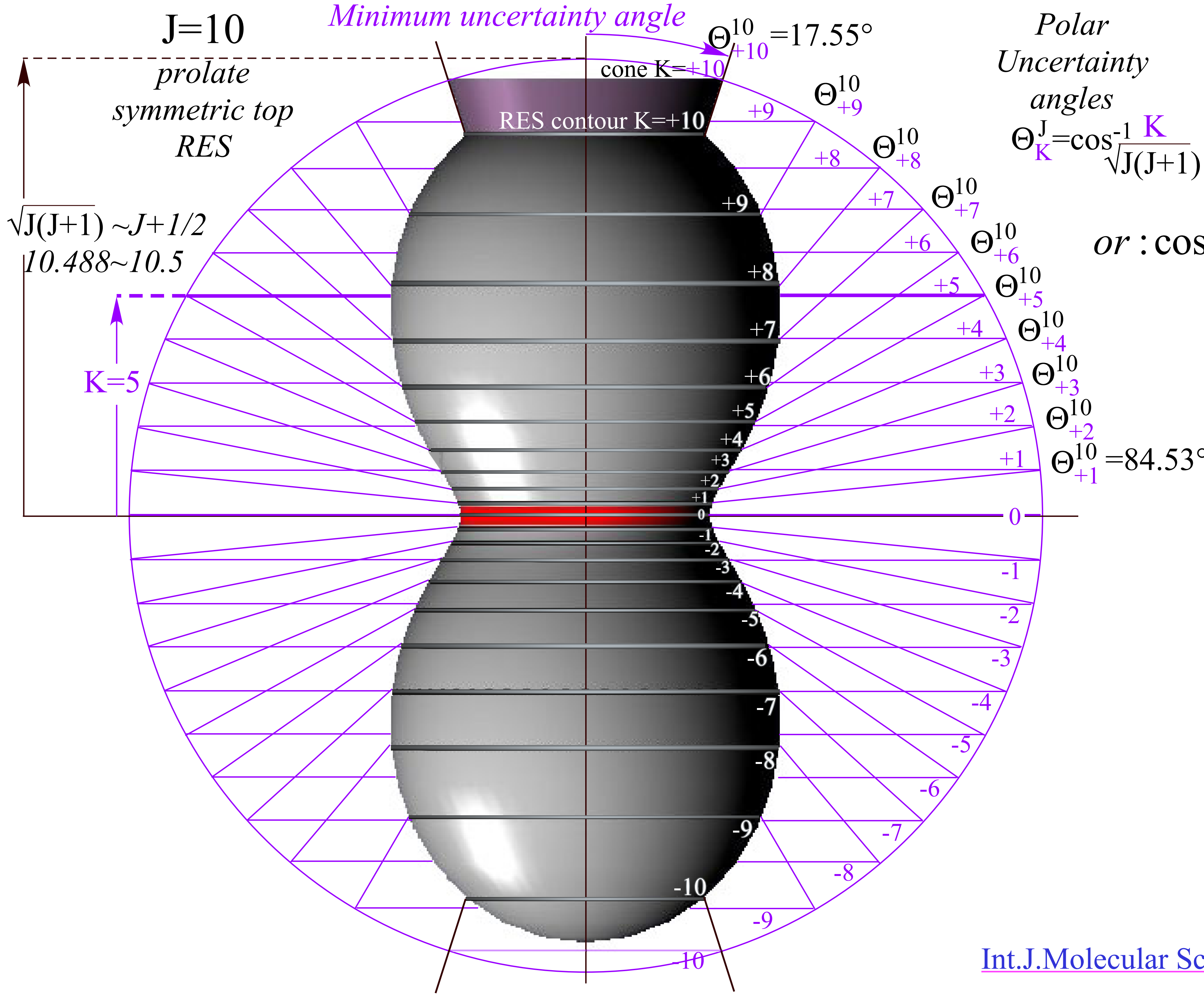
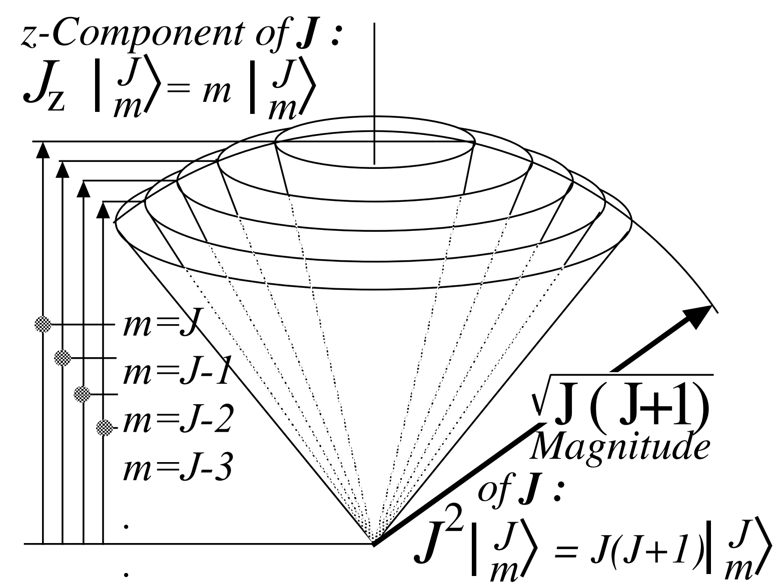
$n = K = \mathbf{J}_z = \sqrt{J(J+1)}\cos\Theta$



Polar Uncertainty angles $\Theta^J_K = \cos^{-1}\frac{K}{\sqrt{J(J+1)}}$

(Here this gives exact quantum eigenvalues!)

$or: \cos\Theta^J_K = \frac{K}{\sqrt{J(J+1)}}$



z-Component of $\boldsymbol{J}$: $J_z\left|\begin{matrix} J \\ m \end{matrix}\right\rangle = m\left|\begin{matrix} J \\ m \end{matrix}\right\rangle$

$J^2\left|\begin{matrix} J \\ m \end{matrix}\right\rangle = J(J+1)\left|\begin{matrix} J \\ m \end{matrix}\right\rangle$

Int.J.Molecular Science 14.(2013) Fig.1 p. 730

Wigner D^J_{mn} irreps of U(2)~R(3) give atomic and molecular eigenfunctions $\Psi_{m,n}$ of 3D rotor Hamiltonian $\mathbf{H}=A\mathbf{J}_x^2+B\mathbf{J}_y^2+C\mathbf{J}_z^2$ and angular momentum uncertainty effects.

Review 1. *Angular momentum raise-n-lower operators* $\mathbf{S}_+$ and $\mathbf{S}_-$ Review 2. Angular momentum commutation

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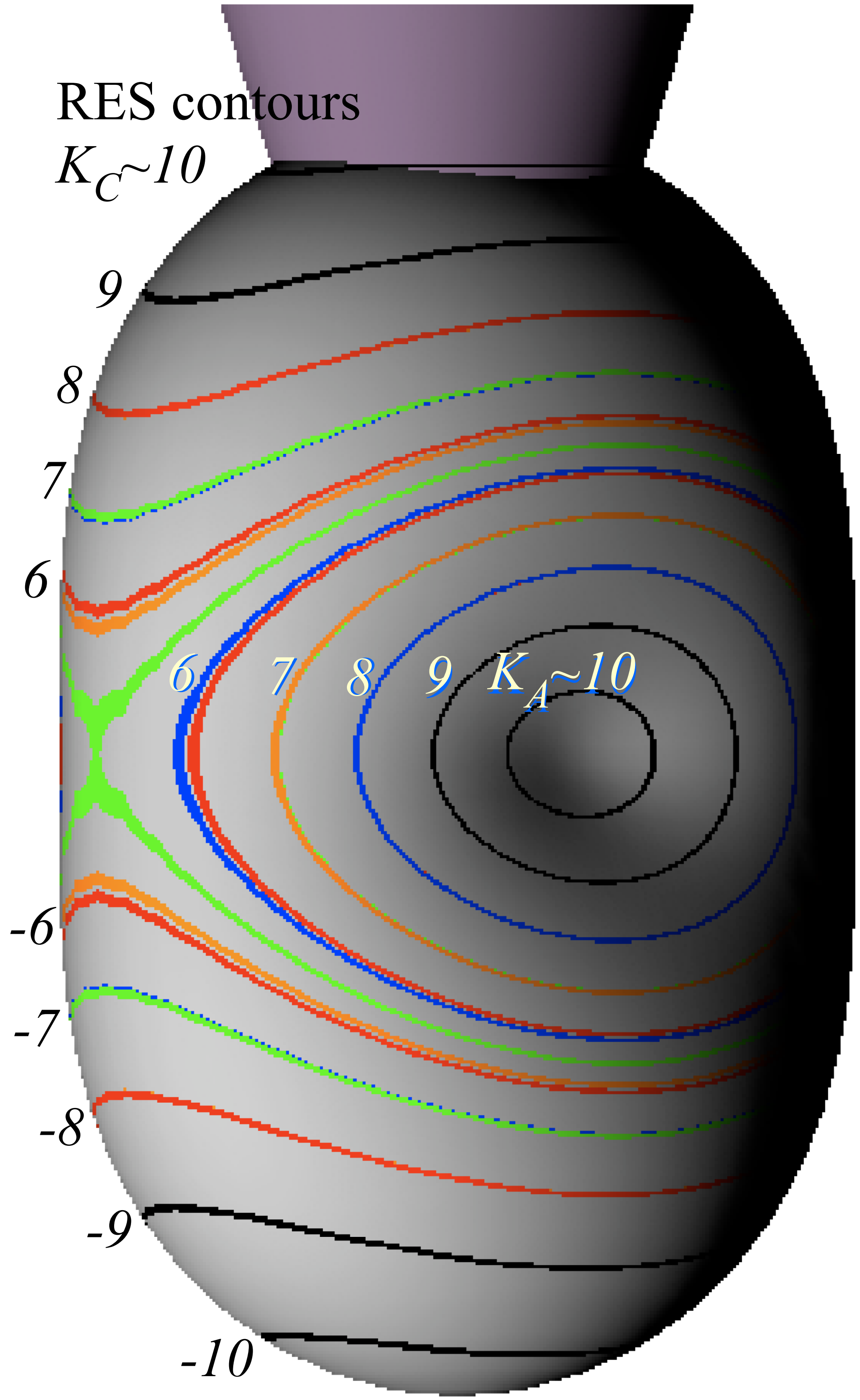
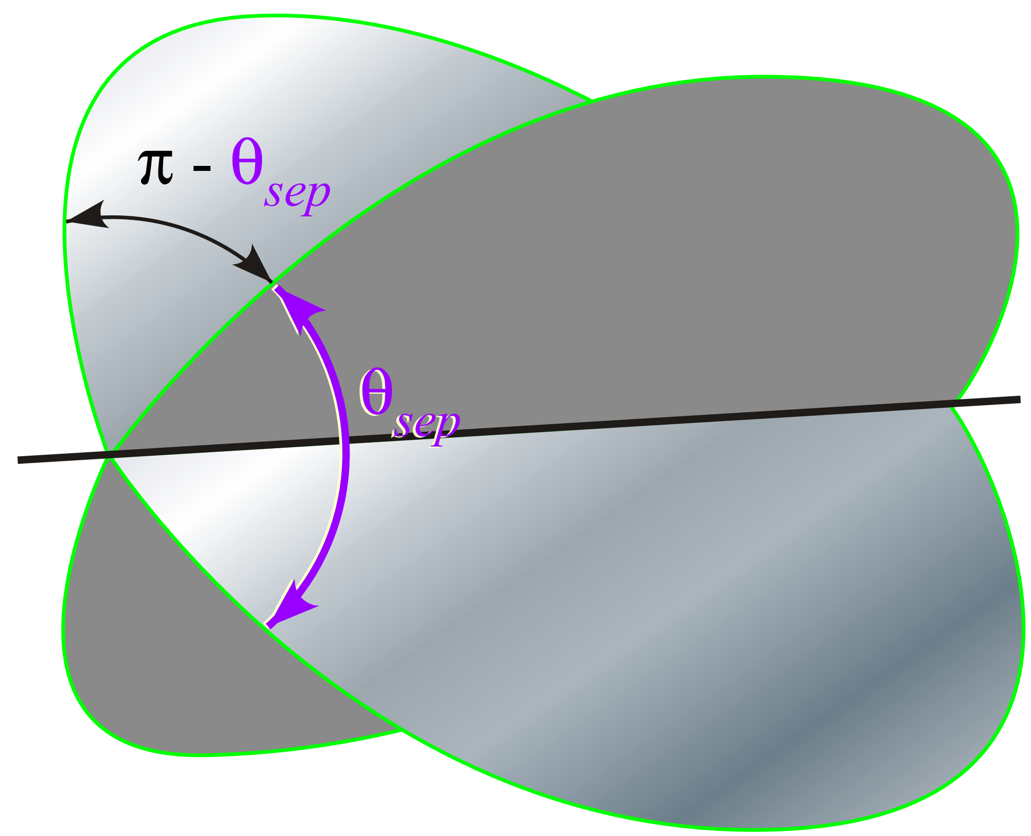
Rotational Energy Surfaces (RE or RES) of asymmetric rotor (for following class)



Separatrix circle pair dihedral angle

$$\theta_{sep} = \text{atan}\left(\frac{A-B}{B-C}\right)$$



Int.J.Molecular Science 14.(2013) Fig.3 p. 733

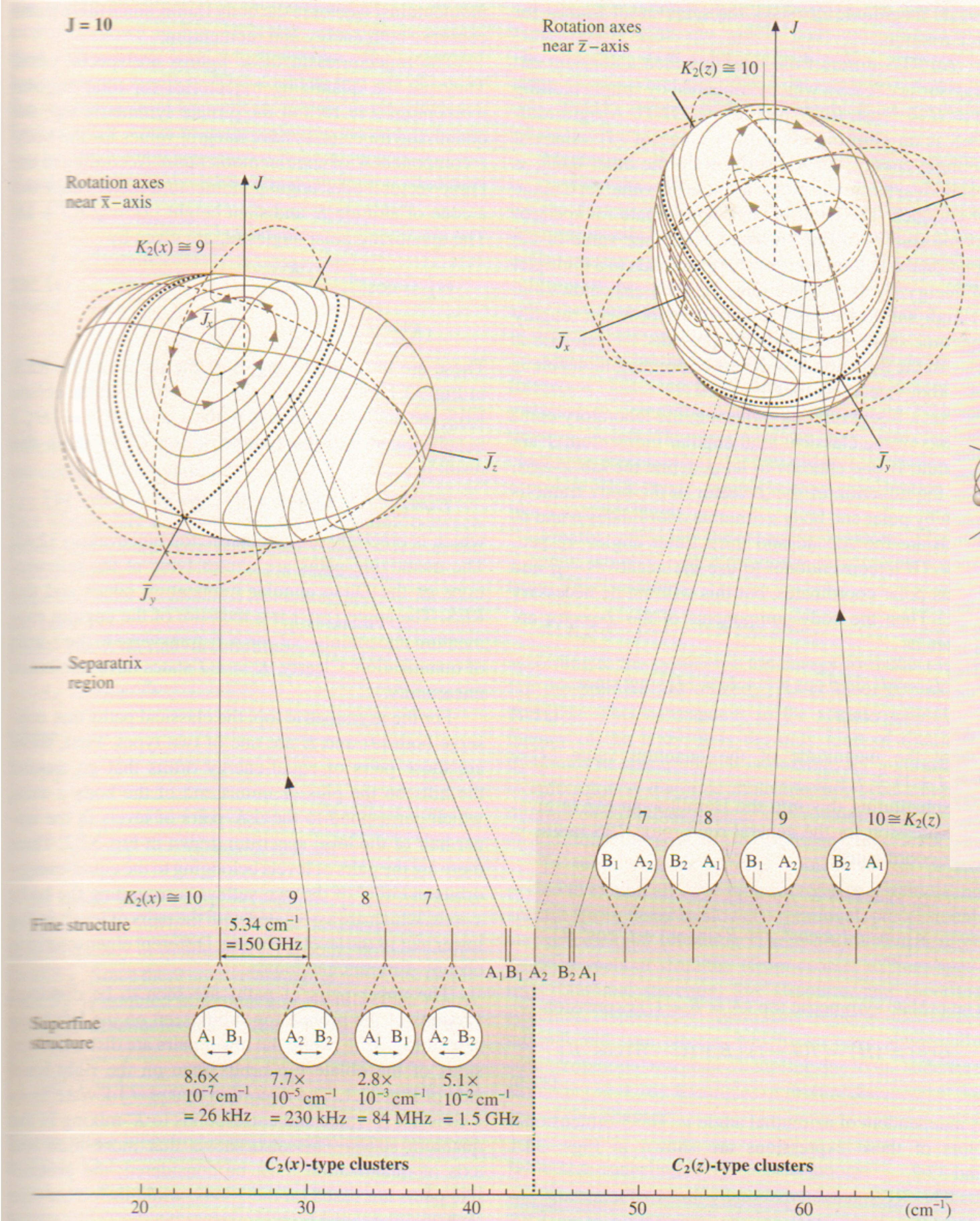
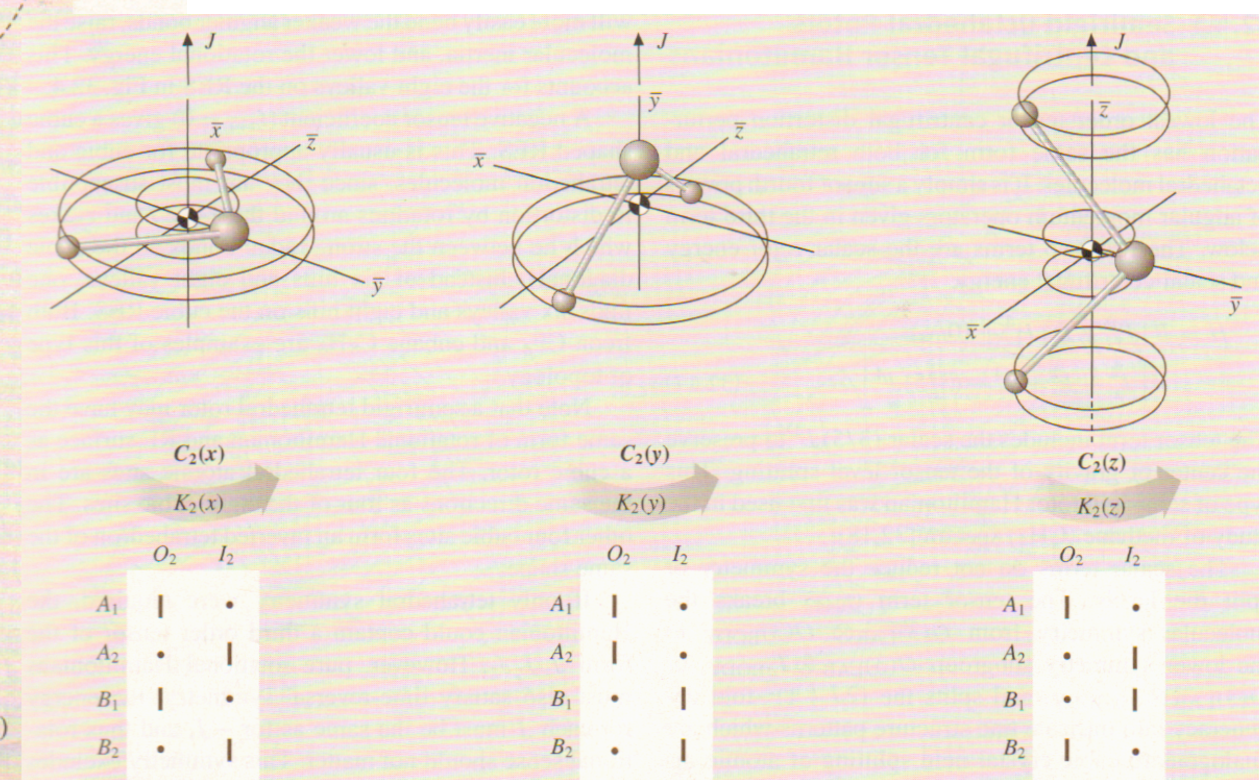


Fig. 32.2 $J = 10$ rotational energy surface and related level spectrum for an asymmetric rigid rotator ($A = 0.2$, $B = 0.4$, $C = 0.6\,\text{cm}^{-1}$)

Examples of Group⊃Sub-group correlation

$D_2 \supset C_2(x)$ $D_2 \supset C_2(y)$ $D_2 \supset C_2(z)$

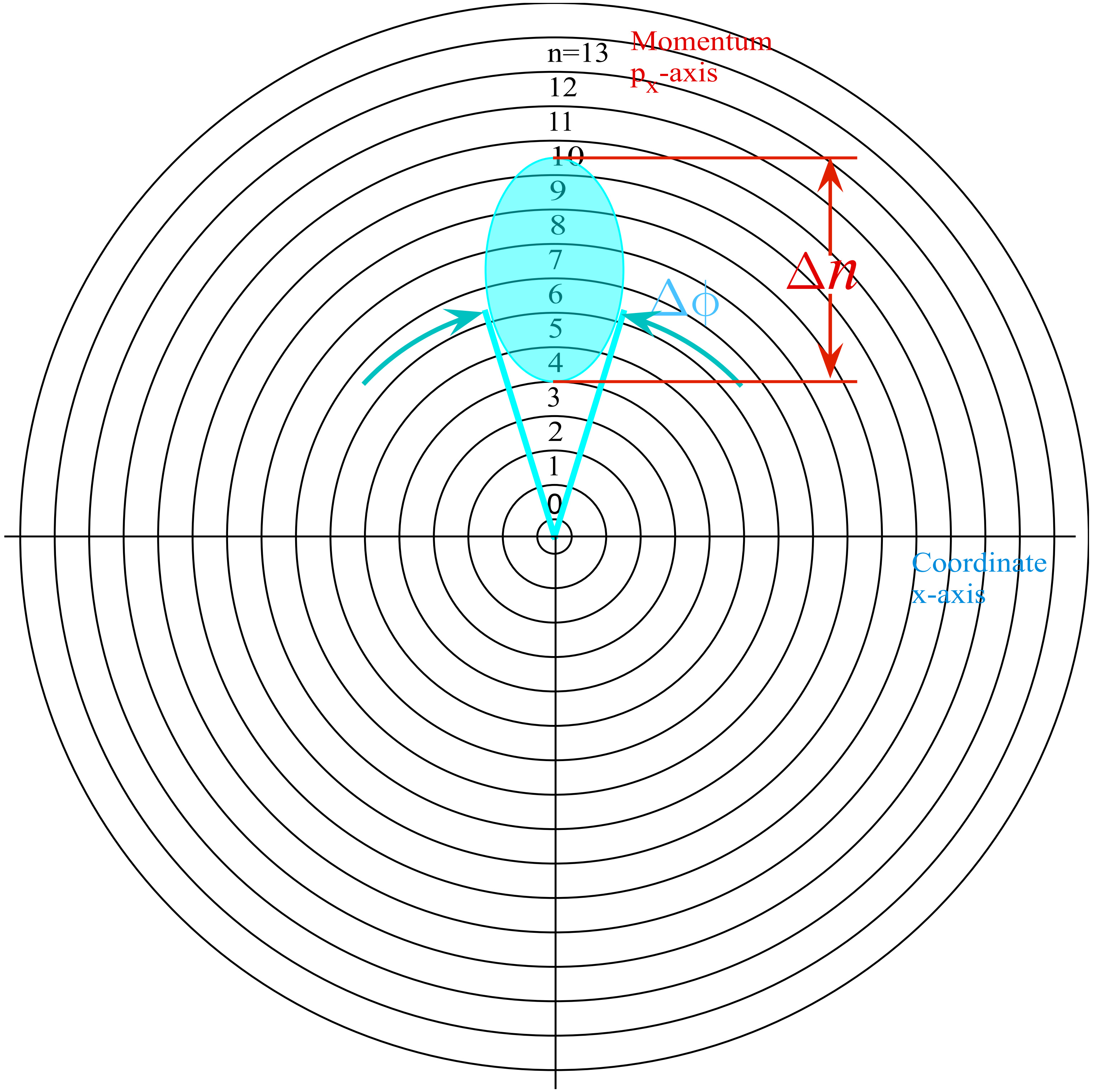


Springer Handbook
of
Atomic, Molecular, and Optical
Physics (2005)
Fig.32.2 and 32.3 p. 495-497

after *QTforCA Unit 8. Ch. 25* Fig. 25.4.2

Properties of 1D-HO coherent state

Coherent wave packet uncertainty relation: $\Delta n \cdot \Delta\phi > \pi / n$



???? Some uncertainty remains about this uncertainty ????