

# Group Theory in Quantum Mechanics

## Lecture 24 (4.25.17)

### Rotational symmetry $U(2) \subset U(3)$ and $O(3)$

(*Int.J.Mol.Sci*, 14, 714(2013) p.755-774 , QTCA Unit 7 Ch. 21-22 )

(PSDS - Ch. 5, 7 )

Review : 2-D  $\mathfrak{a}^\dagger \mathfrak{a}$  algebra of  $U(2)$  representations

Angular momentum generators by  $U(2)$  analysis

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

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

Angular momentum commutation relations

Key Lie theorems

Angular momentum magnitude and uncertainty

Angular momentum uncertainty angle

Generating  $R(3)$  rotation and  $U(2)$  representations

Applications of  $R(3)$  rotation and  $U(2)$  representations

Molecular and nuclear wavefunctions

Molecular and nuclear eigenlevels

Generalized Stern-Gerlach and transformation matrices

Angular momentum cones and high  $J$  properties

*Partial listing of the Harter-Soft/Heyoka LearnIt Web Apps as of April 24, 2017*  
*(Apps are being upgraded as time permits)*

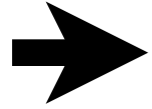
**Production Links - For the students & general public**

[BohrIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/BohrItWeb.html"](http://www.uark.edu/ua/modphys/markup/BohrItWeb.html)  
[BounceIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/BounceItWeb.html"](http://www.uark.edu/ua/modphys/markup/BounceItWeb.html)  
[BoxIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/BoxItWeb.html"](http://www.uark.edu/ua/modphys/markup/BoxItWeb.html)  
[CoulIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/CoulItWeb.html"](http://www.uark.edu/ua/modphys/markup/CoulItWeb.html)  
[Cycloidulum - Production; URL is "http://www.uark.edu/ua/modphys/markup/CycloidulumWeb.html"](http://www.uark.edu/ua/modphys/markup/CycloidulumWeb.html)  
[LearnIt - Production; URL is "<http://www.uark.edu/ua/modphys>" or "http://www.uark.edu/ua/modphys/markup/LearnItWeb.html"](http://www.uark.edu/ua/modphys/markup/LearnItWeb.html)  
[JerkIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/JerkItWeb.html"](http://www.uark.edu/ua/modphys/markup/JerkItWeb.html)  
[Pendulum - Production; URL is "http://www.uark.edu/ua/modphys/markup/PendulumWeb.html"](http://www.uark.edu/ua/modphys/markup/PendulumWeb.html)  
[QuantIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/QuantItWeb.html"](http://www.uark.edu/ua/modphys/markup/QuantItWeb.html)  
[Relativity - Pirelli Entrant; URL is "http://www.uark.edu/ua/pirelli" or "http://www.uark.edu/ua/pirelli/html/default.html"](http://www.uark.edu/ua/pirelli)  
[Trebuchet Production; URL is "http://www.uark.edu/ua/modphys/markup/TrebuchetWeb.html"](http://www.uark.edu/ua/modphys/markup/TrebuchetWeb.html)

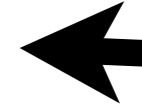
**Testing Links - For internal use and testing by Harter & Heyoka**

[BohrIt - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/BohrItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/BohrItWeb.html)  
[BounceIt - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/BounceItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/BounceItWeb.html)  
[BounceIt Title Page - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/BounceItTitlePage.html"](http://www.uark.edu/ua/modphys/testing/markup/BounceItTitlePage.html)  
[BoxIt - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/BoxItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/BoxItWeb.html)  
[CoulIt - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/CoulItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/CoulItWeb.html)  
[Cycloidulum - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/CycloidulumWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/CycloidulumWeb.html)  
[Harter-Soft Web Apps - Quick Reference - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/JerkItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/JerkItWeb.html)  
[JerkIt - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/JerkItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/JerkItWeb.html)  
[ModernPhysics - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/IntroCover.html"](http://www.uark.edu/ua/modphys/testing/markup/IntroCover.html)  
[Pendulum - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/PendulumWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/PendulumWeb.html)  
[QuantIt - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/QuantItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/QuantItWeb.html)  
[Trebuchet Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/TrebuchetWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/TrebuchetWeb.html)

**[Link to the complete listing of Harter-Soft LearnIt Web Apps and resources for Physics](#)**



Review : 2-D  $\mathfrak{su}(2)$  algebra of  $U(2)$  representations



*Angular momentum generators by  $U(2)$  analysis*

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*Angular momentum cones and high  $J$  properties*

# $U(2)$ -2D-HO Hamiltonian and irreducible representations

$$\mathbf{H} = A(\mathbf{a}_1^\dagger \mathbf{a}_1 + 1/2) + (B - iC)\mathbf{a}_1^\dagger \mathbf{a}_2 + (B + iC)\mathbf{a}_2^\dagger \mathbf{a}_1 + D(\mathbf{a}_2^\dagger \mathbf{a}_2 + 1/2)$$

$$\langle \mathbf{H} \rangle = A(1/2) + D(1/2) +$$

$$\begin{aligned} \mathbf{a}_1^\dagger \mathbf{a}_1 |n_1 n_2\rangle &= n_1 |n_1 n_2\rangle \\ \mathbf{a}_2^\dagger \mathbf{a}_1 |n_1 n_2\rangle &= \sqrt{n_1} \sqrt{n_2 + 1} |n_1 - 1, n_2 + 1\rangle \\ \mathbf{a}_1^\dagger \mathbf{a}_2 |n_1 n_2\rangle &= \sqrt{n_1 + 1} \sqrt{n_2} |n_1 + 1, n_2 - 1\rangle \\ \mathbf{a}_2^\dagger \mathbf{a}_2 |n_1 n_2\rangle &= n_2 |n_1 n_2\rangle \end{aligned}$$

	$ 00\rangle$	$ 01\rangle$	$ 02\rangle$	...	$ 10\rangle$	$ 11\rangle$	$ 12\rangle$	...	$ 20\rangle$	$ 21\rangle$	$ 22\rangle$	...
$\langle 00 $	0			...	.			...				...
$\langle 01 $		$D$		...	$B + iC$	.		...				...
$\langle 02 $			$2D$	...		$\sqrt{2}(B + iC)$	.	...				...
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$				$\ddots$
$\langle 10 $	.	$B - iC$		...	$A$			...	.			...
$\langle 11 $		.	$\sqrt{2}(B - iC)$	...		$A + D$		...	$\sqrt{2}(B + iC)$	.		...
$\langle 12 $				...			$A + 2D$	...		$\sqrt{4}(B + iC)$	.	...
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$
$\langle 20 $					.	$\sqrt{2}(B - iC)$		...	$2A$			...
$\langle 21 $						.	$\sqrt{4}(B - iC)$	...		$2A + D$		...
$\langle 22 $							.	...			$2A + 2D$	...
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$

Example:

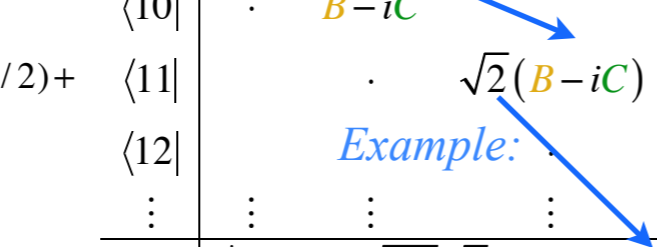
Rearrangement of rows and columns brings the matrix to a block-diagonal form.

$$\mathbf{H} = A(\mathbf{a}_1^\dagger \mathbf{a}_1 + 1/2) + (B - iC)\mathbf{a}_1^\dagger \mathbf{a}_2 + (B + iC)\mathbf{a}_2^\dagger \mathbf{a}_1 + D(\mathbf{a}_2^\dagger \mathbf{a}_2 + 1/2)$$

$$\langle \mathbf{H} \rangle = A(1/2) + D(1/2) +$$

$$\begin{aligned} \mathbf{a}_1^\dagger \mathbf{a}_1 |n_1 n_2\rangle &= n_1 |n_1 n_2\rangle \\ \mathbf{a}_2^\dagger \mathbf{a}_1 |n_1 n_2\rangle &= \sqrt{n_1} \sqrt{n_2 + 1} |n_1 - 1, n_2 + 1\rangle \\ \mathbf{a}_1^\dagger \mathbf{a}_2 |n_1 n_2\rangle &= \sqrt{n_1 + 1} \sqrt{n_2} |n_1 + 1, n_2 - 1\rangle \\ \mathbf{a}_2^\dagger \mathbf{a}_2 |n_1 n_2\rangle &= n_2 |n_1 n_2\rangle \end{aligned}$$

	00⟩	01⟩	02⟩	...	10⟩	11⟩	12⟩	...	20⟩	21⟩	22⟩	...
⟨00	0			...	.			...				...
⟨01		<i>D</i>		...	<i>B + iC</i>	.		...				...
⟨02			<i>2D</i>	...		$\sqrt{2}(B + iC)$	.	...				...
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
⟨10	.	<i>B - iC</i>		...	<i>A</i>			...	.			...
⟨11		.	$\sqrt{2}(B - iC)$	...		<i>A + D</i>		...	$\sqrt{2}(B + iC)$	.		...
⟨12				...			<i>A + 2D</i>	...		$\sqrt{4}(B + iC)$	.	...
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
⟨20				...	.	$\sqrt{2}(B - iC)$		...	<i>2A</i>			...
⟨21				...		.	$\sqrt{4}(B - iC)$	...		<i>2A + D</i>		...
⟨22				...			.	...			<i>2A + 2D</i>	...
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮



Rearrangement of rows and columns brings the matrix to a block-diagonal form.  
 Base states  $|n_1\rangle|n_2\rangle$  with the same total quantum number  $v = n_1 + n_2$  define each block.

$$\mathbf{H} = A(\mathbf{a}_1^\dagger \mathbf{a}_1 + 1/2) + (B - iC)\mathbf{a}_1^\dagger \mathbf{a}_2 + (B + iC)\mathbf{a}_2^\dagger \mathbf{a}_1 + D(\mathbf{a}_2^\dagger \mathbf{a}_2 + 1/2)$$

$$\langle \mathbf{H} \rangle = A(1/2) + D(1/2) +$$

$$\begin{aligned} \mathbf{a}_1^\dagger \mathbf{a}_1 |n_1 n_2\rangle &= n_1 |n_1 n_2\rangle \\ \mathbf{a}_2^\dagger \mathbf{a}_1 |n_1 n_2\rangle &= \sqrt{n_1} \sqrt{n_2 + 1} |n_1 - 1, n_2 + 1\rangle \\ \mathbf{a}_1^\dagger \mathbf{a}_2 |n_1 n_2\rangle &= \sqrt{n_1 + 1} \sqrt{n_2} |n_1 + 1, n_2 - 1\rangle \\ \mathbf{a}_2^\dagger \mathbf{a}_2 |n_1 n_2\rangle &= n_2 |n_1 n_2\rangle \end{aligned}$$

	00⟩	01⟩	02⟩	...	10⟩	11⟩	12⟩	...	20⟩	21⟩	22⟩	...
⟨00	0			...	.			...				...
⟨01		D		...	B + iC	.		...				...
⟨02			2D	...		√2(B + iC)	.	...				...
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
⟨10	.	B - iC		...	A			...	.			...
⟨11		.	√2(B - iC)	...		A + D		...	√2(B + iC)	.		...
⟨12				...			A + 2D	...		√4(B + iC)	.	...
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
⟨20				...	.	√2(B - iC)		...	2A			...
⟨21				...		.	√4(B - iC)	...		2A + D		...
⟨22				...				...			2A + 2D	...
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

Example:

Rearrangement of rows and columns brings the matrix to a block-diagonal form.  
 Base states  $|n_1\rangle|n_2\rangle$  with the same total quantum number  $v = n_1 + n_2$  define each block.

Group reorganized  
 "Little-Endian" indexing  
 (...01,02,03..10,11,12,13...  
 20,21,22,23,...)

	00⟩	01⟩	10⟩	02⟩	11⟩	20⟩	03⟩	12⟩	21⟩	30⟩	...
⟨00	0	Vacuum (v=0)									
⟨01		D	B + iC	Fundamental (v=1)							
⟨10		B - iC	A	vibrational sub-space							
⟨02				2D	√2(B + iC)						
⟨11				√2(B - iC)	A + D	√2(B + iC)	Overtone (v=2)				
⟨20					√2(B - iC)	2A	vibrational sub-space				
⟨03							3D	√3(B + iC)			
⟨12							√3(B - iC)	A + 2D	√4(B + iC)		Overtone (v=3)
⟨21								√4(B - iC)	2A + D	√3(B + iC)	vibrational sub-space
⟨30									√3(B - iC)	3A	
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

$$\mathbf{H}^A = A(\mathbf{a}_1^\dagger \mathbf{a}_1 + 1/2) + D(\mathbf{a}_2^\dagger \mathbf{a}_2 + 1/2)$$

$$\epsilon_{n_1 n_2}^A = A\left(n_1 + \frac{1}{2}\right) + D\left(n_2 + \frac{1}{2}\right) = \frac{A+D}{2}(n_1 + n_2 + 1) + \frac{A-D}{2}(n_1 - n_2)$$

Setting  $(B=0=C)$  and  $(A=\omega_+)$  and  $(D=\omega_-)$  gives diagonal block matrices.

Review Lect.23 p80-92

	$ 00\rangle$	$ 01\rangle$	$ 10\rangle$	$ 02\rangle$	$ 11\rangle$	$ 20\rangle$	$ 03\rangle$	$ 12\rangle$	$ 21\rangle$	$ 30\rangle$	...
$\langle 00 $	0										
$\langle 01 $		$\omega_-$									
$\langle 10 $			$\omega_+$								
$\langle 02 $				$2\omega_-$							
$\langle 11 $					$\omega_+ + \omega_-$						
$\langle 20 $						$2\omega_+$					
$\langle 03 $							$3\omega_-$				
$\langle 12 $								$\omega_+ + 2\omega_-$			
$\langle 21 $									$2\omega_+ + \omega_-$		
$\langle 30 $										$3\omega_+$	
$\vdots$											

$$\begin{aligned} \omega_+ - \omega_- &= \Omega \\ &= \sqrt{(2B)^2 + (2C)^2 + (A - D)^2} \\ &= A - D \end{aligned}$$

$$\langle \mathbf{H} \rangle = A(\mathbf{1}/2) + D(\mathbf{1}/2) +$$

$$\mathbf{H}^A = A(\mathbf{a}_1^\dagger \mathbf{a}_1 + \mathbf{1}/2) + D(\mathbf{a}_2^\dagger \mathbf{a}_2 + \mathbf{1}/2)$$

$$\begin{aligned} \epsilon_{n_1 n_2}^A &= A\left(n_1 + \frac{1}{2}\right) + D\left(n_2 + \frac{1}{2}\right) = \frac{A+D}{2}(n_1 + n_2 + 1) + \frac{A-D}{2}(n_1 - n_2) \\ &= \Omega_0(n_1 + n_2 + 1) + \frac{\Omega}{2}(n_1 - n_2) = \Omega_0(v+1) + \Omega m \end{aligned}$$

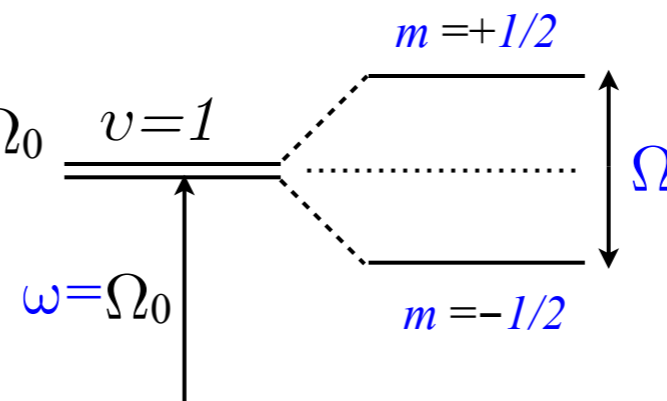
Define *total quantum number*  $v=2j$  and half-difference or *asymmetry quantum number*  $m$

$$v = n_1 + n_2 = 2j$$

$$j = \frac{n_1 + n_2}{2} = \frac{v}{2}$$

$$m = \frac{n_1 - n_2}{2}$$

$v+1=2j+1$  multiplies *base frequency*  $\omega = \Omega_0$   
 $m$  multiplies *beat frequency*  $\Omega$



$$\omega_+ = \Omega_0 + \Omega\left(+\frac{1}{2}\right)$$

$$\omega_- = \Omega_0 + \Omega\left(-\frac{1}{2}\right)$$

Setting  $(B=0=C)$  and  $(A=\omega_+)$  and  $(D=\omega_-)$  gives diagonal block matrices.

	$ 00\rangle$	$ 01\rangle$	$ 10\rangle$	$ 02\rangle$	$ 11\rangle$	$ 20\rangle$	$ 03\rangle$	$ 12\rangle$	$ 21\rangle$	$ 30\rangle$	...
$\langle 00 $	0										
$\langle 01 $		$\omega_-$									
$\langle 10 $			$\omega_+$								
$\langle 02 $				$2\omega_-$							
$\langle 11 $					$\omega_+ + \omega_-$						
$\langle 20 $						$2\omega_+$					
$\langle 03 $							$3\omega_-$				
$\langle 12 $								$\omega_+ + 2\omega_-$			
$\langle 21 $									$2\omega_+ + \omega_-$		
$\langle 30 $										$3\omega_+$	
$\vdots$											

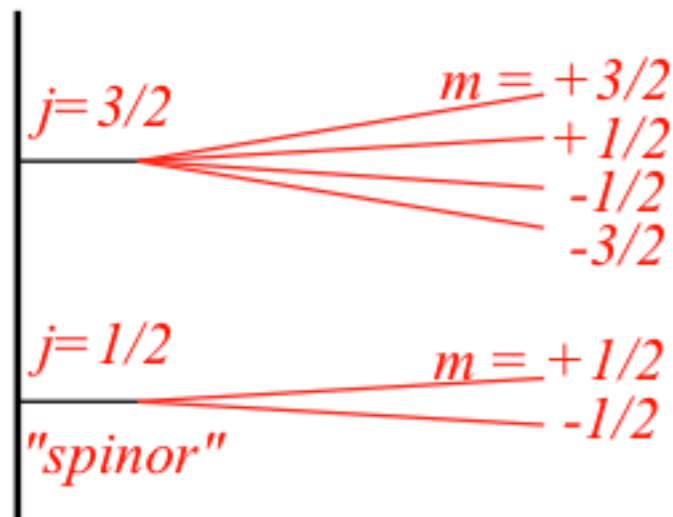
$$\omega_+ - \omega_- = \Omega$$

$$= \sqrt{(2B)^2 + (2C)^2 + (A - D)^2}$$

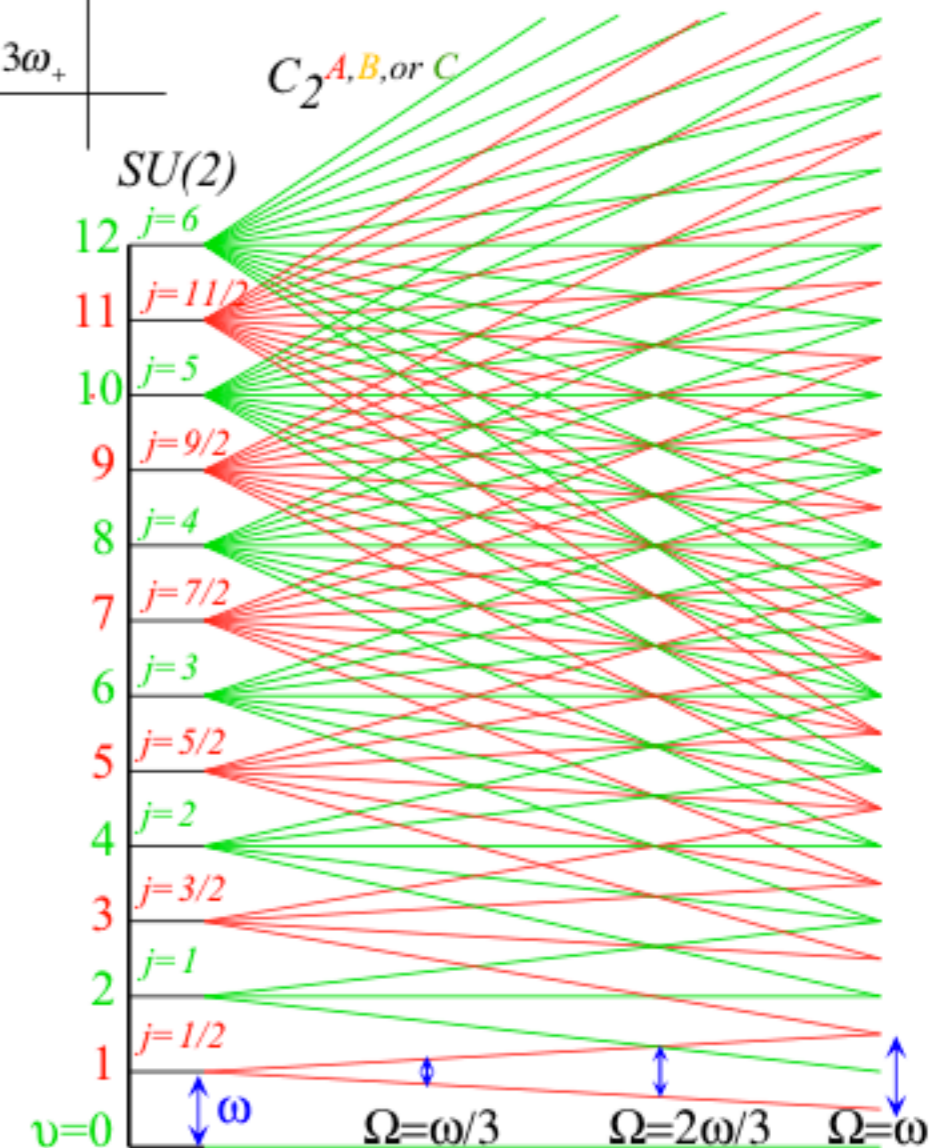
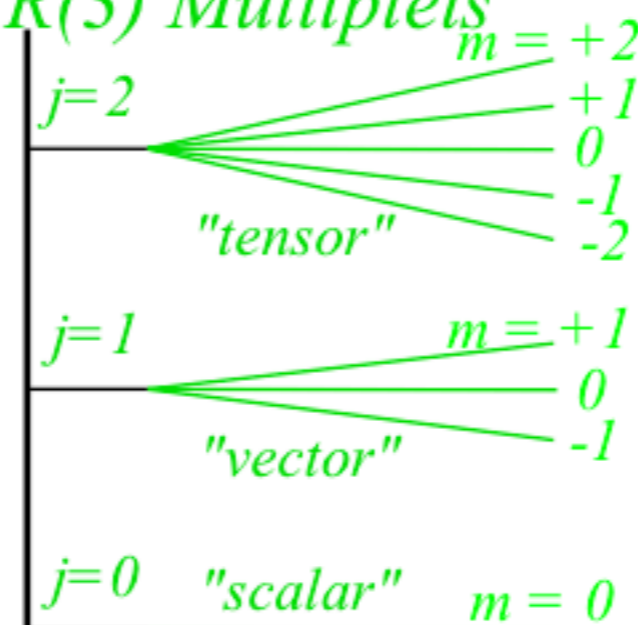
$$= A - D$$

$$\langle \mathbf{H} \rangle = A(1/2) + D(1/2) +$$

### SU(2) Multiplets



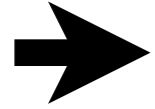
### R(3) Multiplets



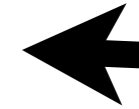


Review : 2-D  $\mathfrak{a}^{\dagger}\mathfrak{a}$  algebra of  $U(2)$  representations

Review Lect.23 p99-103



*Angular momentum generators by  $U(2)$  analysis*  
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( $\nu=1$ ) or ( $j=1/2$ ) block **H** matrices of U(2) oscillator

Use irreps of unit operator  $\mathbf{S}_0 = \mathbf{1}$  and spin operators  $\{\mathbf{S}_X, \mathbf{S}_Y, \mathbf{S}_Z\}$ . (also known as:  $\{\mathbf{S}_B, \mathbf{S}_C, \mathbf{S}_A\}$ )

$$\begin{pmatrix} A & B-iC \\ B+iC & D \end{pmatrix} = \frac{A+D}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + 2B \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} + 2C \begin{pmatrix} 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 \end{pmatrix} + (A-D) \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$$

( $\nu=1$ ) or ( $j=1/2$ ) block **H** matrices of U(2) oscillator

Use irreps of unit operator  $\mathbf{S}_0 = \mathbf{1}$  and spin operators  $\{\mathbf{S}_X, \mathbf{S}_Y, \mathbf{S}_Z\}$ . (also known as:  $\{\mathbf{S}_B, \mathbf{S}_C, \mathbf{S}_A\}$ )

$$\begin{pmatrix} A & B-iC \\ B+iC & D \end{pmatrix} = \frac{A+D}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + 2B \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} + 2C \begin{pmatrix} 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 \end{pmatrix} + (A-D) \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$$

( $\nu=2$ ) or ( $j=1$ ) 3-by-3 block uses their vector irreps.

$$\begin{pmatrix} 2A & \sqrt{2}(B-iC) & \cdot \\ \sqrt{2}(B+iC) & A+D & \sqrt{2}(B-iC) \\ \cdot & \sqrt{2}(B+iC) & 2D \end{pmatrix} = (A+D) \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} + 2B \begin{pmatrix} \cdot & \frac{\sqrt{2}}{2} & \cdot \\ \frac{\sqrt{2}}{2} & \cdot & \frac{\sqrt{2}}{2} \\ \cdot & \frac{\sqrt{2}}{2} & \cdot \end{pmatrix} + 2C \begin{pmatrix} \cdot & -i\frac{\sqrt{2}}{2} & \cdot \\ i\frac{\sqrt{2}}{2} & \cdot & -i\frac{\sqrt{2}}{2} \\ \cdot & i\frac{\sqrt{2}}{2} & \cdot \end{pmatrix} + (A-D) \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$$

( $\nu=1$ ) or ( $j=1/2$ ) block **H** matrices of U(2) oscillator

Use irreps of unit operator  $\mathbf{S}_0 = \mathbf{1}$  and spin operators  $\{\mathbf{S}_X, \mathbf{S}_Y, \mathbf{S}_Z\}$ . (also known as:  $\{\mathbf{S}_B, \mathbf{S}_C, \mathbf{S}_A\}$ )

$$\begin{pmatrix} A & B-iC \\ B+iC & D \end{pmatrix} = \frac{A+D}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + 2B \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} + 2C \begin{pmatrix} 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 \end{pmatrix} + (A-D) \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$$

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( $\nu=3$ ) or ( $j=3/2$ ) 4-by-4 block uses Dirac spinor irreps.

$$\begin{pmatrix} 3A & \sqrt{3}(B-iC) & & \\ \sqrt{3}(B+iC) & 2A+D & \sqrt{4}(B-iC) & \\ & \sqrt{4}(B+iC) & A+2D & \sqrt{3}(B-iC) \\ & & \sqrt{3}(B+iC) & 3D \end{pmatrix} = \frac{3(A+D)}{2} \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 \end{pmatrix} + 2B \begin{pmatrix} \cdot & \frac{\sqrt{3}}{2} & \cdot & \cdot \\ \frac{\sqrt{3}}{2} & \cdot & \frac{\sqrt{4}}{2} & \cdot \\ \cdot & \frac{\sqrt{4}}{2} & \cdot & \frac{\sqrt{3}}{2} \\ \cdot & \cdot & \frac{\sqrt{3}}{2} & \cdot \end{pmatrix} + 2C \begin{pmatrix} \cdot & -\frac{i\sqrt{3}}{2} & \cdot & \cdot \\ i\frac{\sqrt{3}}{2} & \cdot & -i\frac{\sqrt{4}}{2} & \cdot \\ \cdot & i\frac{\sqrt{4}}{2} & \cdot & -i\frac{\sqrt{3}}{2} \\ \cdot & \cdot & i\frac{\sqrt{3}}{2} & \cdot \end{pmatrix} + (A-D) \begin{pmatrix} \frac{3}{2} & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{2} & \cdot & \cdot \\ \cdot & \cdot & -\frac{1}{2} & \cdot \\ \cdot & \cdot & \cdot & -\frac{3}{2} \end{pmatrix}$$

( $\nu=1$ ) or ( $j=1/2$ ) block **H** matrices of U(2) oscillator

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( $\nu=2j$ ) or ( $2j+1$ )-by- $(2j+1)$  block uses  $D^{(j)}(\mathbf{s}_\mu)$  irreps of U(2) or R(3).

$$\langle \mathbf{H} \rangle^{j\text{-block}} = 2j\Omega_0 \langle \mathbf{1} \rangle^j + \Omega_X \langle \mathbf{s}_X \rangle^j + \Omega_Y \langle \mathbf{s}_Y \rangle^j + \Omega_Z \langle \mathbf{s}_Z \rangle^j$$

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All  $j$ -block matrix operators factor into raise-n-lower operators  $\mathbf{s}_\pm = \mathbf{s}_X \pm i\mathbf{s}_Y$  plus the diagonal  $\mathbf{s}_Z$

$$\langle \mathbf{H} \rangle^{j\text{-block}} = 2j\Omega_0 \langle \mathbf{1} \rangle^j + \left[ (\Omega_X - i\Omega_Y) \langle \mathbf{s}_X + i\mathbf{s}_Y \rangle^j + (\Omega_X + i\Omega_Y) \langle \mathbf{s}_X - i\mathbf{s}_Y \rangle^j \right] / 2 + \Omega_Z \langle \mathbf{s}_Z \rangle^j$$

Review : 2-D  $\mathfrak{a}^{\dagger}\mathfrak{a}$  algebra of  $U(2)$  representations

Review Lect.23 p105-111

Angular momentum generators by  $U(2)$  analysis

Angular momentum raise-n-lower operators  $\mathbf{s}_+$  and  $\mathbf{s}_-$

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

Angular momentum commutation relations

Key Lie theorems

Angular momentum magnitude and uncertainty

Angular momentum uncertainty angle

Generating  $R(3)$  rotation and  $U(2)$  representations

Applications of  $R(3)$  rotation and  $U(2)$  representations

Molecular and nuclear wavefunctions

Molecular and nuclear eigenstates

Generalized Stern-Gerlach and transformation matrices

Angular momentum cones and high  $J$  properties

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

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*  $\mathbf{a}^\dagger \mathbf{a}$

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



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

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

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

to raise angular momentum by one  $\hbar$  unit

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

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

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  $\mathbf{a}^\dagger \mathbf{a}$

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

Hamilton-Pauli-Jordan representation of  $\mathbf{s}_Z$  is:

$$\langle \mathbf{s}_Z \rangle^{(\frac{1}{2})} = D^{(\frac{1}{2})}(\mathbf{s}_Z) = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$$

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

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

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

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

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

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  $\downarrow$

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

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

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-D  $\mathfrak{a}^\dagger \mathfrak{a}$  algebra of  $U(2)$  representations

Review Lect.23 p113-125

Angular momentum generators by  $U(2)$  analysis

Angular momentum raise-n-lower operators  $\mathbf{s}_+$  and  $\mathbf{s}_-$

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

Angular momentum commutation relations

Key Lie theorems

Angular momentum magnitude and uncertainty

Angular momentum uncertainty angle

Generating  $R(3)$  rotation and  $U(2)$  representations

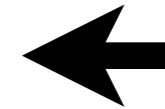
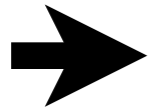
Applications of  $R(3)$  rotation and  $U(2)$  representations

Molecular and nuclear wavefunctions

Molecular and nuclear eigenstates

Generalized Stern-Gerlach and transformation matrices

Angular momentum cones and high  $J$  properties



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

$U(2)$  boson oscillator states  $|n_1, n_2\rangle$

Oscillator total quanta:  $\nu = (n_1 + n_2)$

$$|n_1 n_2\rangle = \frac{(\mathbf{a}_1^\dagger)^{n_1} (\mathbf{a}_2^\dagger)^{n_2}}{\sqrt{n_1! n_2!}} |0 0\rangle$$



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

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

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Oscillator  $\mathbf{a}^\dagger \mathbf{a} \dots$

$$\mathbf{a}_1^\dagger \mathbf{a}_2 |n_1 n_2\rangle = \sqrt{n_1 + 1} \sqrt{n_2} |n_1 + 1, n_2 - 1\rangle$$

$$\mathbf{a}_2^\dagger \mathbf{a}_1 |n_1 n_2\rangle = \sqrt{n_1} \sqrt{n_2 + 1} |n_1 - 1, n_2 + 1\rangle$$

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

$$\begin{aligned} \mathbf{a}_1^\dagger \mathbf{a}_2 |n_1 n_2\rangle &= \sqrt{n_1+1} \sqrt{n_2} |n_1+1, n_2-1\rangle \Rightarrow \mathbf{s}_+ \begin{Bmatrix} j \\ m \end{Bmatrix} = \sqrt{j+m+1} \sqrt{j-m} \begin{Bmatrix} j \\ m+1 \end{Bmatrix} \\ \mathbf{a}_2^\dagger \mathbf{a}_1 |n_1 n_2\rangle &= \sqrt{n_1} \sqrt{n_2+1} |n_1-1, n_2+1\rangle \Rightarrow \mathbf{s}_- \begin{Bmatrix} j \\ m \end{Bmatrix} = \sqrt{j+m} \sqrt{j-m+1} \begin{Bmatrix} j \\ m-1 \end{Bmatrix} \end{aligned} \quad \left. \begin{aligned} \mathbf{a}_1^\dagger \mathbf{a}_1 |n_1 n_2\rangle &= n_1 |n_1 n_2\rangle \\ \mathbf{a}_2^\dagger \mathbf{a}_2 |n_1 n_2\rangle &= n_2 |n_1 n_2\rangle \end{aligned} \right\}$$



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$j=1$  vector  $\mathbf{s}_+$

$$D^1(\mathbf{s}_+) = D^1(\mathbf{s}_x + i\mathbf{s}_y) = \begin{pmatrix} \cdot & \frac{\sqrt{2}}{2} & \cdot \\ \frac{\sqrt{2}}{2} & \cdot & \frac{\sqrt{2}}{2} \\ \cdot & \frac{\sqrt{2}}{2} & \cdot \end{pmatrix} + i \begin{pmatrix} \cdot & -i\frac{\sqrt{2}}{2} & \cdot \\ i\frac{\sqrt{2}}{2} & \cdot & -i\frac{\sqrt{2}}{2} \\ \cdot & i\frac{\sqrt{2}}{2} & \cdot \end{pmatrix} = \begin{pmatrix} \cdot & \sqrt{2} & \cdot \\ 0 & \cdot & \sqrt{2} \\ \cdot & 0 & \cdot \end{pmatrix}$$

...and  $\mathbf{s}_z$

$$D^1(\mathbf{s}_z) = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$$

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$$|n_\uparrow n_\downarrow\rangle = \frac{(\mathbf{a}_\uparrow^\dagger)^{n_\uparrow} (\mathbf{a}_\downarrow^\dagger)^{n_\downarrow}}{\sqrt{n_\uparrow! n_\downarrow!}} |0 0\rangle = \frac{(\mathbf{a}_\uparrow^\dagger)^{j+m} (\mathbf{a}_\downarrow^\dagger)^{j-m}}{\sqrt{(j+m)! (j-m)!}} |0 0\rangle = |j, m\rangle$$

Oscillator  $\mathbf{a}^\dagger \mathbf{a}$  give  $\mathbf{s}_+$  and  $\mathbf{s}_-$  matrices.

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

$$\mathbf{a}_1^\dagger \mathbf{a}_2 |n_1 n_2\rangle = \sqrt{n_1+1} \sqrt{n_2} |n_1+1, n_2-1\rangle \Rightarrow \mathbf{s}_+ |j, m\rangle = \sqrt{j+m+1} \sqrt{j-m} |j, m+1\rangle$$

$$\mathbf{a}_2^\dagger \mathbf{a}_1 |n_1 n_2\rangle = \sqrt{n_1} \sqrt{n_2+1} |n_1-1, n_2+1\rangle \Rightarrow \mathbf{s}_- |j, m\rangle = \sqrt{j+m} \sqrt{j-m+1} |j, m-1\rangle$$

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

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

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

$$D^1(\mathbf{s}_Z) = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$$

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

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

$$D^{\frac{3}{2}}(\mathbf{s}_Z) = \begin{pmatrix} \frac{3}{2} & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{2} & \cdot & \cdot \\ \cdot & \cdot & -\frac{1}{2} & \cdot \\ \cdot & \cdot & \cdot & -\frac{3}{2} \end{pmatrix}$$

$U(2)$  boson oscillator states  $|n_1, n_2\rangle = R(3)$  spin or rotor states  $|j, m\rangle$

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

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

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

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

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

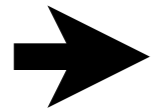
$$D^2(\mathbf{s}_Z) = \begin{pmatrix} 2 & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot & -1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & -2 \end{pmatrix}$$

Review : 2-D  $\mathfrak{su}(2)$  algebra of  $U(2)$  representations

Angular momentum generators by  $U(2)$  analysis

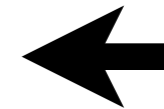
Angular momentum raise-n-lower operators  $\mathbf{s}_+$  and  $\mathbf{s}_-$

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



Angular momentum commutation relations

Key Lie theorems



Angular momentum magnitude and uncertainty

Angular momentum uncertainty angle

Generating  $R(3)$  rotation and  $U(2)$  representations

Applications of  $R(3)$  rotation and  $U(2)$  representations

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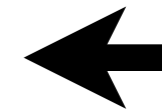
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*QED*

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*Q.E.D.*

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



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### General eigen-commutation theorem:

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

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

## Angular momentum commutation relations

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

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

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

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### 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:  $\mathbf{s}_- = \mathbf{e}_{21}$

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

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*Q.E.D.*

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

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U(2) Oscillator  
eigensolutions:

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

Review : 2-D  $\mathfrak{su}(2)$  algebra of  $U(2)$  representations

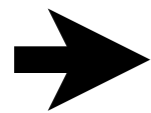
Angular momentum generators by  $U(2)$  analysis

Angular momentum raise-n-lower operators  $\mathbf{s}_+$  and  $\mathbf{s}_-$

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

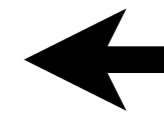
Angular momentum commutation relations

Key Lie theorems



Angular momentum magnitude and uncertainty

Angular momentum uncertainty angle



Generating  $R(3)$  rotation and  $U(2)$  representations

Applications of  $R(3)$  rotation and  $U(2)$  representations

Molecular and nuclear wavefunctions

Molecular and nuclear eigenstates

Generalized Stern-Gerlach and transformation matrices

Angular momentum cones and high  $J$  properties

*Angular momentum magnitude and uncertainty*

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

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

$$m = (n_1 - n_2)/2$$

R(3) angular quanta in  $n_1 = j + m$  and  $n_2 = j - m$  give R(3) eigenvalue formula.

$$\mathbf{s} \cdot \mathbf{s} \left| \begin{matrix} j \\ m \end{matrix} \right\rangle = \frac{1}{4} \left[ 2(j + m + 1)(j - m) + 2(j - m + 1)(j + m) + 4m^2 \right] \left| \begin{matrix} j \\ m \end{matrix} \right\rangle$$

$$n_1 = j + m$$

$$n_2 = j - m$$

Has very simple  $j$ -formula...

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

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

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

In terms of  $\mathbf{a}$ -operators the squared momentum operator is

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

Using  $\mathbf{a}_m \mathbf{a}_n^\dagger = \mathbf{a}_n^\dagger \mathbf{a}_m + \delta_{mn} \mathbf{1}$  gives  $\mathbf{s} \cdot \mathbf{s}$  as number operators.

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

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

Eigenvalue formula is then found. (Replace number-operator  $\mathbf{a}_k^\dagger \mathbf{a}_k$  with its number  $n_k$ )

$$\begin{aligned} \mathbf{s} \cdot \mathbf{s} |n_1 n_2\rangle &= \frac{1}{4} \left[ 2(n_2 + 1)n_1 + 2(n_1 + 1)n_2 + (n_1 - n_2)(n_1 - n_2) \right] |n_1 n_2\rangle \\ &= \frac{1}{4} \left[ 2n_1 + 2n_2 + 4n_1 n_2 + (n_1 - n_2)(n_1 - n_2) \right] |n_1 n_2\rangle \end{aligned}$$

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

$$m = (n_1 - n_2)/2$$

R(3) angular quanta in  $n_1 = j + m$  and  $n_2 = j - m$  give R(3) eigenvalue formula.

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$$n_1 = j + m$$

$$n_2 = j - m$$

Has very simple  $j$ -formula...

# 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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U(2) eigenvalue formula is then found.

$$\begin{aligned} \mathbf{s} \cdot \mathbf{s} |n_1 n_2\rangle &= \frac{1}{4} \left[ 2(n_2 + 1)n_1 + 2(n_1 + 1)n_2 + (n_1 - n_2)(n_1 - n_2) \right] |n_1 n_2\rangle \\ &= \frac{1}{4} \left[ 2n_1 + 2n_2 + 4n_1 n_2 + (n_1 - n_2)(n_1 - n_2) \right] |n_1 n_2\rangle \end{aligned}$$

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$$n_1 = j + m$$

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For Large  $j$ :

$$\text{Magnitude of angular momentum } |\mathbf{s}| \text{ approaches } j + 1/2: |\mathbf{s}| \left| \begin{smallmatrix} j \\ m \end{smallmatrix} \right\rangle = \sqrt{\mathbf{s} \cdot \mathbf{s}} \left| \begin{smallmatrix} j \\ m \end{smallmatrix} \right\rangle = \sqrt{j(j + 1)} \left| \begin{smallmatrix} j \\ m \end{smallmatrix} \right\rangle \cong \left( j + \frac{1}{2} \right) \left| \begin{smallmatrix} j \\ m \end{smallmatrix} \right\rangle$$

Review : 2-D  $\mathfrak{a}^\dagger\mathfrak{a}$  algebra of  $U(2)$  representations

Angular momentum generators by  $U(2)$  analysis

Angular momentum raise-n-lower operators  $\mathbf{s}_+$  and  $\mathbf{s}_-$

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

Angular momentum commutation relations

Key Lie theorems

Angular momentum magnitude and uncertainty

Angular momentum uncertainty angle

Generating  $R(3)$  rotation and  $U(2)$  representations

Applications of  $R(3)$  rotation and  $U(2)$  representations

Molecular and nuclear wavefunctions

Molecular and nuclear eigenstates

Generalized Stern-Gerlach and transformation matrices

Angular momentum cones and high  $J$  properties

## *Angular momentum uncertainty angle*

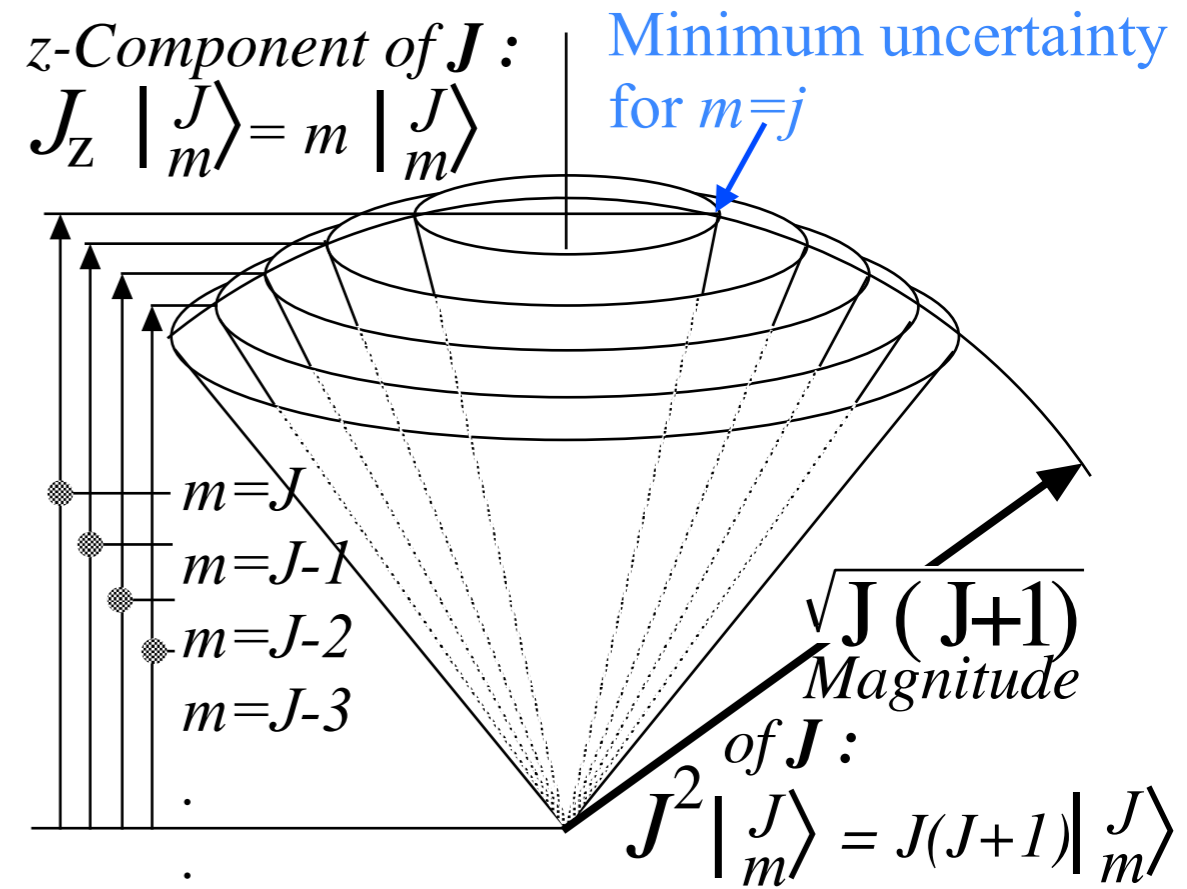
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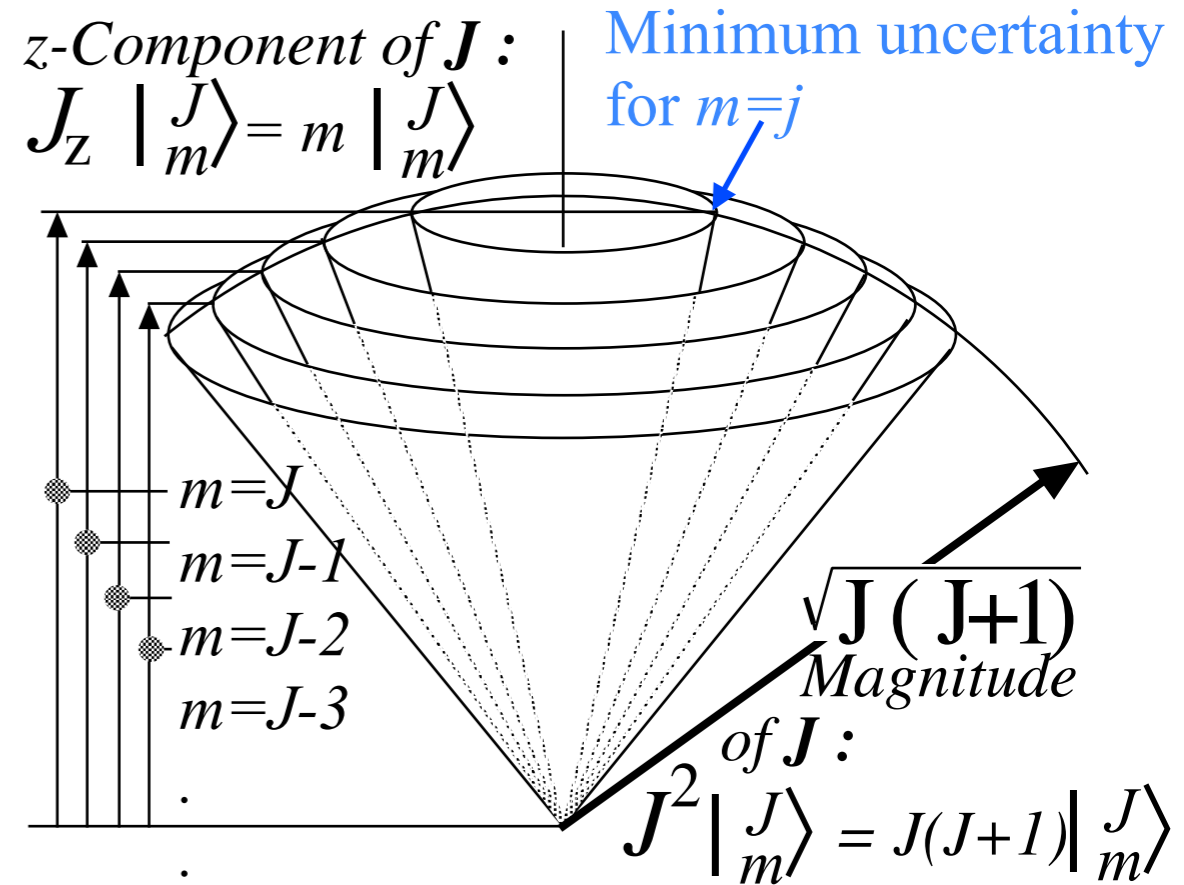




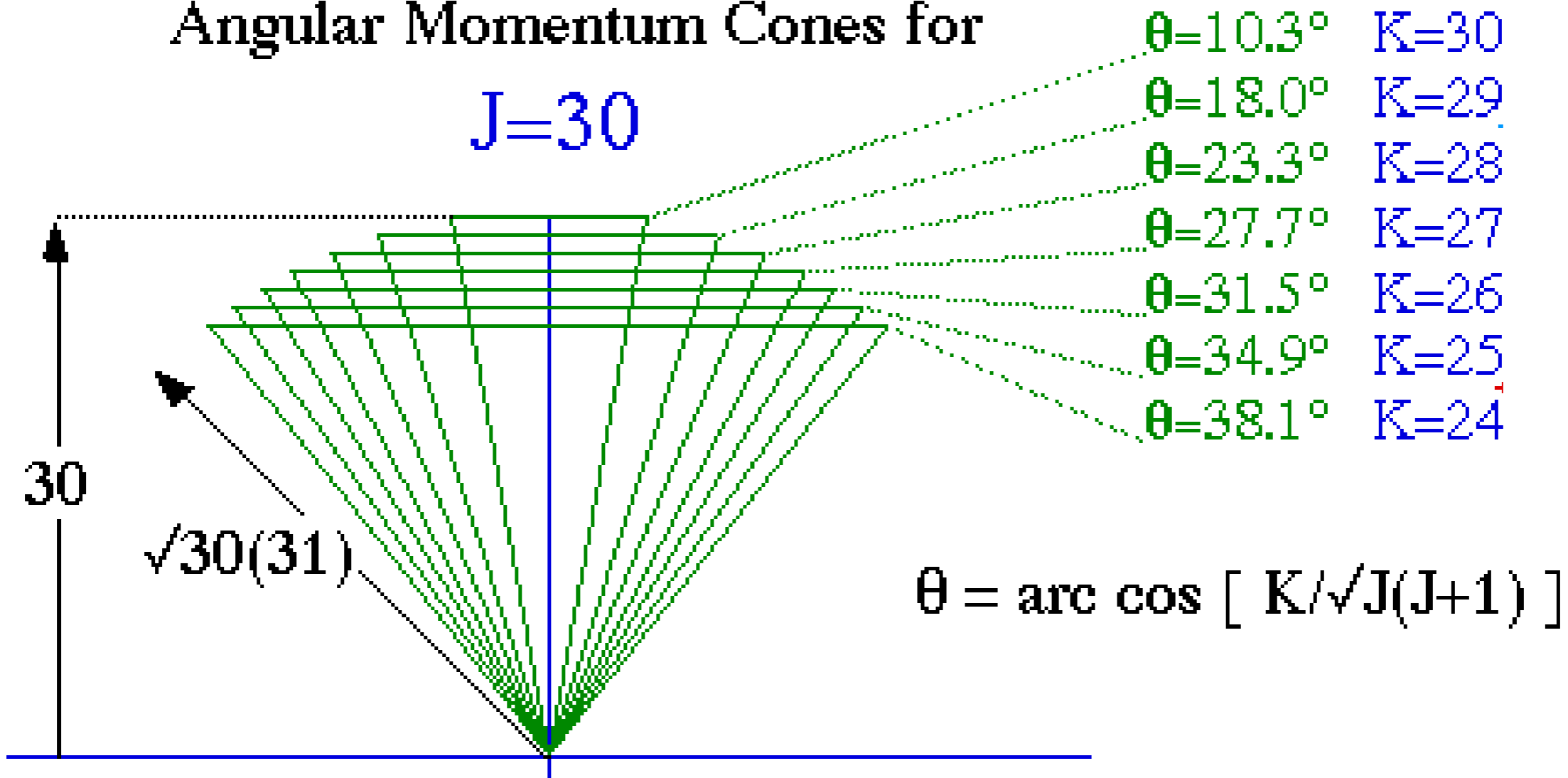
# Angular momentum uncertainty angle

The *angular momentum uncertainty angle*  $\Theta_m^j$  is given by:

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## Angular Momentum Cones for J=30



Review : 2-D  $\mathfrak{a}^{\dagger}\mathfrak{a}$  algebra of  $U(2)$  representations

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➔ *Generating  $R(3)$  rotation and  $U(2)$  representations*

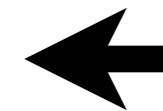
*Applications of  $R(3)$  rotation and  $U(2)$  representations*

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## Generating $R(3)$ rotation and $U(2)$ representations

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

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

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Corresponding transformation of the fundamental creation operators

$$\mathbf{a}_{1'}^\dagger = D_{11}^{1/2}(\alpha\beta\gamma)\mathbf{a}_1^\dagger + D_{21}^{1/2}(\alpha\beta\gamma)\mathbf{a}_2^\dagger = e^{-i\frac{\alpha+\gamma}{2}} \cos\frac{\beta}{2} \mathbf{a}_1^\dagger + e^{i\frac{\alpha-\gamma}{2}} \sin\frac{\beta}{2} \mathbf{a}_2^\dagger$$

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**Problem:** Find corresponding transformation  $D^{(j)}(\alpha\beta\gamma)$  matrix for a ( $\nu=2j$ )-oscillator state ( $\nu=2j$ )-quantum state is rotated to a new "prime" basis.

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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  $j+n-\ell = n-m+k$

$$= \frac{\sum_{\ell} \sum_k \binom{j+n}{\ell} \binom{j-n}{k} (D_{11})^\ell (D_{21})^{j+n-\ell} (D_{12})^k (D_{22})^{j-n-k}}{\sqrt{(j+n)!(j-n)!} \ell!(j+n-\ell)!k!(j-n-k)!} (\mathbf{a}_1^\dagger)^{\ell+k} (\mathbf{a}_2^\dagger)^{2j-\ell-k} |00\rangle = \frac{\sum_m \sum_k \binom{j+n}{j+m-k} \binom{j-n}{n-m+k} (D_{11})^{j+m-k} (D_{21})^{n-m+k} (D_{12})^k (D_{22})^{j-n-k}}{\sqrt{(j+n)!(j-n)!} (j+m-k)!(n-m+k)!k!(j-n-k)!} (\mathbf{a}_1^\dagger)^{j+m} (\mathbf{a}_2^\dagger)^{j-m} |00\rangle$$

## Generating $R(3)$ rotation and $U(2)$ representations

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

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

Corresponding transformation of the fundamental creation operators

$$\mathbf{a}_{1'}^\dagger = D_{11}^{1/2}(\alpha\beta\gamma) \mathbf{a}_1^\dagger + D_{21}^{1/2}(\alpha\beta\gamma) \mathbf{a}_2^\dagger = e^{-i\frac{\alpha+\gamma}{2}} \cos \frac{\beta}{2} \mathbf{a}_1^\dagger + e^{i\frac{\alpha-\gamma}{2}} \sin \frac{\beta}{2} \mathbf{a}_2^\dagger$$

$$\mathbf{a}_{2'}^\dagger = D_{12}^{1/2}(\alpha\beta\gamma) \mathbf{a}_1^\dagger + D_{22}^{1/2}(\alpha\beta\gamma) \mathbf{a}_2^\dagger = -e^{-i\frac{\alpha-\gamma}{2}} \sin \frac{\beta}{2} \mathbf{a}_1^\dagger + e^{i\frac{\alpha+\gamma}{2}} \cos \frac{\beta}{2} \mathbf{a}_2^\dagger$$

**Problem:** Find corresponding transformation  $D^{(j)}(\alpha\beta\gamma)$  matrix for a ( $\nu=2j$ )-oscillator state ( $\nu=2j$ )-quantum state is rotated to a new "prime" basis.

$$\mathbf{R}(\alpha\beta\gamma) |j\rangle = \frac{(\mathbf{a}_{1'}^\dagger)^{j+n} (\mathbf{a}_{2'}^\dagger)^{j-n}}{\sqrt{(j+n)!(j-n)!}} |00\rangle = \frac{(D_{11}\mathbf{a}_1^\dagger + D_{21}\mathbf{a}_2^\dagger)^{j+n} (D_{21}\mathbf{a}_1^\dagger + D_{22}\mathbf{a}_2^\dagger)^{j-n}}{\sqrt{(j+n)!(j-n)!}} |00\rangle$$

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

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

And general  *$SU(2)$  irreducible representation for Euler angles  $(\alpha\beta\gamma)$* .

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

$k$ -sum limited by ( $-integer$ )! $=\infty$  and  $0!=1=1!$



Review : 2-D  $\mathfrak{su}(2)$  algebra of  $U(2)$  representations

Angular momentum generators by  $U(2)$  analysis

Angular momentum raise-n-lower operators  $\mathbf{s}_+$  and  $\mathbf{s}_-$

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

Angular momentum commutation relations

Key Lie theorems

Move to Lect. 25 for up-to-date graphics

Angular momentum magnitude and uncertainty

Angular momentum uncertainty angle

Generating  $R(3)$  rotation and  $U(2)$  representations

➔ Applications of  $R(3)$  rotation and  $U(2)$  representations ←

Molecular and nuclear wavefunctions

Molecular and nuclear eigenlevels

Generalized Stern-Gerlach and transformation matrices

Angular momentum cones and high  $J$  properties

## Applications of $R(3)$ rotation and $U(2)$ representations

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

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

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

*Move to Lect. 25 for up-to-date graphics*

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

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

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

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

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# Applications of $R(3)$ rotation and $U(2)$ representations

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## 3-D linear-circular polarization T-matrix.

$$\begin{pmatrix} \langle 1|1 \rangle_x & \langle 1|1 \rangle_y & \langle 1|1 \rangle_z \\ \langle 0|1 \rangle_x & \langle 0|1 \rangle_y & \langle 0|1 \rangle_z \\ \langle -1|1 \rangle_x & \langle -1|1 \rangle_y & \langle -1|1 \rangle_z \end{pmatrix} = \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \end{pmatrix}$$

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$$\begin{pmatrix} \langle 1|1 \rangle_x & \langle 1|1 \rangle_y & \langle 1|1 \rangle_z \\ \langle 0|1 \rangle_x & \langle 0|1 \rangle_y & \langle 0|1 \rangle_z \\ \langle -1|1 \rangle_x & \langle -1|1 \rangle_y & \langle -1|1 \rangle_z \end{pmatrix} = \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \end{pmatrix}$$

## Applying T-matrix:

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

# Applications of R(3) rotation and U(2) representations

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$$\begin{pmatrix} \langle 1|1 \rangle_x & \langle 1|1 \rangle_y & \langle 1|1 \rangle_z \\ \langle 0|1 \rangle_x & \langle 0|1 \rangle_y & \langle 0|1 \rangle_z \\ \langle -1|1 \rangle_x & \langle -1|1 \rangle_y & \langle -1|1 \rangle_z \end{pmatrix} = \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \end{pmatrix}$$

## Applying T-matrix:

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

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



# Applications of $R(3)$ rotation and $U(2)$ representations

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

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

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

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

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

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

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

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

## Dipole ( $j=\ell=1$ ) wave functions

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

$$D_{0,0}^{1*}(\phi, \theta) = \cos\theta = \frac{z}{r}$$

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

## 3-D linear-circular polarization T-matrix:

$$\begin{pmatrix} \langle 1|1 \rangle_x & \langle 1|1 \rangle_y & \langle 1|1 \rangle_z \\ \langle 0|1 \rangle_x & \langle 0|1 \rangle_y & \langle 0|1 \rangle_z \\ \langle -1|1 \rangle_x & \langle -1|1 \rangle_y & \langle -1|1 \rangle_z \end{pmatrix} = \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \end{pmatrix}$$

## Applying T-matrix:

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

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

$$\begin{pmatrix} D_{x,x}^1(\alpha\beta\gamma) & D_{x,y}^1 & D_{x,z}^1 \\ D_{y,x}^1 & D_{y,y}^1 & D_{y,z}^1 \\ D_{z,x}^1 & D_{z,y}^1 & D_{z,z}^1 \end{pmatrix} = \begin{pmatrix} \cos\alpha \cos\beta \cos\gamma - \sin\alpha \sin\gamma & -\cos\alpha \cos\beta \sin\gamma - \sin\alpha \cos\gamma & \cos\alpha \sin\beta \\ \sin\alpha \cos\beta \cos\gamma + \cos\alpha \sin\gamma & -\sin\alpha \cos\beta \sin\gamma + \cos\alpha \cos\gamma & \sin\alpha \sin\beta \\ -\cos\gamma \sin\beta & \sin\gamma \sin\beta & \cos\beta \end{pmatrix}$$

# Applications of $R(3)$ rotation and $U(2)$ representations

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

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

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

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

$$Y_0^1(\phi, \theta) = \sqrt{\frac{3}{4\pi}} \cos\theta$$

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

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

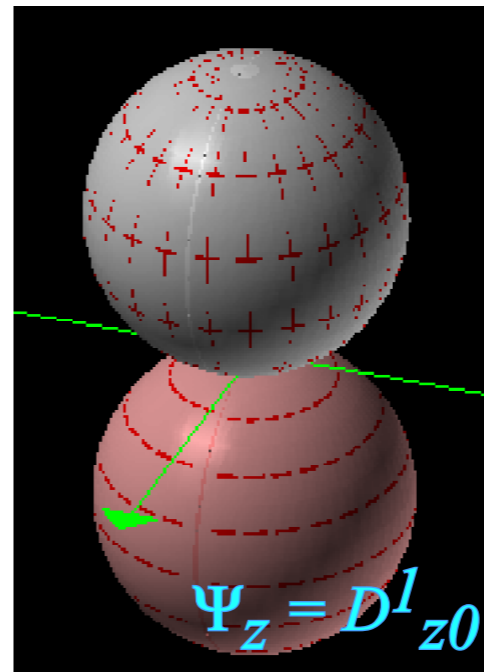
$$Y_m^\ell(\phi, \theta) = D_{m, n=0}^{\ell*}(\phi, \theta, 0) \sqrt{\frac{2\ell+1}{4\pi}}$$

## Dipole ( $j=\ell=1$ ) wave functions

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

$$D_{0,0}^{1*}(\phi, \theta) = \cos\theta = \frac{z}{r}$$

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

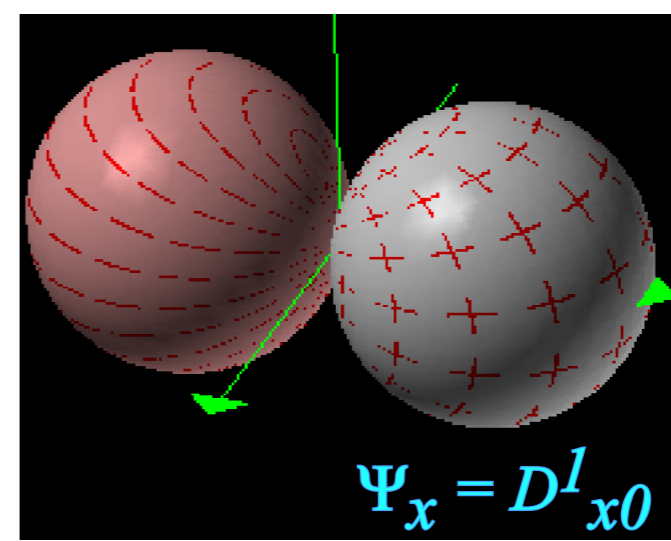
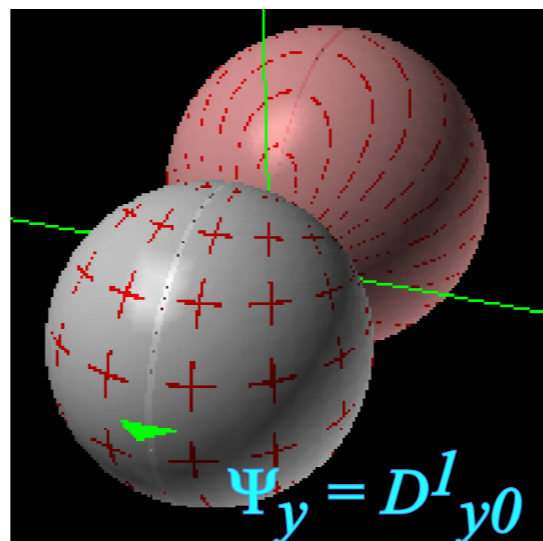


$j = 1$   
Standing  
 $p$ -Waves

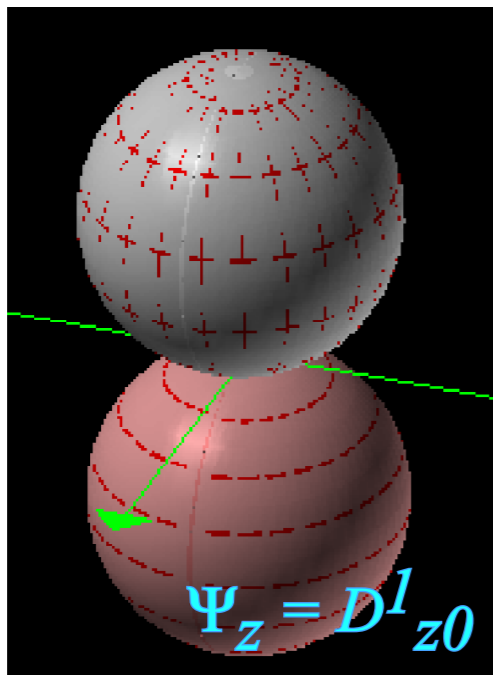
$$\Psi_x^1(\phi, \theta) = D_{x,z}^1(\phi, \theta, 0) = \cos\phi \sin\theta$$

$$\Psi_y^1(\phi, \theta) = D_{y,z}^1(\phi, \theta, 0) = \sin\phi \sin\theta$$

$$\Psi_z^1(\phi, \theta) = D_{z,z}^1(\phi, \theta, 0) = \cos\theta$$

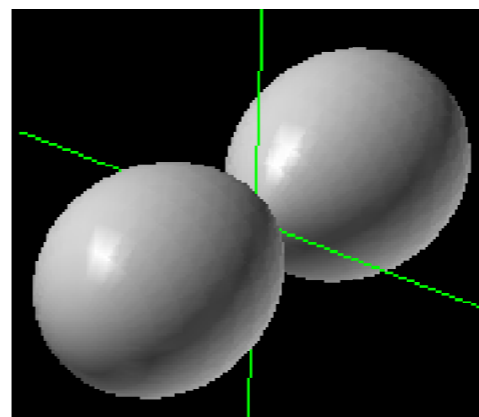


[QuantIt web simulation: Visualizing D representations](#)

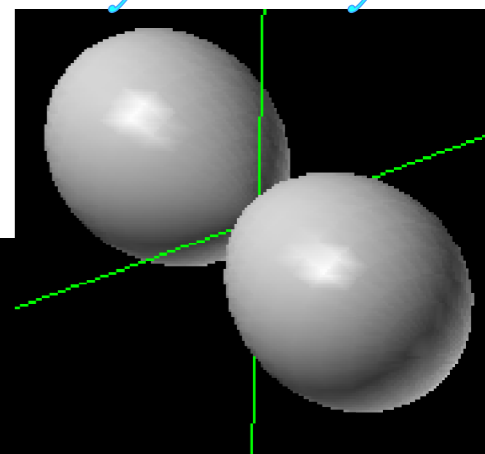


$j = 1$   
Standing  
 $p$ -Waves

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

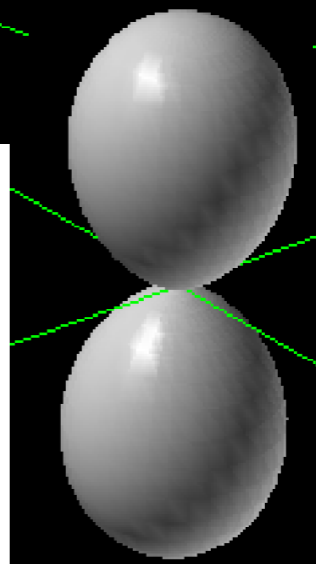


$$|\Psi_y|^2 = |D^1_{y0}|^2$$



Standing  $p$ -Wave  
Distributions

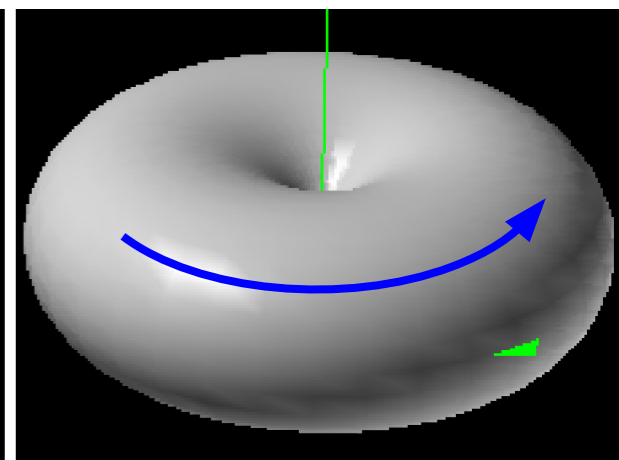
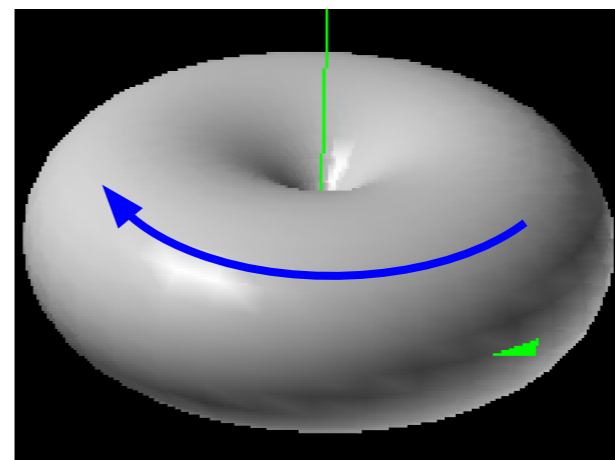
$$|\Psi_z|^2 = |D^1_{z0}|^2$$



Moving  $p$ -Wave  
Distributions

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

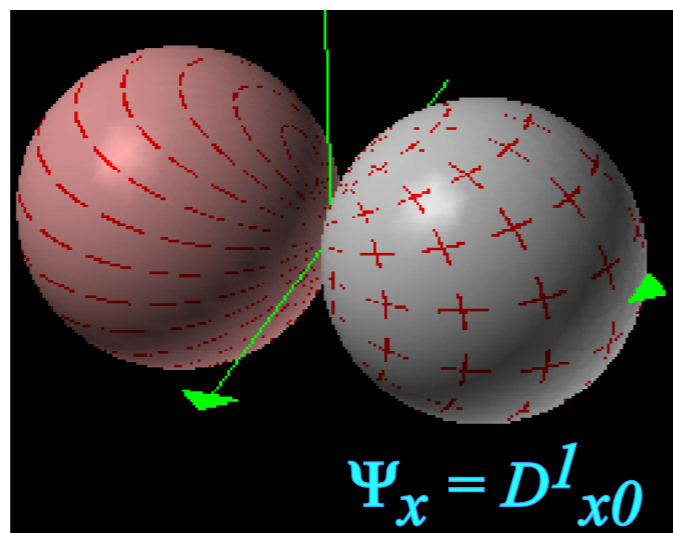
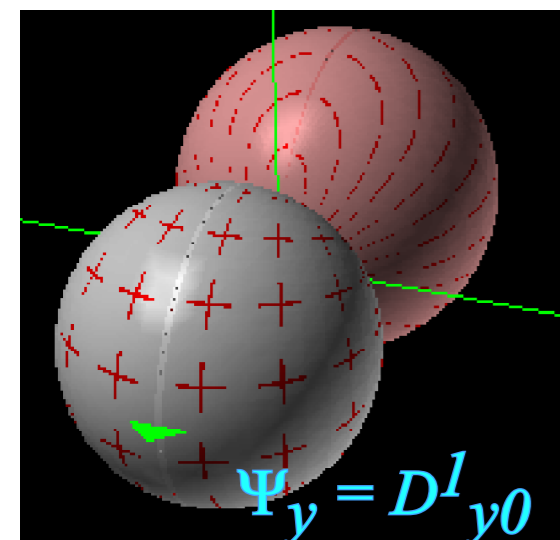
$$|\Psi_1|^2 = |D^1_{10}|^2$$



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

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

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



## Applications of $R(3)$ rotation and $U(2)$ representations

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

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

# Applications of $R(3)$ rotation and $U(2)$ representations

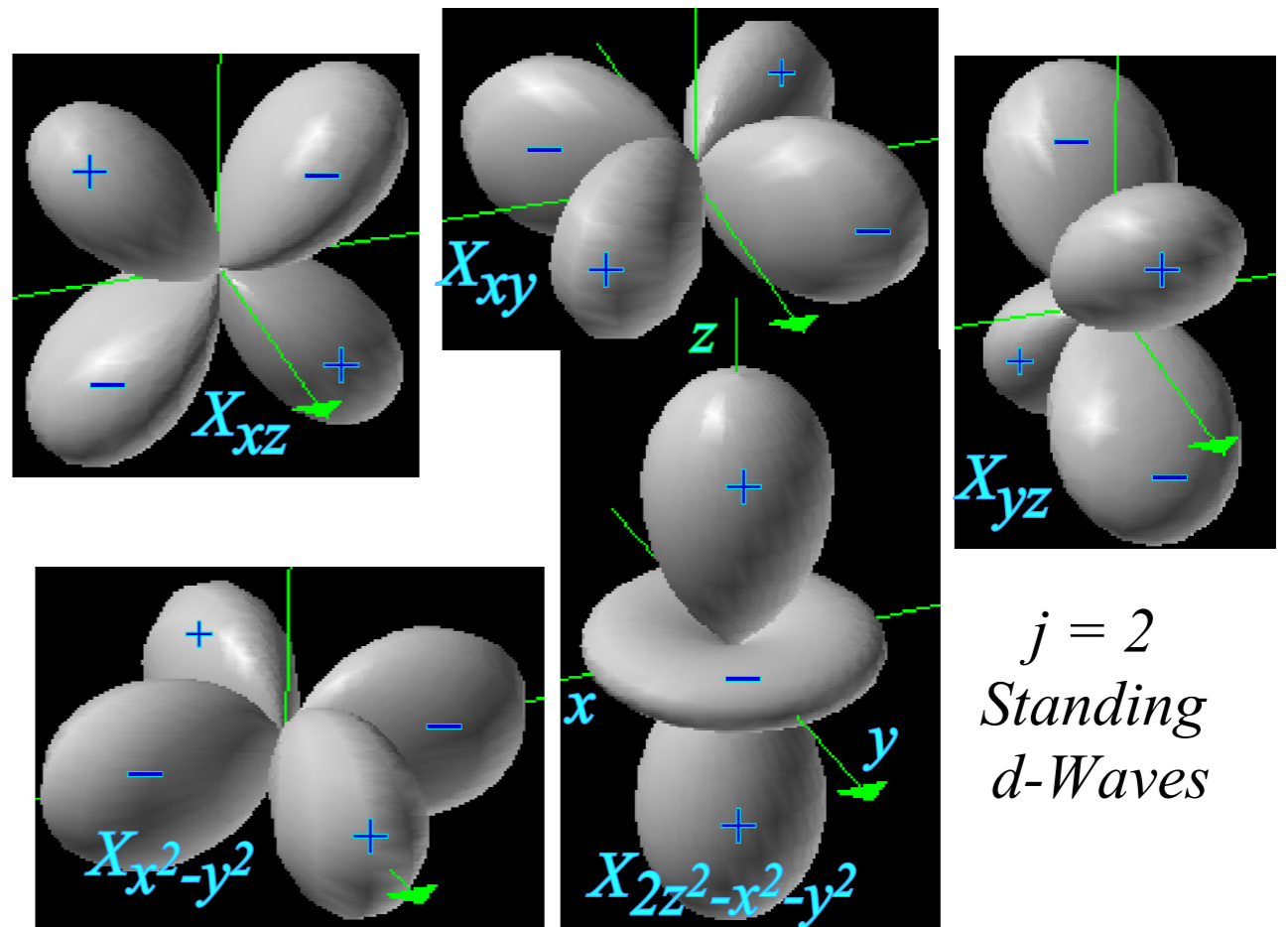
## Tensor ( $j=\ell=2$ ) representation

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

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

$$\begin{aligned} \sqrt{4\pi/5} Y_{m=2}^{\ell=2}(\phi\theta) &= D_{2,0}^{2*}(\phi\theta 0) = \sqrt{\frac{3}{8}} e^{i2\phi} \sin^2\theta = \sqrt{\frac{3}{8}} \frac{(x+iy)^2}{r^2} \\ \sqrt{4\pi/5} Y_{m=1}^{\ell=2}(\phi\theta) &= D_{1,0}^{2*}(\phi\theta 0) = -\sqrt{\frac{3}{2}} e^{i\phi} \sin\theta \cos\theta = -\sqrt{\frac{3}{2}} \frac{(x+iy)z}{r^2} \\ \sqrt{4\pi/5} Y_{m=0}^{\ell=2}(\phi\theta) &= D_{0,0}^{2*}(\phi\theta 0) = \frac{3\cos^2\theta-1}{2} = \frac{3z^2-r^2}{2r^2} \\ \sqrt{4\pi/5} Y_{m=-1}^{\ell=2}(\phi\theta) &= D_{-1,0}^{2*}(\phi\theta 0) = \sqrt{\frac{3}{2}} e^{-i\phi} \sin\theta \cos\theta = \sqrt{\frac{3}{2}} \frac{(x-iy)z}{r^2} \\ \sqrt{4\pi/5} Y_{m=-2}^{\ell=2}(\phi\theta) &= D_{-2,0}^{2*}(\phi\theta 0) = \sqrt{\frac{3}{8}} e^{-i2\phi} \sin^2\theta = \sqrt{\frac{3}{8}} \frac{(x-iy)^2}{r^2} \end{aligned}$$

$$X_q^k = r^k D_{q,0}^{k*} = \sqrt{\frac{4\pi}{2k+1}} r^k Y_q^k$$



$j = 2$   
Standing  
 $d$ -Waves

[QuantIt web simulation:](#)  
[Visualizing  \$D\$  representations](#)

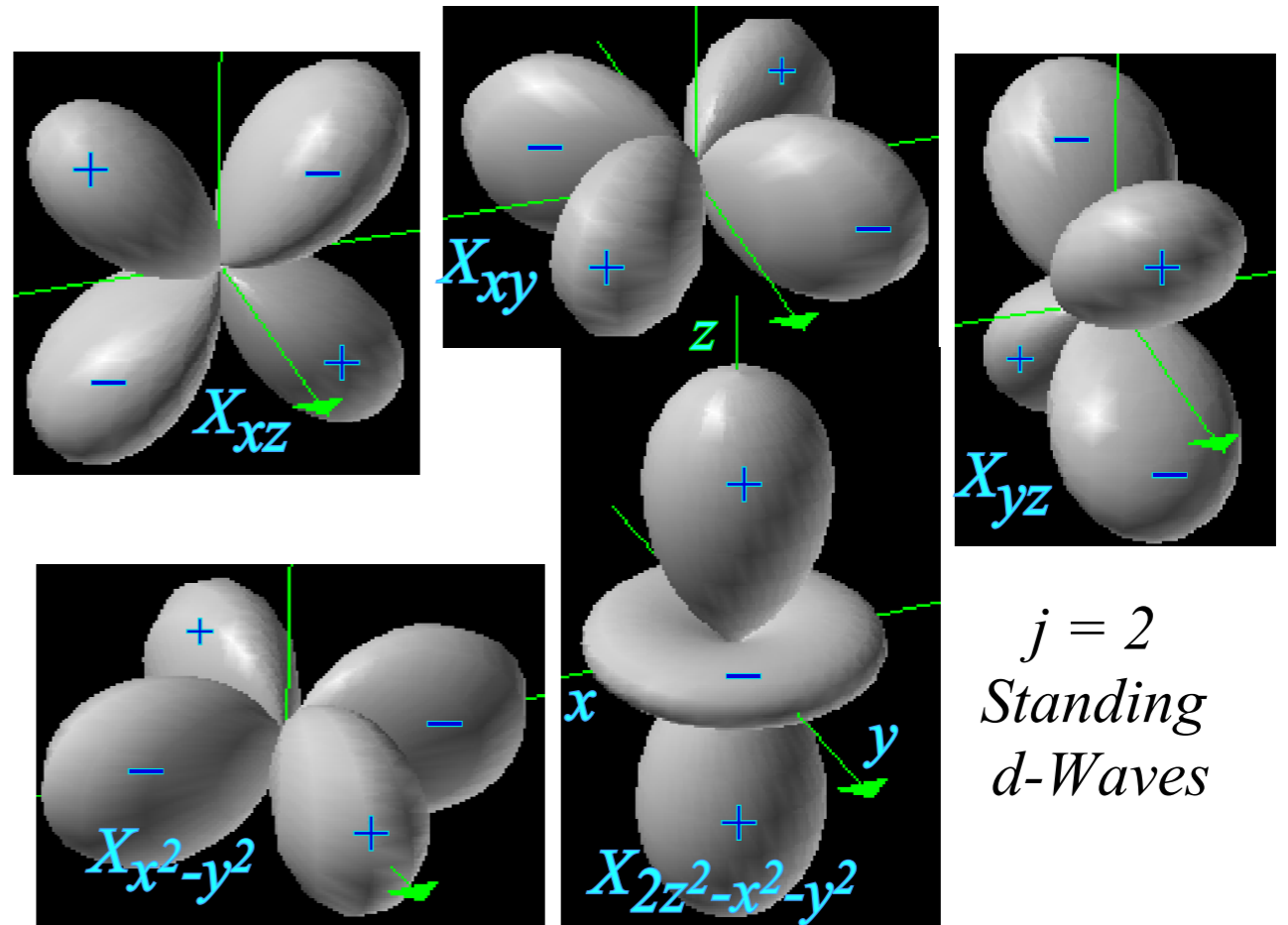
# Applications of $R(3)$ rotation and $U(2)$ representations

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

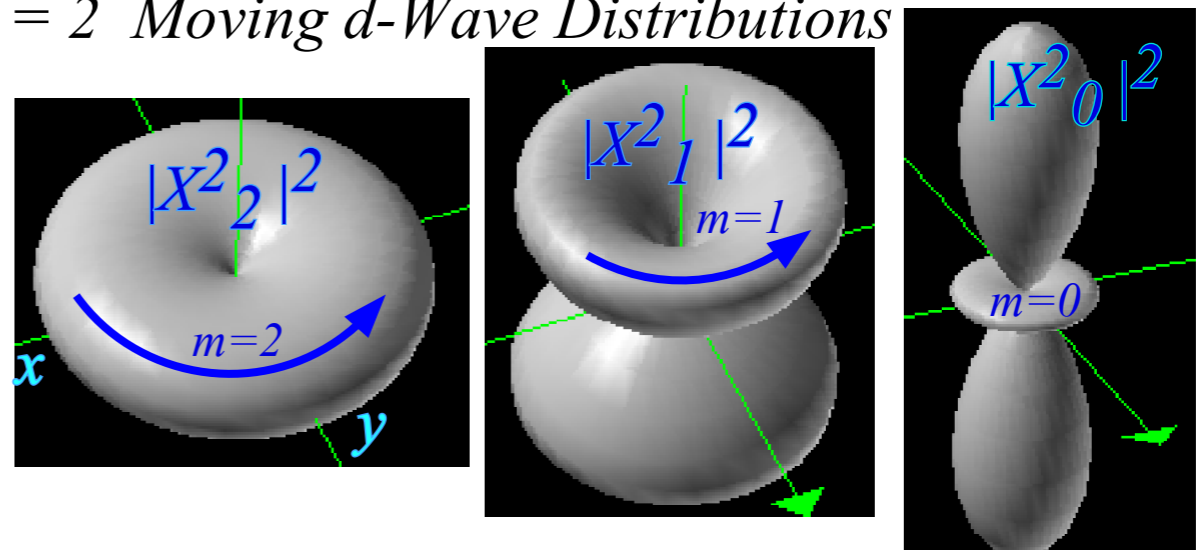
Spherical  $2^k$ -multipole functions  $X_q^k$  or  $X$ -functions are  $D^*$ -functions times the  $k^{\text{th}}$  power of radius ( $r^k$ ).

$$\begin{aligned} \sqrt{4\pi/5} Y_{m=2}^{\ell=2}(\phi\theta) &= D_{2,0}^{2*}(\phi\theta) = \sqrt{\frac{3}{8}} e^{i2\phi} \sin^2 \theta &= \sqrt{\frac{3}{8}} \frac{(x+iy)^2}{r^2} \\ \sqrt{4\pi/5} Y_{m=1}^{\ell=2}(\phi\theta) &= D_{1,0}^{2*}(\phi\theta) = -\sqrt{\frac{3}{2}} e^{i\phi} \sin \theta \cos \theta &= -\sqrt{\frac{3}{2}} \frac{(x+iy)z}{r^2} \\ \sqrt{4\pi/5} Y_{m=0}^{\ell=2}(\phi\theta) &= D_{0,0}^{2*}(\phi\theta) = \frac{3\cos^2 \theta - 1}{2} &= \frac{3z^2 - r^2}{2r^2} \\ \sqrt{4\pi/5} Y_{m=-1}^{\ell=2}(\phi\theta) &= D_{-1,0}^{2*}(\phi\theta) = \sqrt{\frac{3}{2}} e^{-i\phi} \sin \theta \cos \theta &= \sqrt{\frac{3}{2}} \frac{(x-iy)z}{r^2} \\ \sqrt{4\pi/5} Y_{m=-2}^{\ell=2}(\phi\theta) &= D_{-2,0}^{2*}(\phi\theta) = \sqrt{\frac{3}{8}} e^{-i2\phi} \sin^2 \theta &= \sqrt{\frac{3}{8}} \frac{(x-iy)^2}{r^2} \end{aligned}$$

$$X_q^k = r^k D_{q,0}^{k*} = \sqrt{\frac{4\pi}{2k+1}} r^k Y_q^k$$



## $j = 2$ Moving $d$ -Wave Distributions



Review : 2-D  $\mathfrak{su}(2)$  algebra of  $U(2)$  representations

Angular momentum generators by  $U(2)$  analysis

Angular momentum raise-n-lower operators  $\mathbf{s}_+$  and  $\mathbf{s}_-$

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

Angular momentum commutation relations

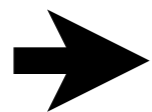
Key Lie theorems

Angular momentum magnitude and uncertainty

Angular momentum uncertainty angle

Generating  $R(3)$  rotation and  $U(2)$  representations

Applications of  $R(3)$  rotation and  $U(2)$  representations

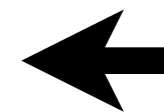


Molecular and nuclear wavefunctions

Molecular and nuclear eigenlevels

Generalized Stern-Gerlach and transformation matrices

Angular momentum cones and high  $J$  properties



## *Applications of $R(3)$ rotation and $U(2)$ representations*

### *Molecular and nuclear wavefunctions*

For  $SU(2)$  and  $R(3)$ , sum over rotations is an integral over Euler angles  $(\alpha\beta\gamma)$ .

For integral- $j=0, 1, 2,..$  the  $R(3)$  integral over polar angle  $\beta$  ranges from 0 to  $\pi$ .

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



## Applications of $R(3)$ rotation and $U(2)$ representations

### Molecular and nuclear wavefunctions

For  $SU(2)$  and  $R(3)$ , sum over rotations is an integral over Euler angles  $(\alpha\beta\gamma)$ .

For integral- $j=0, 1, 2,..$  the  $R(3)$  integral over polar angle  $\beta$  ranges from 0 to  $\pi$ .

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Same applies to the generators  $\mathbf{s}_Z$  or  $\mathbf{J}_Z$  of  $SU(2)$  or  $R(3)$ .

$$\mathbf{s}_Z |j_{m,n}\rangle = m |j_{m,n}\rangle \quad \bar{\mathbf{s}}_Z |j_{m,n}\rangle = -n |j_{m,n}\rangle$$

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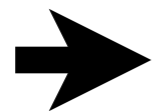
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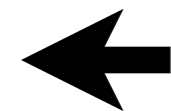
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*Applications of R(3) rotation and U(2) representations*

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The reversed sign is a nuisance, so let us define *reversed momentum operators* that give a positive sign.

$$\mathbf{s}_{\bar{Z}} \left| \begin{smallmatrix} j \\ m, n \end{smallmatrix} \right\rangle = +n \left| \begin{smallmatrix} j \\ m, n \end{smallmatrix} \right\rangle \quad \mathbf{s}_{\bar{Z}} = -\bar{\mathbf{s}}_Z$$



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$$\mathbf{H}_{\text{symmetric top}} = B\mathbf{J}_{\bar{X}}^2 + B\mathbf{J}_{\bar{Y}}^2 + A\mathbf{J}_{\bar{Z}}^2 \quad (\text{Molecular spin is labeled } \mathbf{J} \text{ instead of } \mathbf{s})$$

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Eigensolution equations:

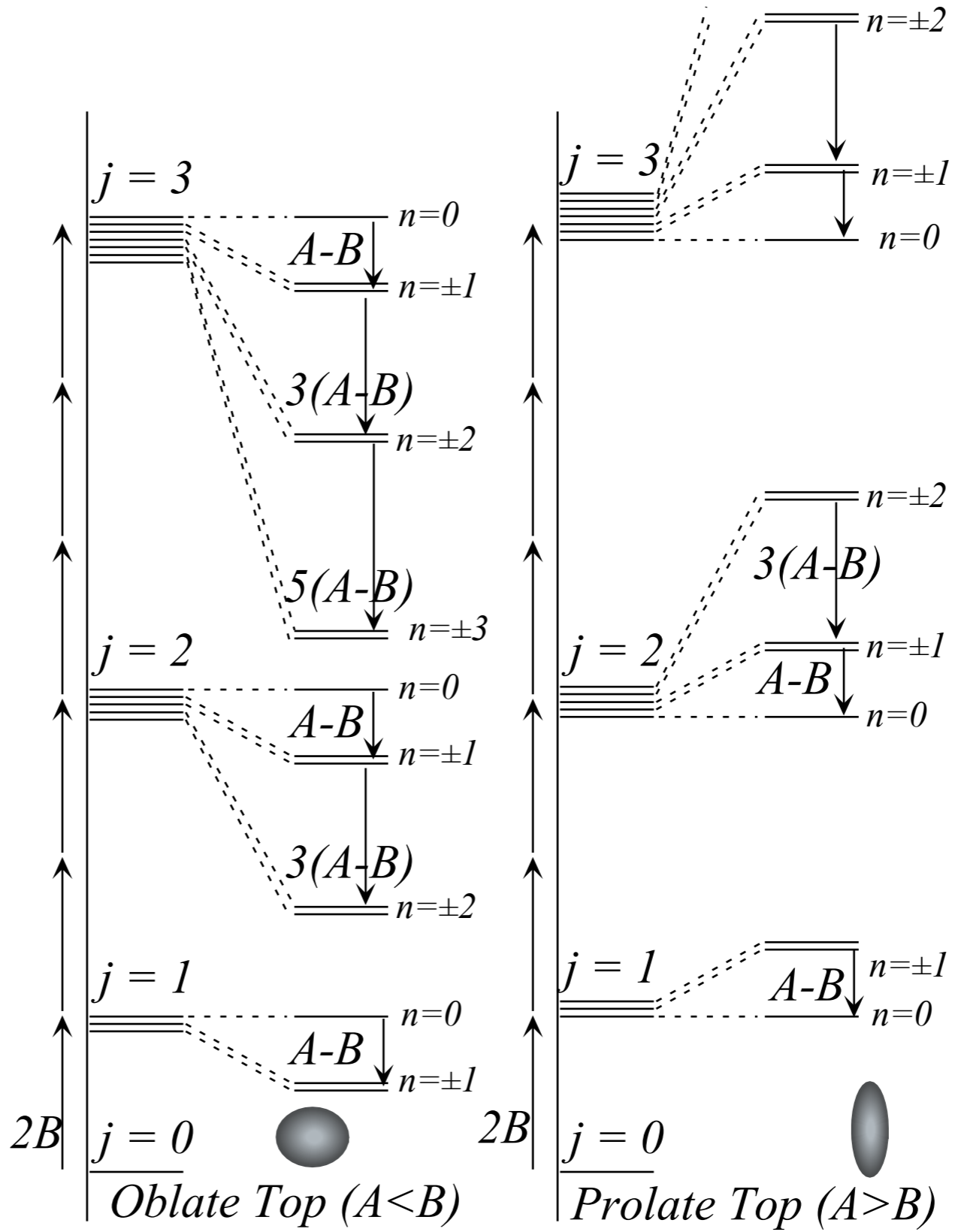
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Eigenvalue and energy level spectrum is shown next.

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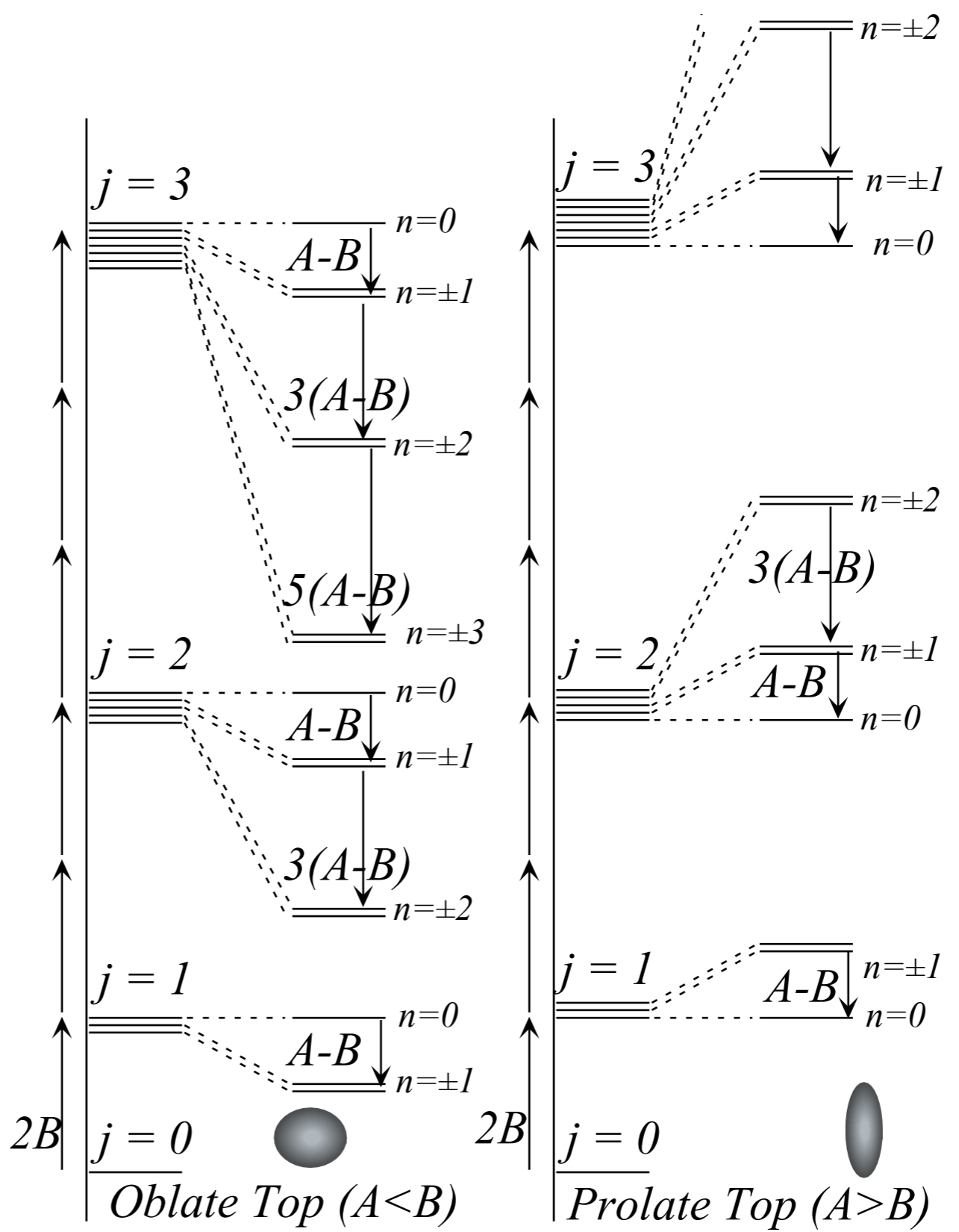


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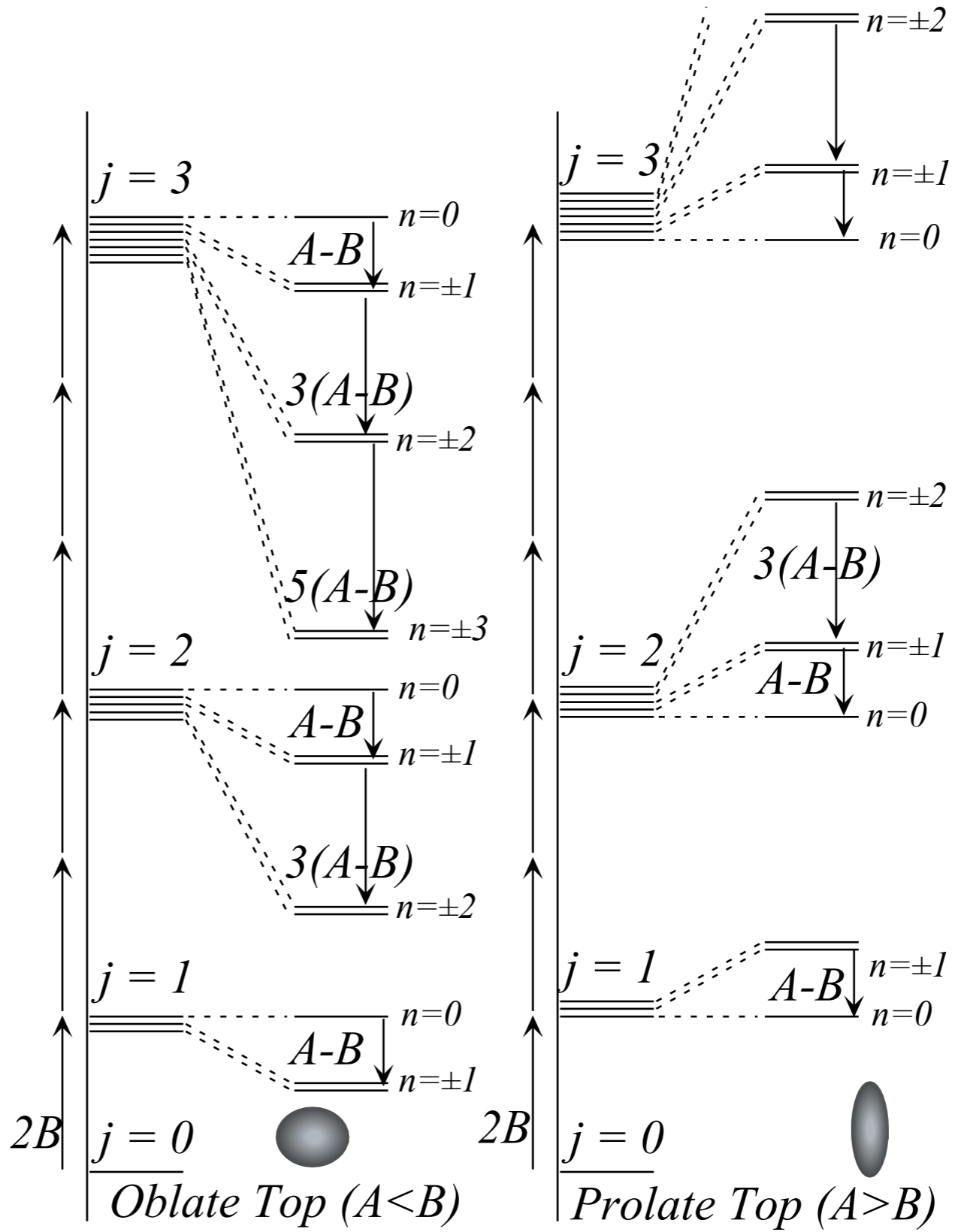
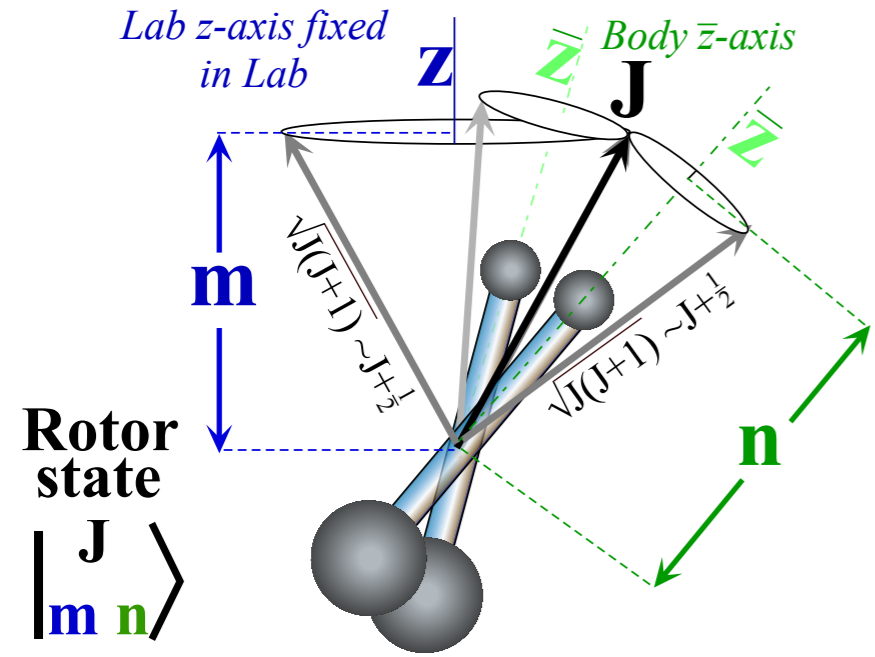


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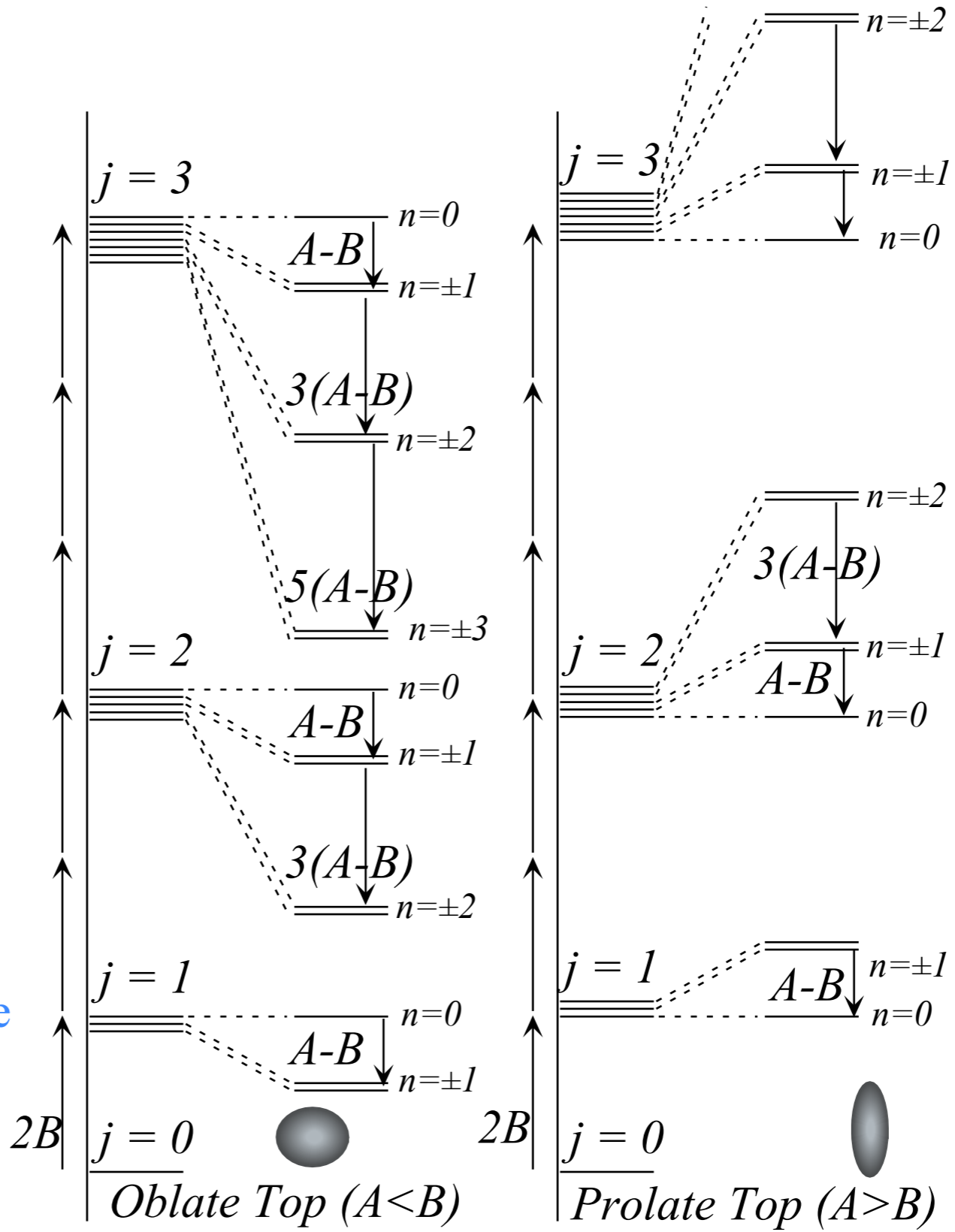
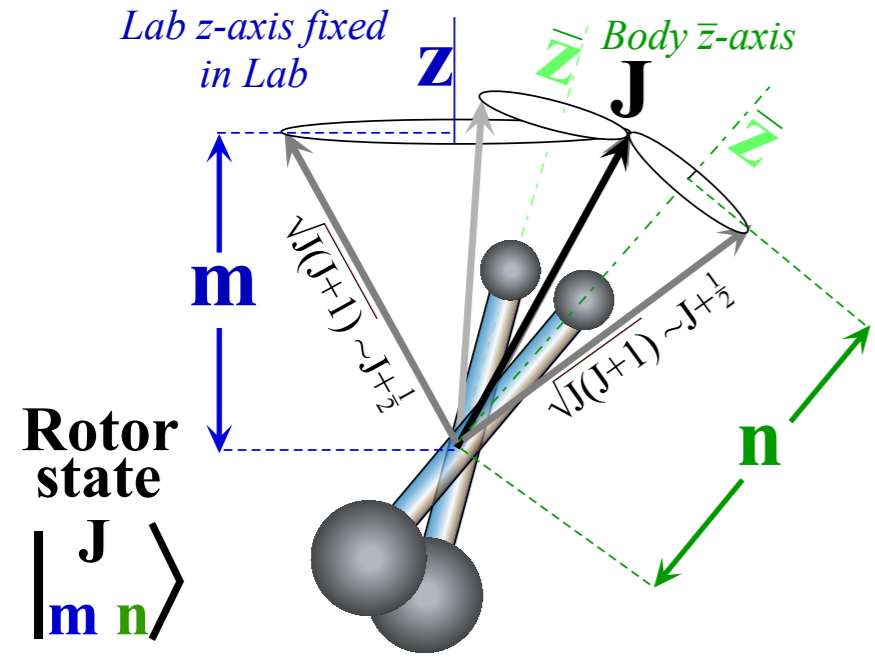


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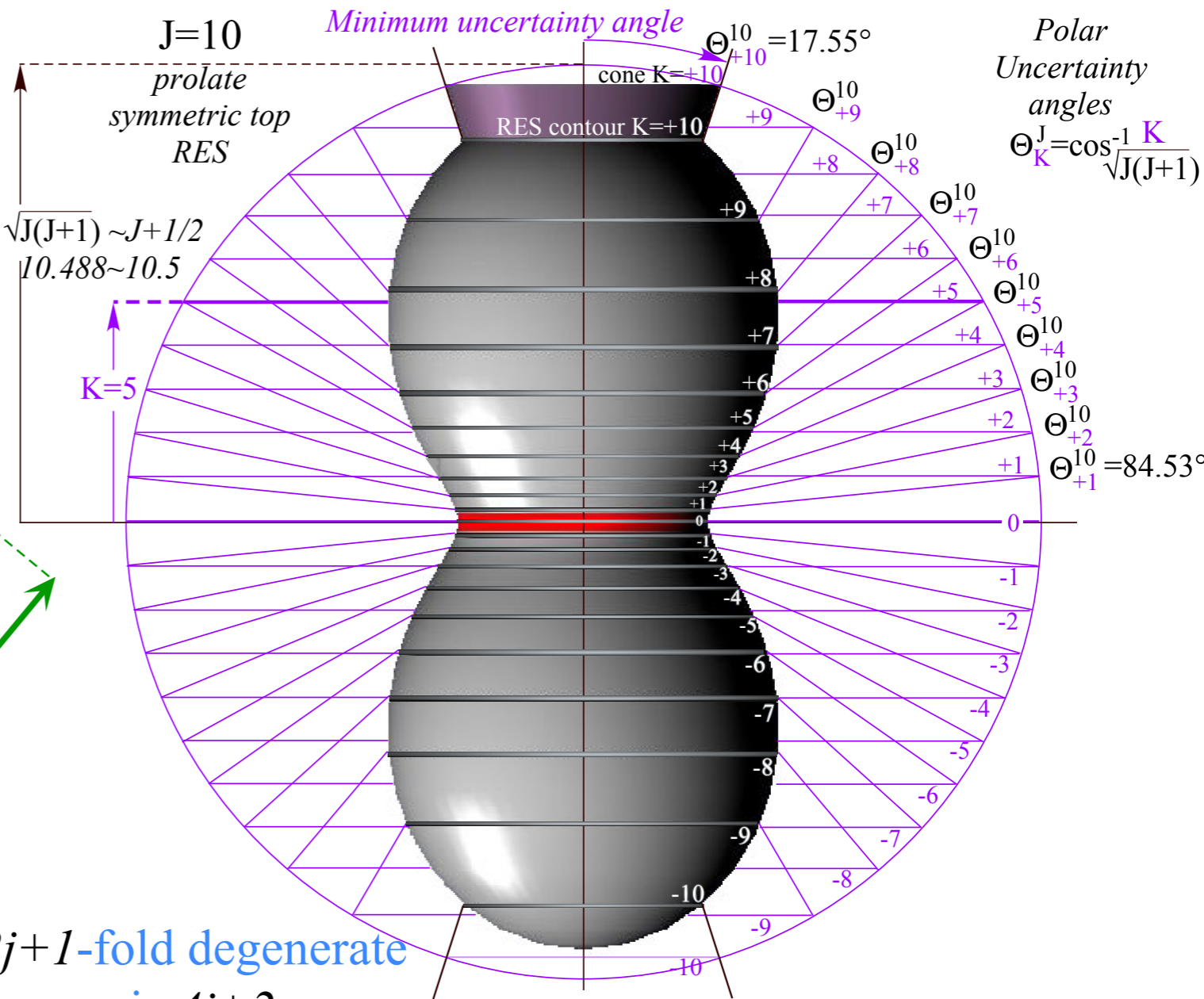
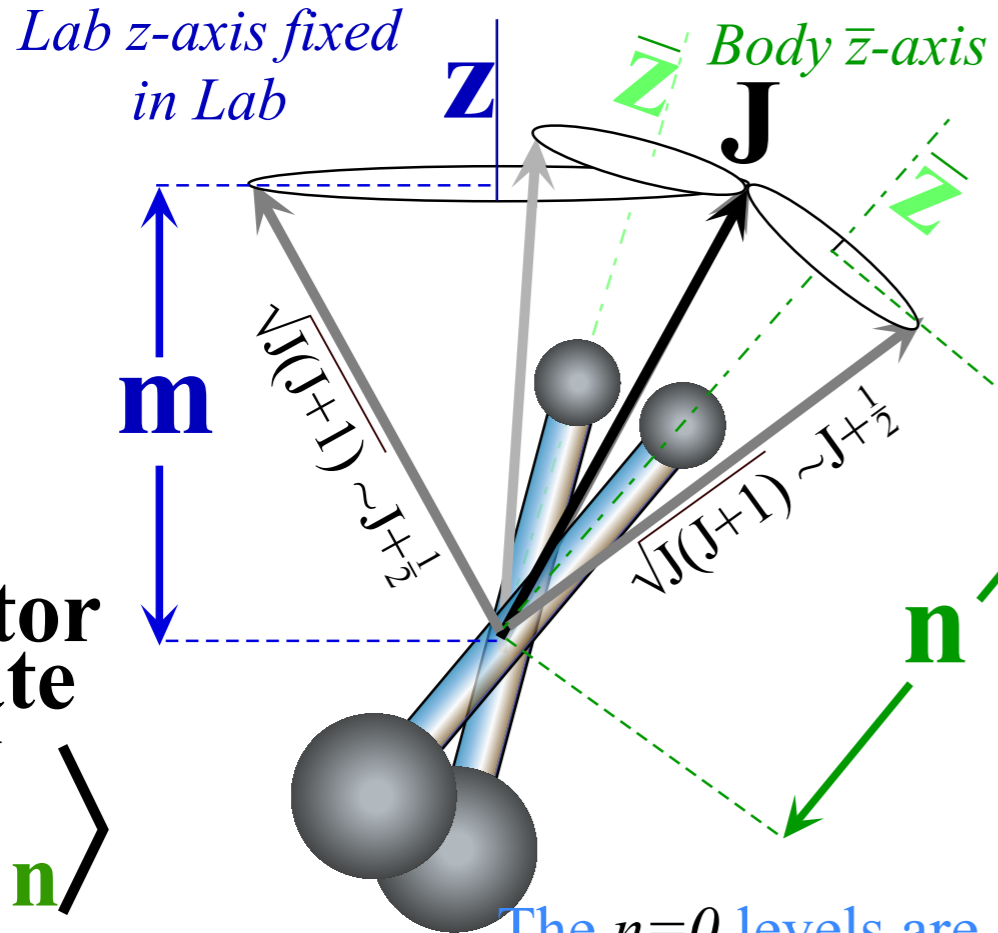
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$$T_0^0 = \mathbf{J} \cdot \mathbf{J} = \langle J \rangle^2 = (J_x^2 + J_y^2 + J_z^2),$$

$$T_0^2 = \frac{1}{2} \langle J \rangle^2 (3 \cos^2 \beta - 1) = \frac{1}{2} (2J_z^2 - J_x^2 - J_y^2),$$

$$H = B T_0^0 + \frac{2}{3} (A - B) T_0^2$$

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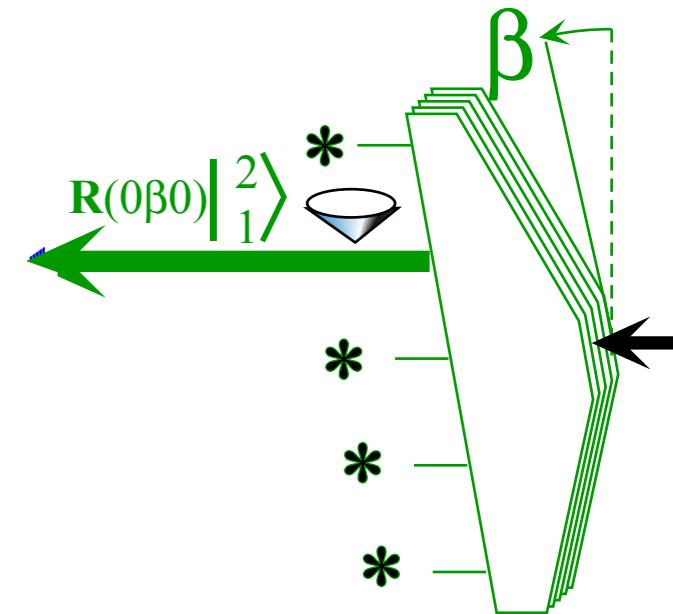
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*Applications of  $R(3)$  rotation and  $U(2)$  representations*

*Generalized Stern-Gerlach and transformation matrices*

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



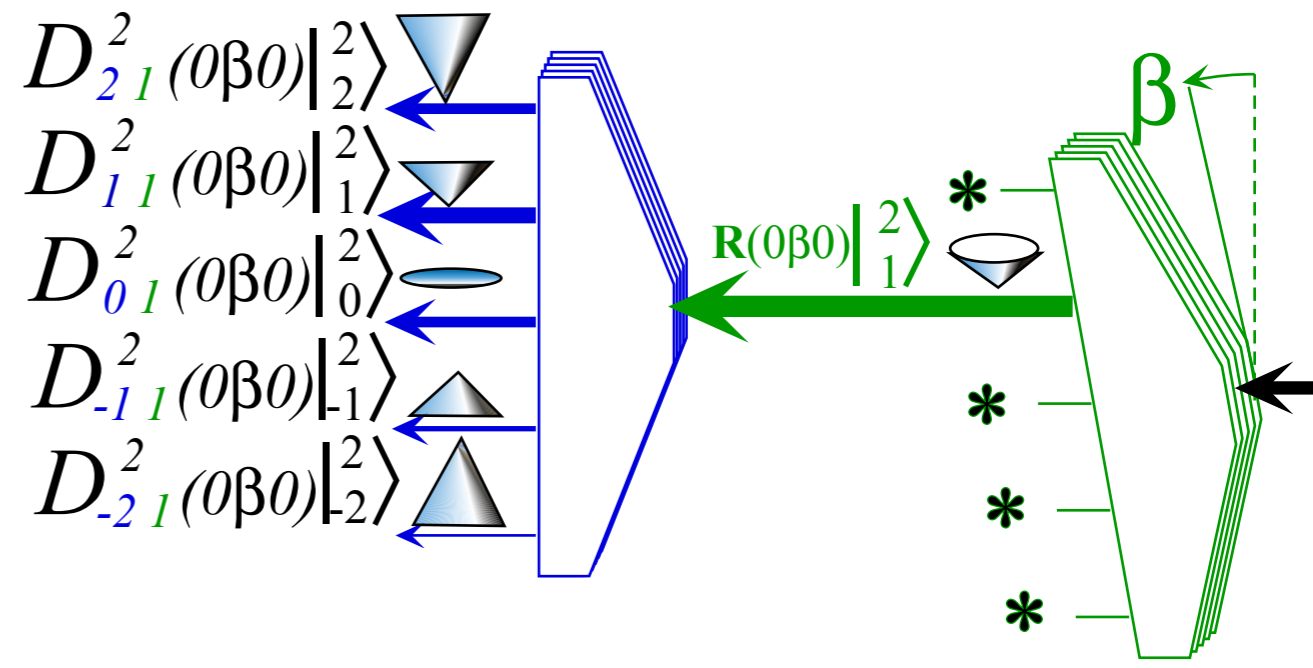
Applications of  $R(3)$  rotation and  $U(2)$  representations

Generalized Stern-Gerlach and transformation matrices

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

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

$$\begin{aligned} \mathbf{R}(0\beta 0) |^j_m\rangle &= \sum_{m'=-j}^j |^j_{m'}\rangle \langle^j_{m'} | \mathbf{R}(0\beta 0) |^j_m\rangle \\ &= \sum_{m'=-j}^j |^j_{m'}\rangle D^j_{m'm}(0\beta 0) \end{aligned}$$



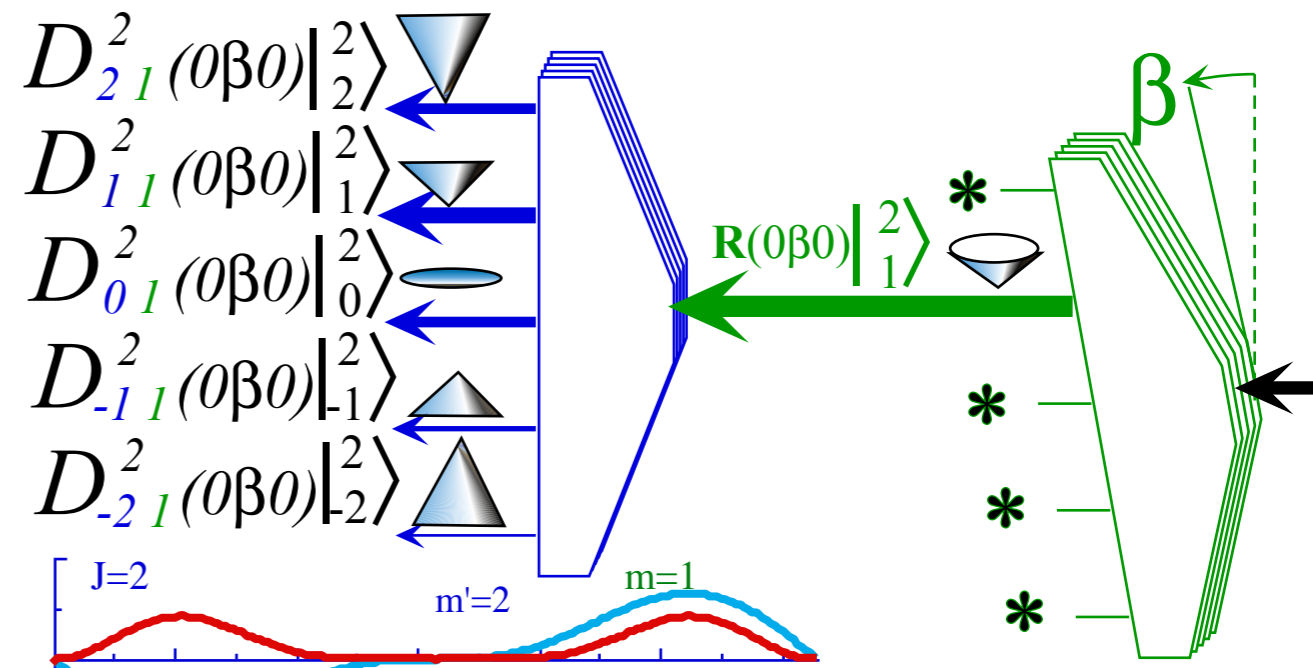
Applications of  $R(3)$  rotation and  $U(2)$  representations

Generalized Stern-Gerlach and transformation matrices

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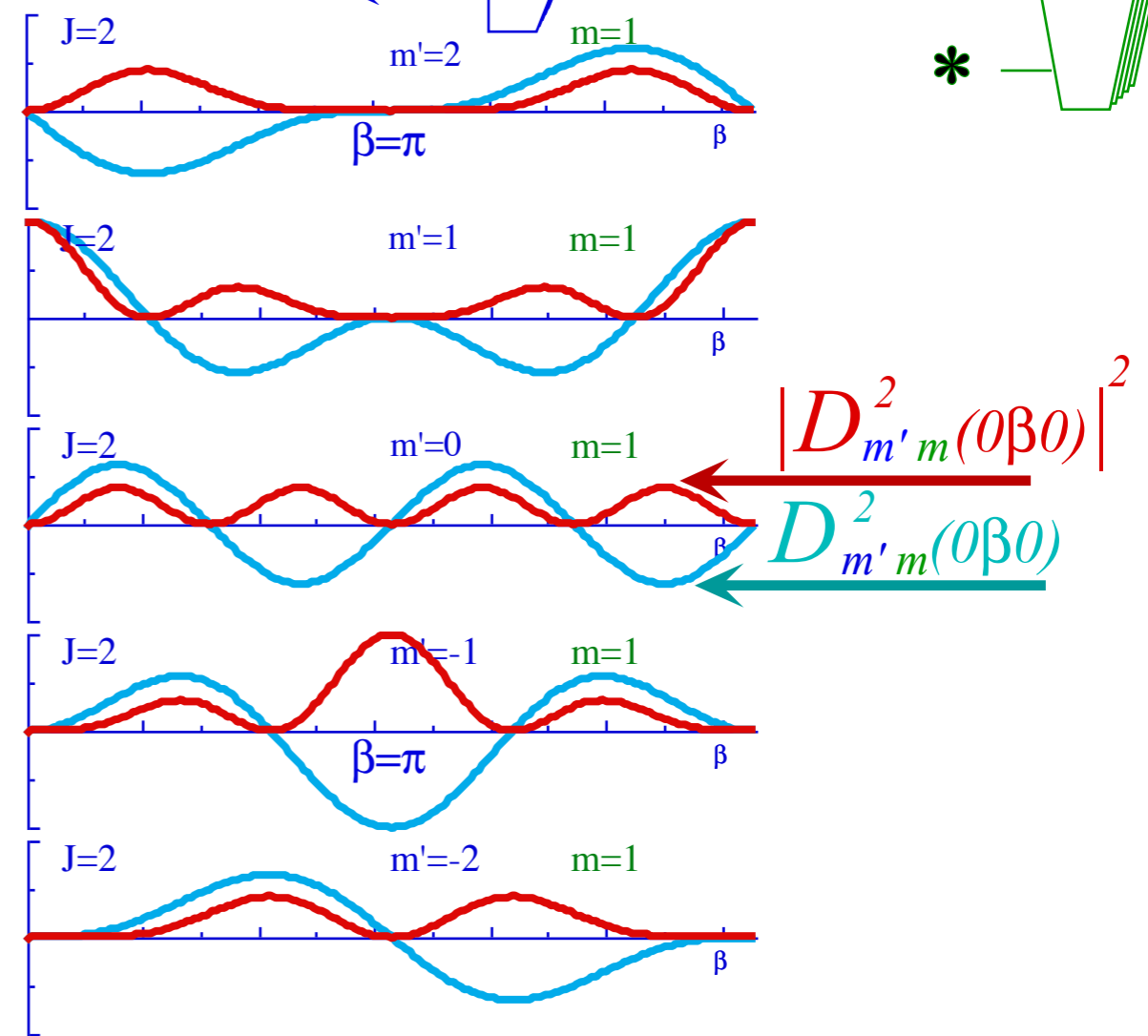
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Overlap of state  $\mathbf{R}(\alpha\beta\gamma) |^2_1\rangle$  with unrotated  $|^{j=2}_{m'}\rangle$  is the corresponding D-matrix element.

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



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

**Polarization analysis:** Suppose a spin- $j$  state  $\mathbf{R}(0\beta 0) |j^2_m\rangle$  exits an analyzer rotated by  $\beta$  and then enters a vertical ( $\beta=0$ ) analyzer that forces it to choose from unrotated states  $|j^2_{m'}\rangle$

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

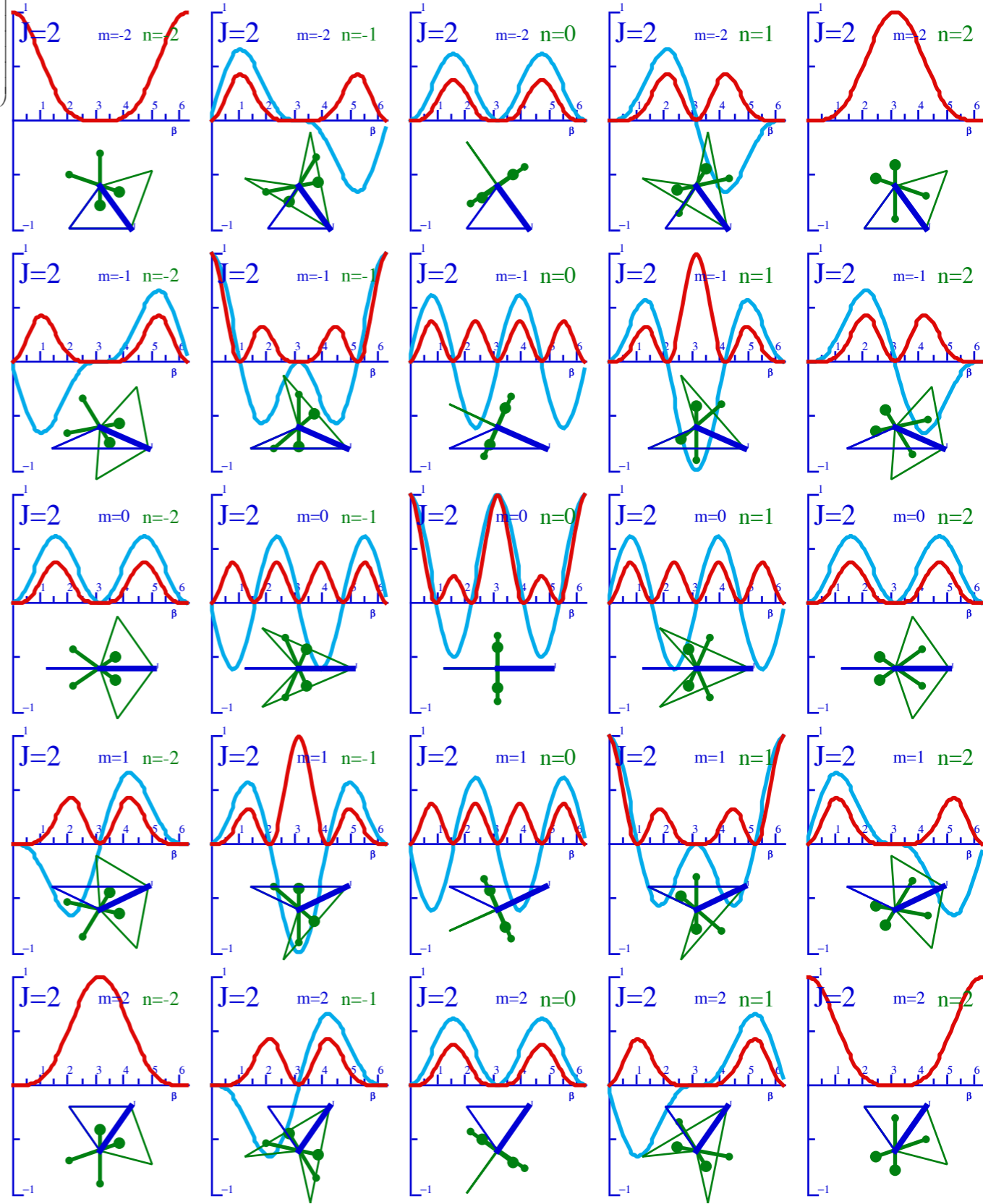
$$\begin{aligned} \mathbf{R}(0\beta 0) |j^2_m\rangle &= \sum_{m'=-j}^j |j^2_{m'}\rangle \langle j^2_{m'} | \mathbf{R}(0\beta 0) |j^2_m\rangle \\ &= \sum_{m'=-j}^j |j^2_{m'}\rangle D^j_{m'm}(0\beta 0) \end{aligned}$$

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

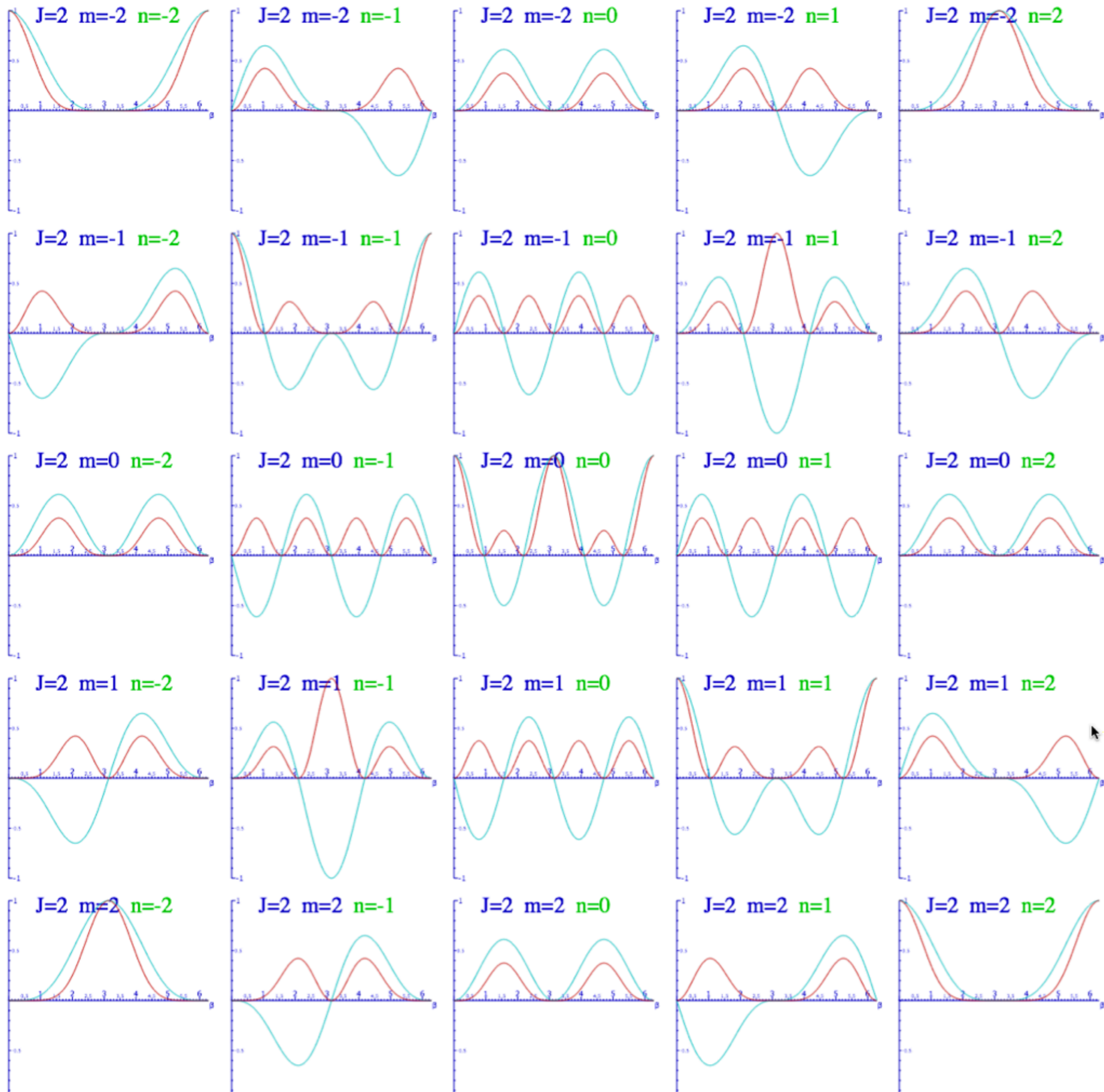
$$\langle j^2_{m'} | \mathbf{R}(\alpha\beta\gamma) |j^2_1\rangle = \delta^{j'2} D^2_{m'1}(\alpha\beta\gamma) = \langle j^2_{m'} | 1^2 \rangle_R$$

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

[QuantIt web simulation:](#)  
[Visualizing D representations](#)



$D_{m'n}^j(0\beta0)$   
 plotted  
 vs.  $\beta$   
 for fixed  
 $j, m', n$



Review : 2-D  $\mathfrak{su}(2)$  algebra of  $U(2)$  representations

Angular momentum generators by  $U(2)$  analysis

Angular momentum raise-n-lower operators  $\mathbf{s}_+$  and  $\mathbf{s}_-$

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

Angular momentum commutation relations

Key Lie theorems

Angular momentum magnitude and uncertainty

Angular momentum uncertainty angle

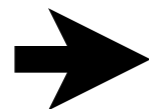
Generating  $R(3)$  rotation and  $U(2)$  representations

Applications of  $R(3)$  rotation and  $U(2)$  representations

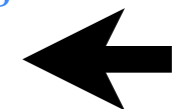
Molecular and nuclear wavefunctions

Molecular and nuclear eigenlevels

Generalized Stern-Gerlach and transformation matrices



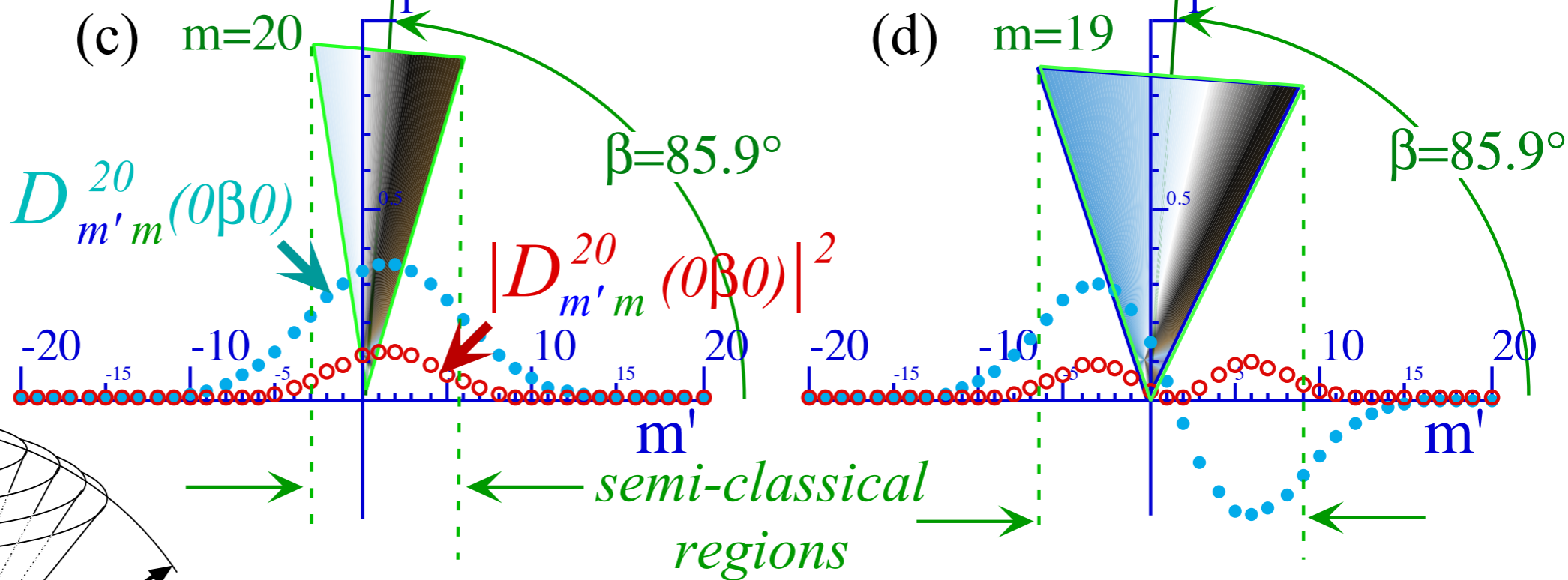
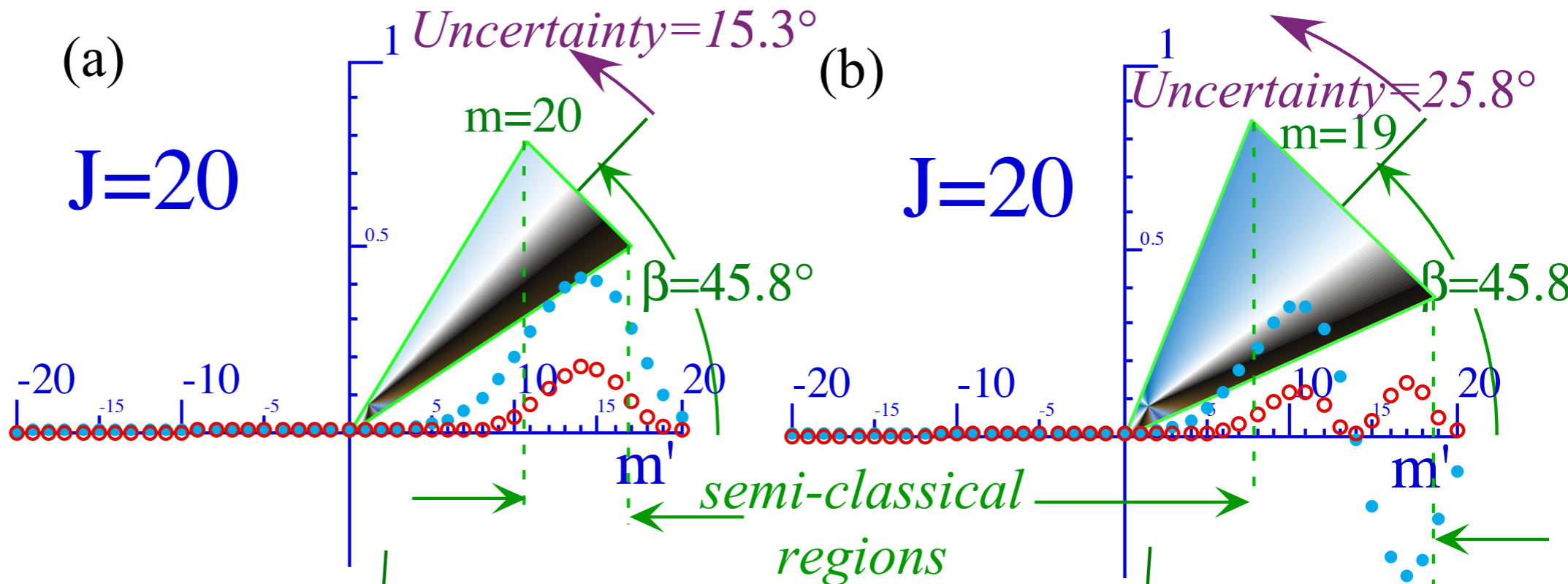
Angular momentum cones and high  $J$  properties



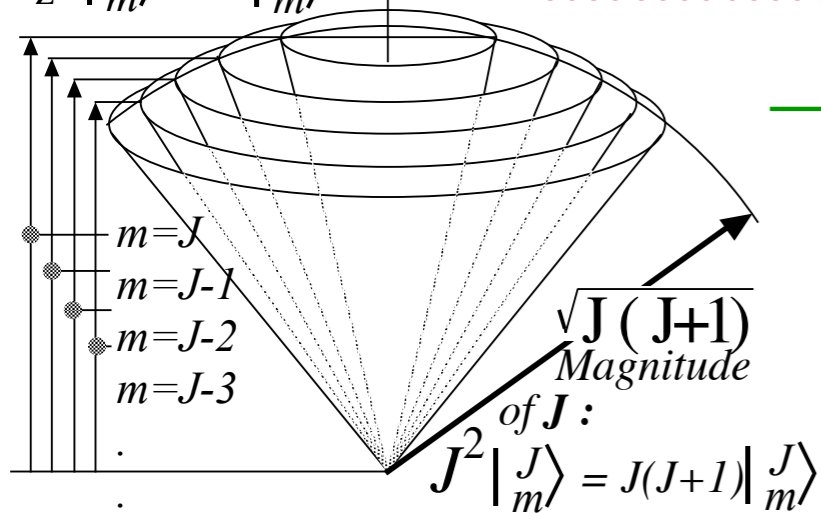


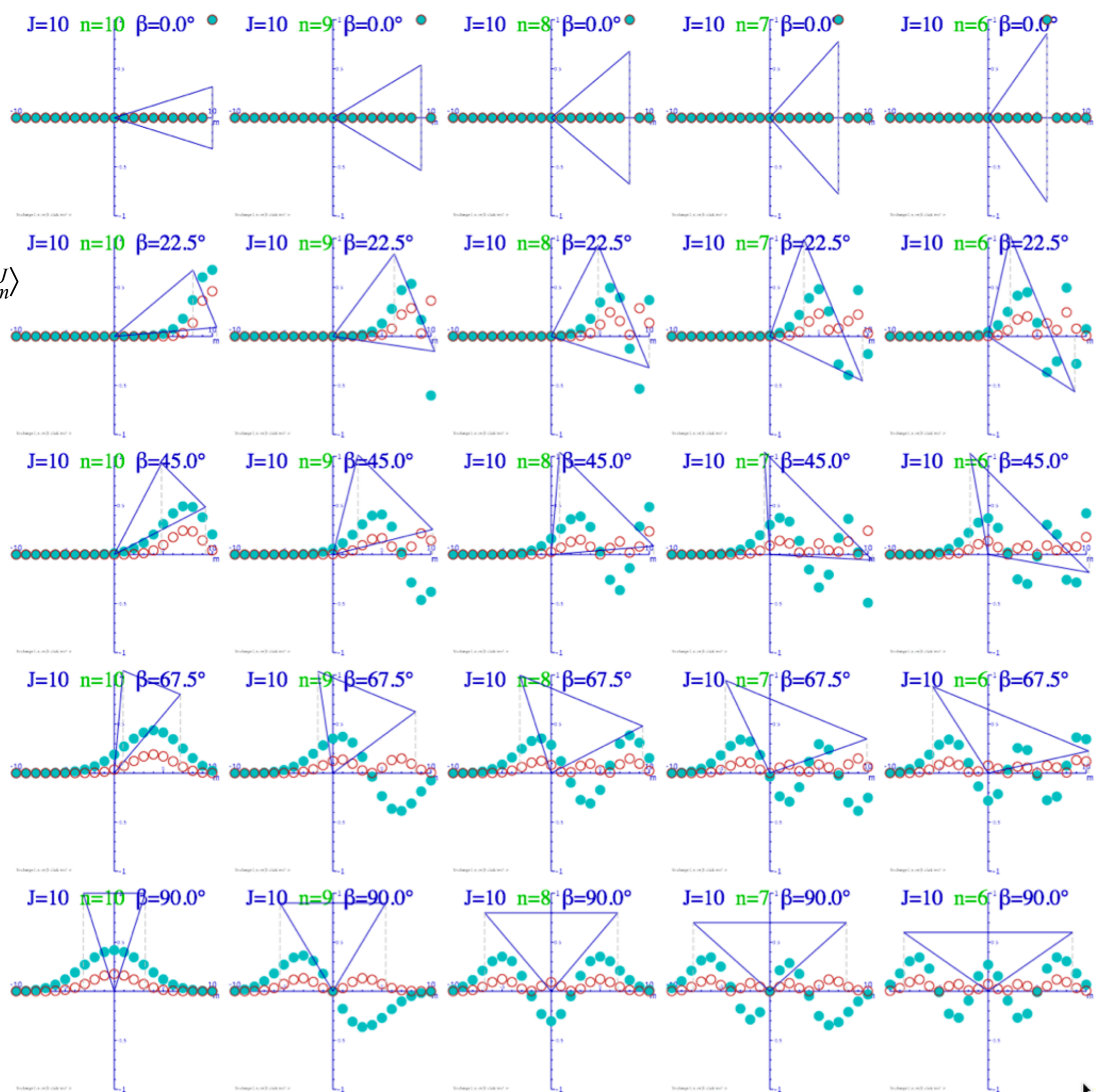
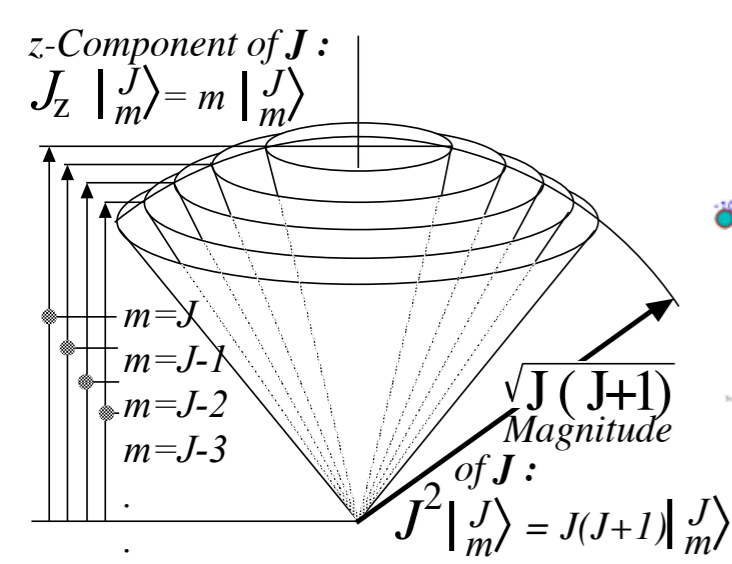
# Angular momentum cones and high $J$ properties

$D_{m'm}^J(0\beta0)$   
plotted  
vs.  $m'$   
for fixed  
 $J, \beta, m$

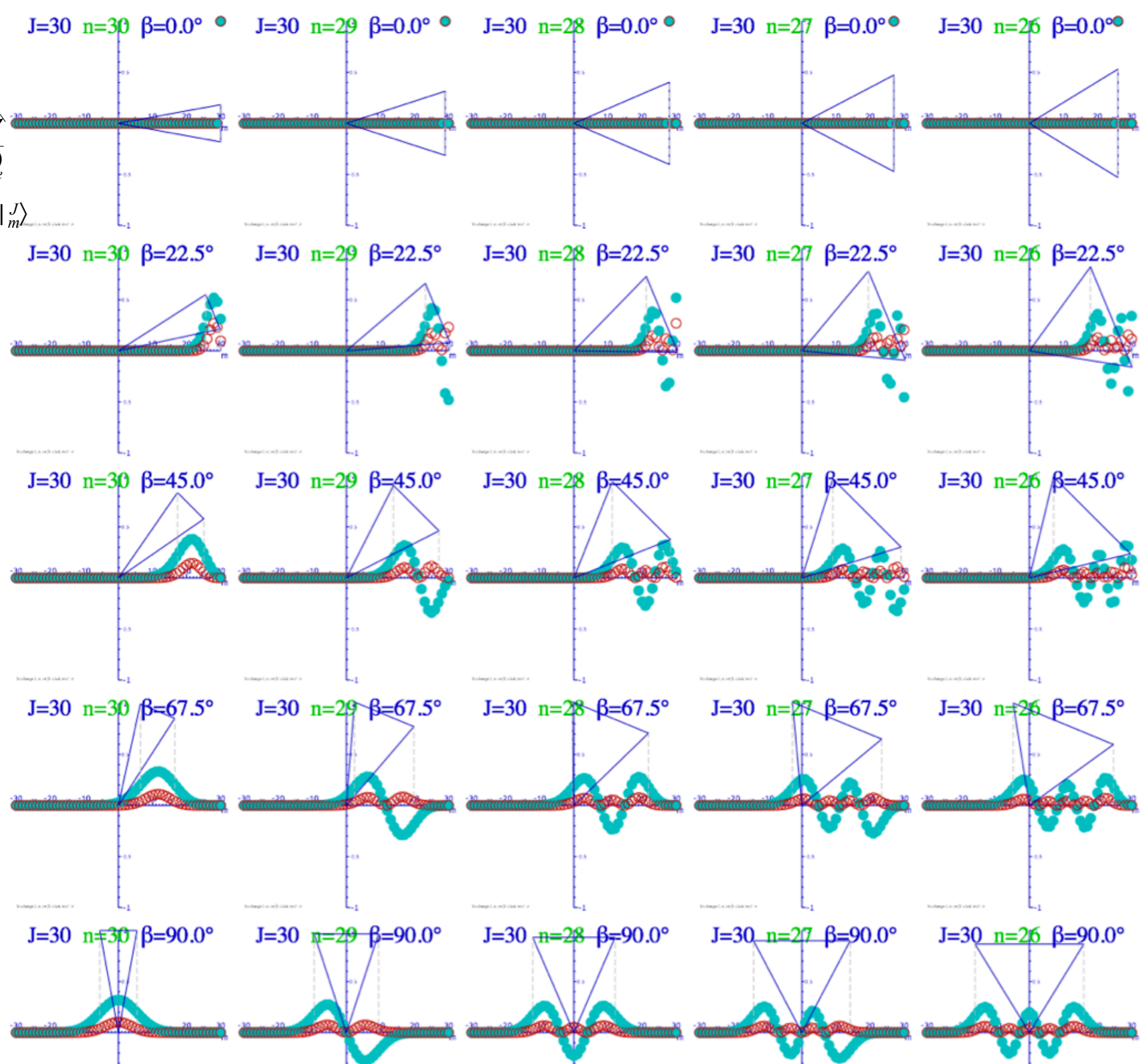
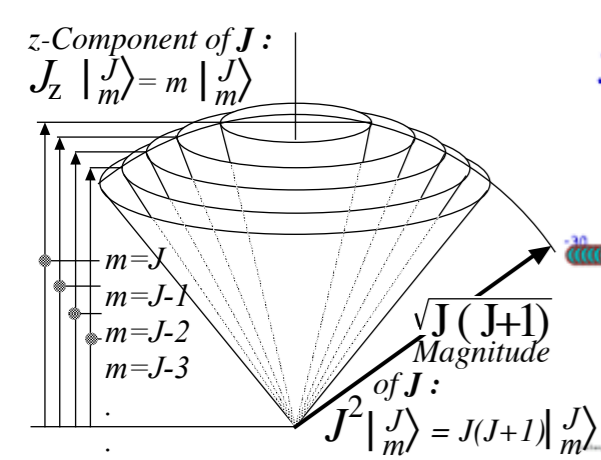


$z$ -Component of  $\mathbf{J}$  :  
 $J_z |J, m\rangle = m |J, m\rangle$



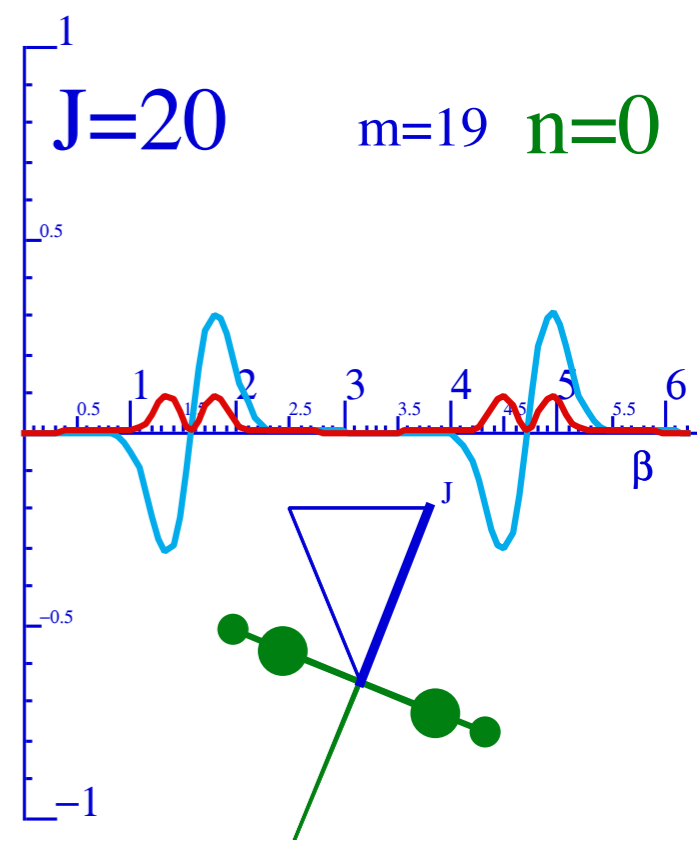
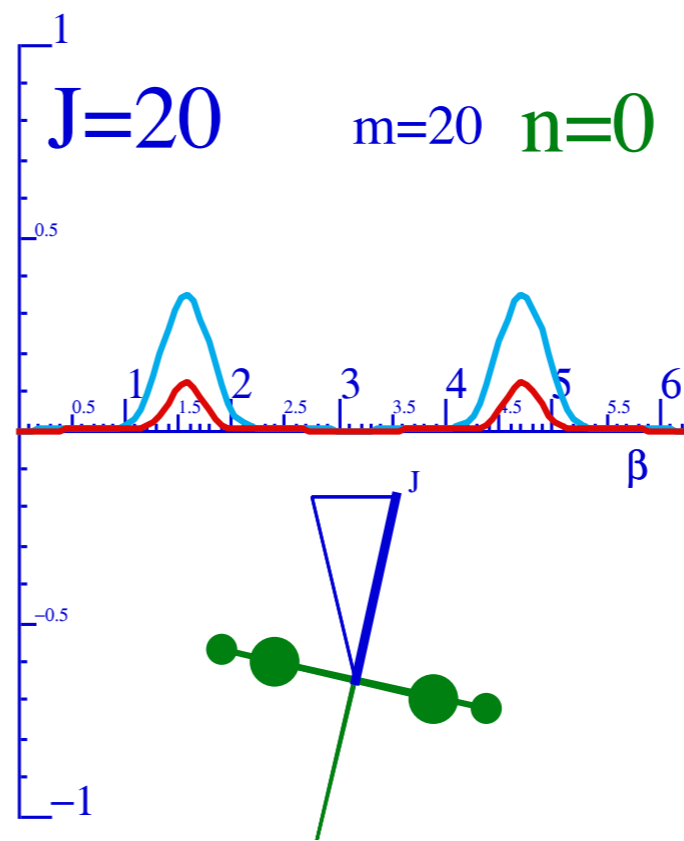
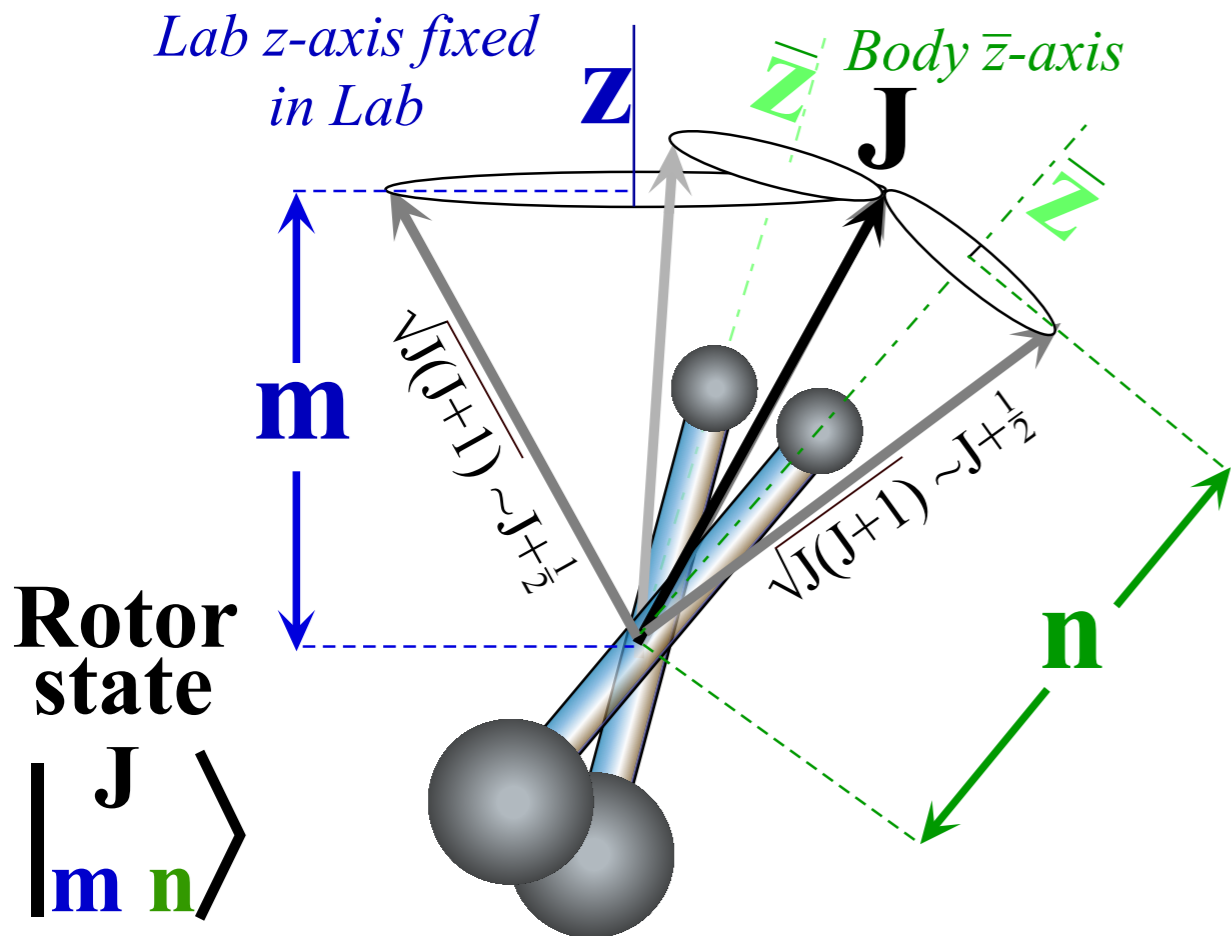


$D^{J=10}_{m,n}(0\beta 0)$   
 plotted  
 vs.  $m$   
 for fixed  
 $J=10, \beta, n$



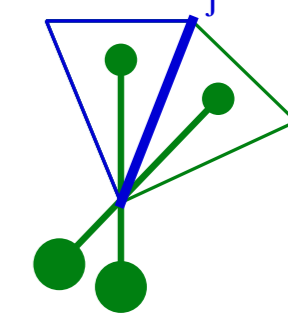
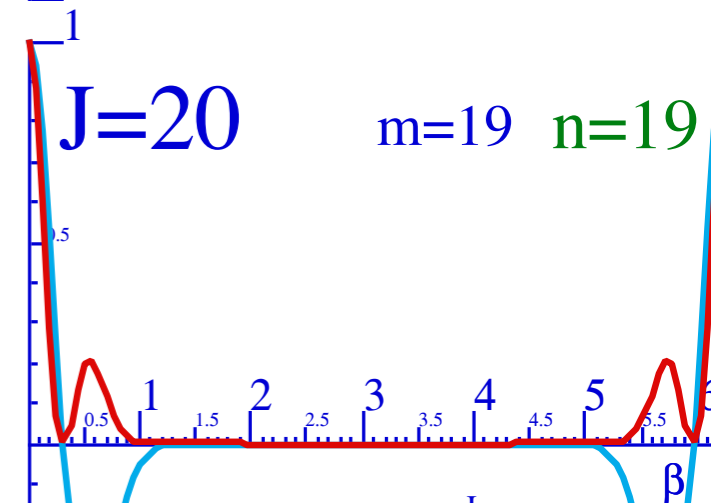
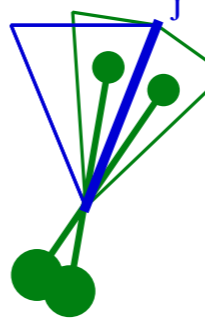
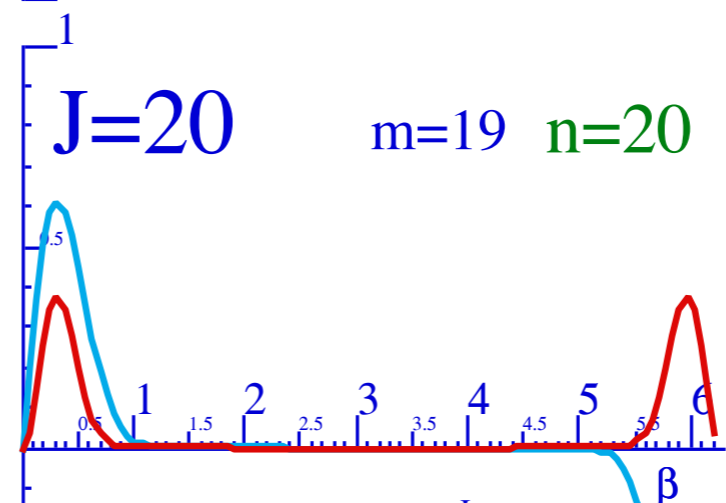
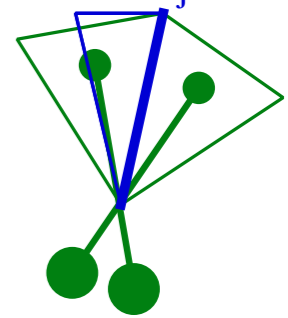
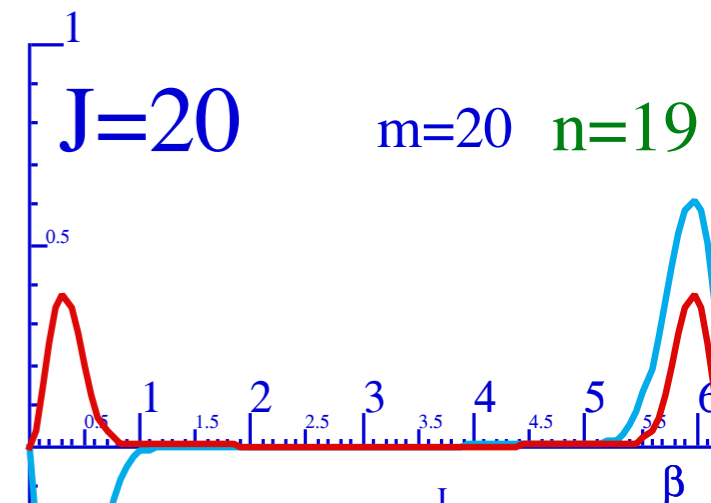
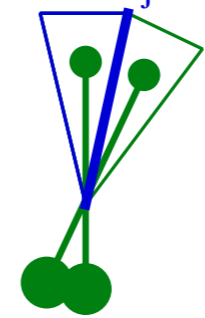
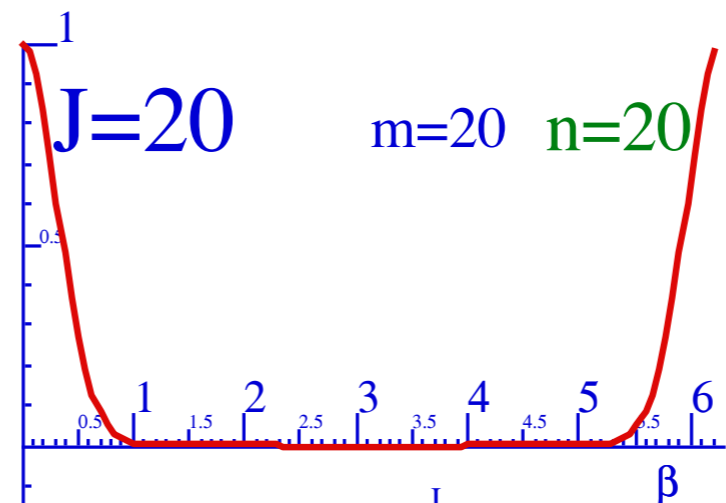
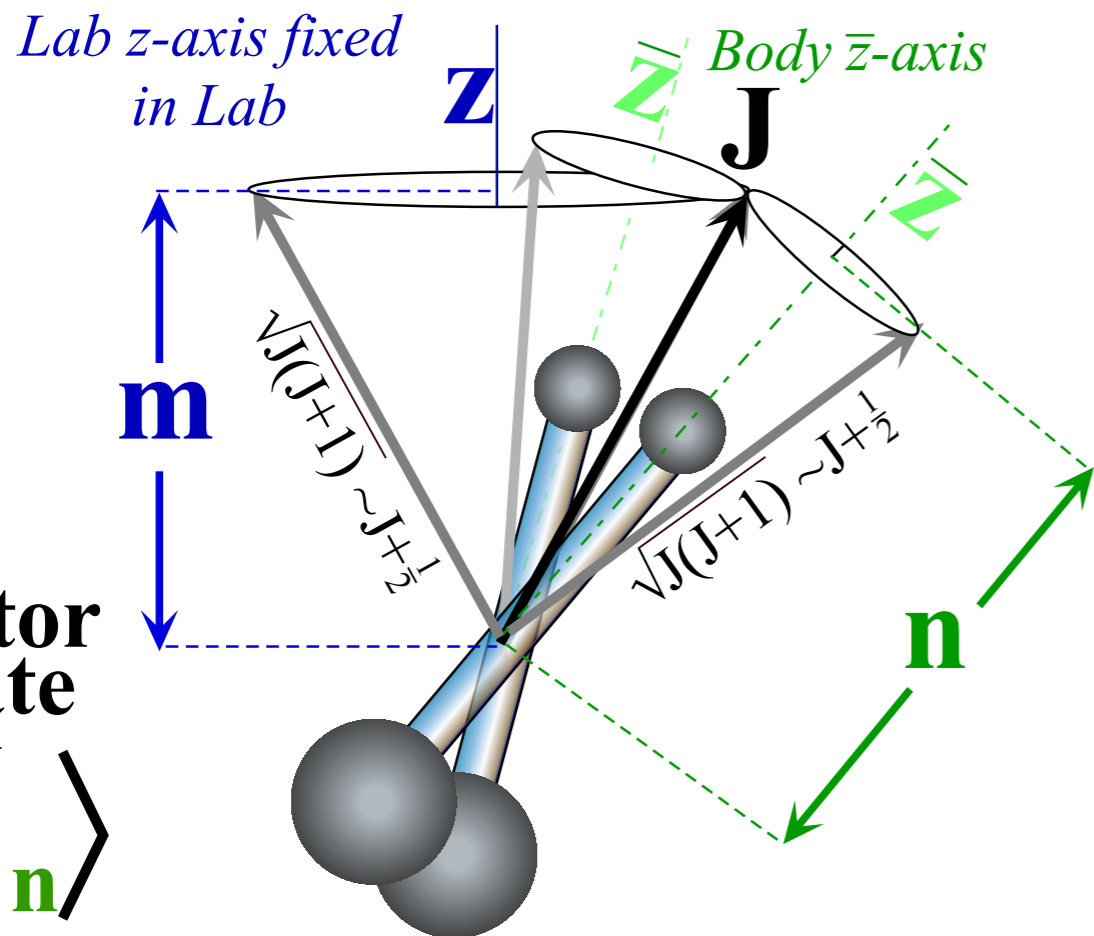
$D^{J=30}_{m,n}(0|\beta 0)$   
 plotted  
 vs.  $m$   
 for fixed  
 $J=30, \beta, n$

$D_{m,n}^{J=20}(0\beta0)$   
 plotted  
 vs.  $\beta$   
 for fixed  
 $J=20, m, n$



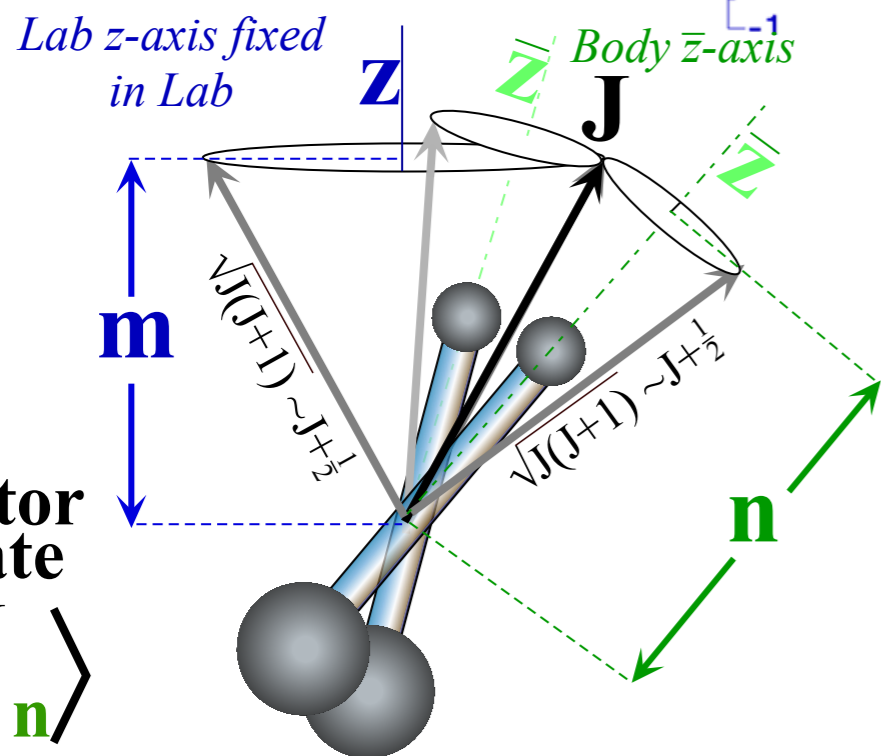
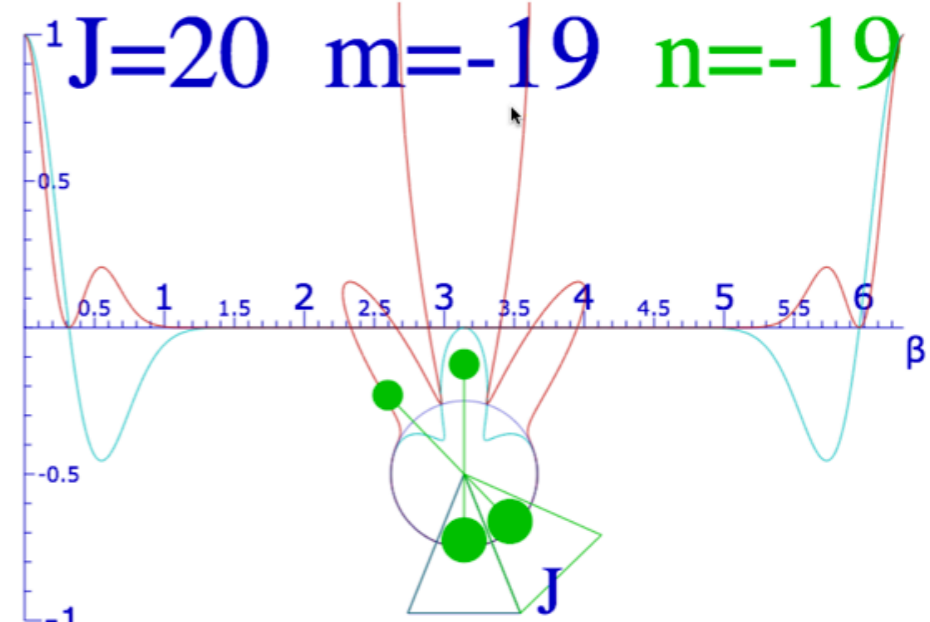
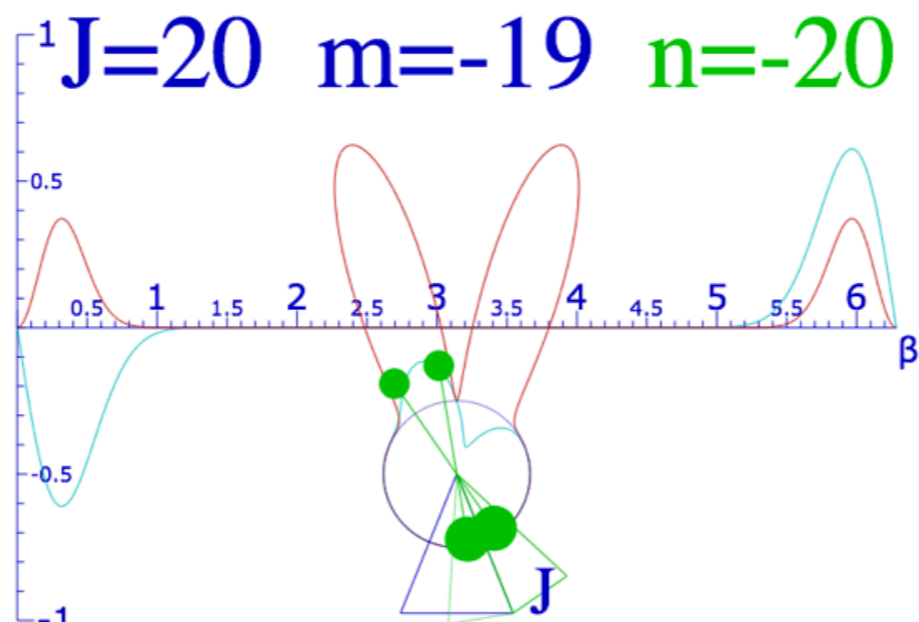
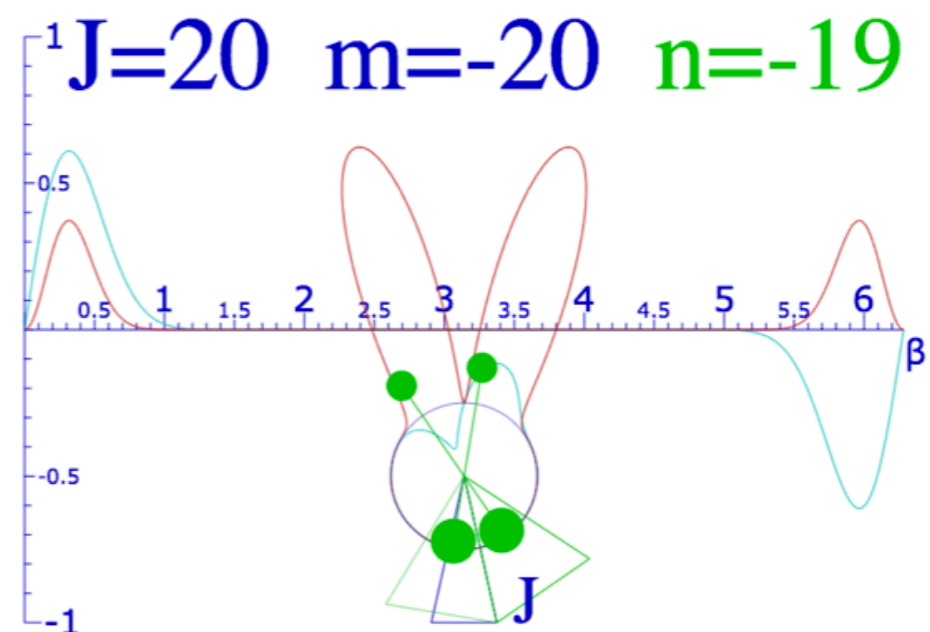
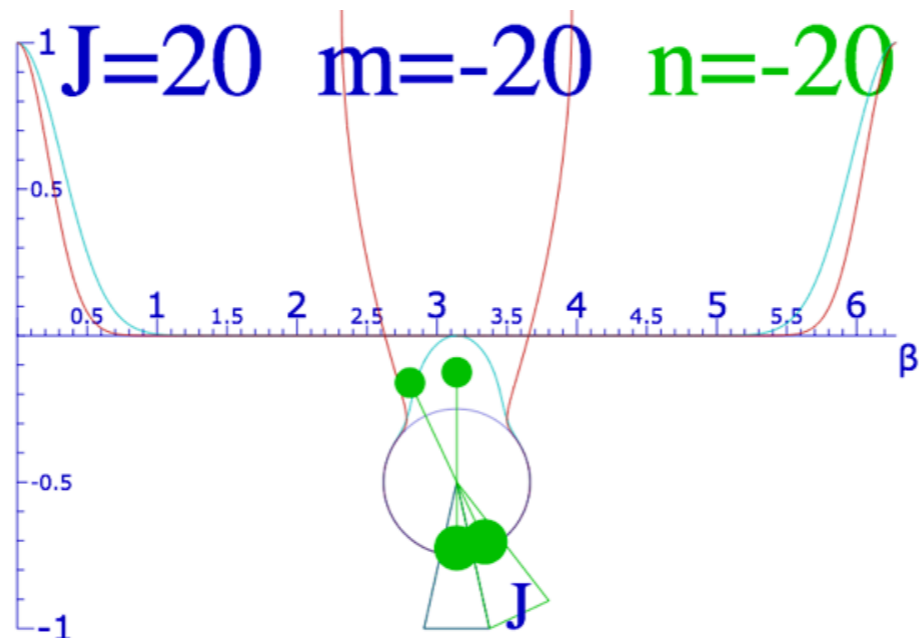
$D_{m,n}^J(0\beta0)$  plotted vs.  $\beta$  for fixed  $J, m, n$

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



*QuantIt web simulation:  
 Visualizing D representations*

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



QuantIt web simulation:  
 Visualizing  $D$  representations

*Partial listing of the Harter-Soft/Heyoka LearnIt Web Apps as of April 24, 2017*  
*(Apps are being upgraded as time permits)*

**Production Links - *For the students & general public***

[BohrIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/BohrItWeb.html"](http://www.uark.edu/ua/modphys/markup/BohrItWeb.html)  
[BounceIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/BounceItWeb.html"](http://www.uark.edu/ua/modphys/markup/BounceItWeb.html)  
[BoxIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/BoxItWeb.html"](http://www.uark.edu/ua/modphys/markup/BoxItWeb.html)  
[CoulIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/CoulItWeb.html"](http://www.uark.edu/ua/modphys/markup/CoulItWeb.html)  
[Cycloidulum - Production; URL is "http://www.uark.edu/ua/modphys/markup/CycloidulumWeb.html"](http://www.uark.edu/ua/modphys/markup/CycloidulumWeb.html)  
[LearnIt - Production; URL is "<http://www.uark.edu/ua/modphys>" or "http://www.uark.edu/ua/modphys/markup/LearnItWeb.html"](http://www.uark.edu/ua/modphys/markup/LearnItWeb.html)  
[JerkIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/JerkItWeb.html"](http://www.uark.edu/ua/modphys/markup/JerkItWeb.html)  
[Pendulum - Production; URL is "http://www.uark.edu/ua/modphys/markup/PendulumWeb.html"](http://www.uark.edu/ua/modphys/markup/PendulumWeb.html)  
[QuantIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/QuantItWeb.html"](http://www.uark.edu/ua/modphys/markup/QuantItWeb.html)  
[Relativity - Pirelli Entrant; URL is "http://www.uark.edu/ua/pirelli" or "http://www.uark.edu/ua/pirelli/html/default.html"](http://www.uark.edu/ua/pirelli)  
[Trebuchet Production; URL is "http://www.uark.edu/ua/modphys/markup/TrebuchetWeb.html"](http://www.uark.edu/ua/modphys/markup/TrebuchetWeb.html)

**Testing Links - *For internal use and testing by Harter & Heyoka***

[BohrIt - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/BohrItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/BohrItWeb.html)  
[BounceIt - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/BounceItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/BounceItWeb.html)  
[BounceIt Title Page - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/BounceItTitlePage.html"](http://www.uark.edu/ua/modphys/testing/markup/BounceItTitlePage.html)  
[BoxIt - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/BoxItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/BoxItWeb.html)  
[CoulIt - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/CoulItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/CoulItWeb.html)  
[Cycloidulum - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/CycloidulumWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/CycloidulumWeb.html)  
[Harter-Soft Web Apps - Quick Reference - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/JerkItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/JerkItWeb.html)  
[JerkIt - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/JerkItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/JerkItWeb.html)  
[ModernPhysics - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/IntroCover.html"](http://www.uark.edu/ua/modphys/testing/markup/IntroCover.html)  
[Pendulum - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/PendulumWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/PendulumWeb.html)  
[QuantIt - Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/QuantItWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/QuantItWeb.html)  
[Trebuchet Testing; URL is "http://www.uark.edu/ua/modphys/testing/markup/TrebuchetWeb.html"](http://www.uark.edu/ua/modphys/testing/markup/TrebuchetWeb.html)

**[Link to the complete listing of Harter-Soft LearnIt Web Apps and resources for Physics](#)**