Introduction to Rotational Eigenstates and Spectra IV
(PSDS - Ch. 5, 7)

Review: Asymmetric rotor levels of $H = A J_x^2 + B J_y^2 + C J_z^2$ and RES plots
$D_2 \supset C_2$ symmetry correlation

Review: Spherical rotor levels and RES plots
Spectral fine structure of $SF_6, SiF_4, C_8H_8,\ldots$
$O \supset C_4$ and $O \supset C_3$ symmetry correlation


Details of $P(88) \nu_4 SF_6$ and $P(88) \nu_4 CF_4$ spectral structure and implications

Beginning theory
Rovibronic nomograms and PQR structure
Rovibronic energy surfaces (RES) and cone geometry
Spin symmetry correlation, tunneling, and entanglement

Hyperfine vs. superfine structure (Case 1. vs Case 2.)
Spin-0 nuclei give Bose Exclusion

The spin-symmetry species mixing problem
Analogy between PE surface dynamics and RES
Rotational Energy Eigenvalue Surfaces (REES)
Review: Asymmetric rotor levels of $H = A J_x^2 + B J_y^2 + C J_z^2$ and RES plots $D_2 \supset C_2$ symmetry correlation
Asymmetric Top Eigensolutions Related to RE Surface and semi-classical J-phase paths

precessing J vector

Note: $A_1B_1A_2B_2$ "monodromy"

after QTforCA Unit 8. Ch. 25 Fig. 25.4.1

$J=10$

$J=3$
SEPARATRIX CIRCLE PAIR DIHEDRAL ANGLE

\[ \theta_{sep} = \tan\left(\frac{A-B}{B-C}\right) \]

Int. J. Molecular Science 14. (2013) Fig. 3 p. 733
Fig. 25.4.2  $J = 10$ asymmetric top energy levels and related RE surface paths

($A = 0.2$, $B = 0.4$, $C = 0.6$). Clustered pairs of levels are indicated in magnifying circles that show superfine splittings.
Review: Asymmetric rotor levels of \( H = A J_x^2 + B J_y^2 + C J_z^2 \) and RES plots

\( D_2 \trianglerighteq C_2 \) symmetry correlation
Examples of Group-Sub-group correlation

<table>
<thead>
<tr>
<th>$D_2$</th>
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<th>$R_y$</th>
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<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>$B_1$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$B_2$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
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</table>

<table>
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<tr>
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<th>1&lt;sub&gt;2&lt;/sub&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>.</td>
</tr>
<tr>
<td>$A_2$</td>
<td>.</td>
<td>1</td>
</tr>
<tr>
<td>$B_1$</td>
<td>1</td>
<td>.</td>
</tr>
<tr>
<td>$B_2$</td>
<td>.</td>
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</tbody>
</table>

<table>
<thead>
<tr>
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<th>0&lt;sub&gt;2&lt;/sub&gt;</th>
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</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>.</td>
</tr>
<tr>
<td>$A_2$</td>
<td>.</td>
<td>1</td>
</tr>
<tr>
<td>$B_1$</td>
<td>1</td>
<td>.</td>
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<tr>
<td>$B_2$</td>
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<tr>
<td>$A_1$</td>
<td>1</td>
<td>.</td>
</tr>
<tr>
<td>$A_2$</td>
<td>.</td>
<td>1</td>
</tr>
<tr>
<td>$B_1$</td>
<td>1</td>
<td>.</td>
</tr>
<tr>
<td>$B_2$</td>
<td>1</td>
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</tr>
</tbody>
</table>

Fig. 25.4.3 Correlations between the asymmetric top symmetry $D_2$ and subgroups $C_2(x)$, $C_2(y)$, and $C_2(z)$.
(Reversed color mixing scheme used here)
Review: Spherical rotor levels and RES plots
Spectral fine structure of SF$_6$, SiF$_4$, C$_8$H$_8$,...

$O \supseteq C_4$ and $O \supseteq C_3$ symmetry correlation

Some more examples of $J=30$ levels (including $T^{[6]}$ vs $T^{[4]}$ effects)
Finding Hamiltonian Eigensolutions by Geometry using Uncertainty Cone Angles

\[ \cos \Theta_J^K = \frac{K}{\sqrt{J(J+1)}} \]

**O_h or T_d Spherical Top:** (Hecht Ro-vib Hamiltonian 1960)

\[
H = B \left( J_x^2 + J_y^2 + J_z^2 \right) + t_{440} \left( J_x^4 + J_y^4 + J_z^4 - \frac{3}{5} J^4 \right) + \cdots
\]

\[= BJ^2 + t_{440} \left( T_0^4 + \sqrt{\frac{5}{14}} \left[ T_4^4 + T_{-4}^4 \right] \right) + \cdots \]

J cone intersects J=88 RE surface to give approx. K=J, J-1, J-2... energy levels

RE Surface topo-lines track precessing semi-classical J vector

K = 88

K = 87

K = 86

K = 88

K = 87

K = 86

(next page shows slice)

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Thursday, April 17, 2014
VISUALIZING THE J = 30 LEVELS OF A SPHERICAL TOP

Angular Momentum Cones for J=30

θ = arc cos [ K/√(J+1) ]
VISUALIZING THE J = 30
LEVELS OF A SPHERICAL TOP

Angular Momentum Cones for J = 30

θ = arc cos [ K/√J(J+1) ]

Two molecular examples: SiF$_4$ and C$_8$H$_8$

Angular Momentum Cones for J = 30

θ = 10.3° K = 30
θ = 18.0° K = 29
θ = 23.3° K = 28
θ = 27.7° K = 27
θ = 31.5° K = 26
θ = 34.9° K = 25
θ = 38.1° K = 24

4-fold cutoff 35.3°
Review: Spherical rotor levels and RES plots
Spectral fine structure of $SF_6$, $SiF_4$, $C_8H_8$, ...

$O \supset C_4$ and $O \supset C_3$ symmetry correlation

Some more examples of $J=30$ levels (including $T^{[6]}$ vs $T^{[4]}$ effects)
Octahedral $O \supseteq C_4$ subgroup correlations

$$\chi^\mu_g(O) \begin{array}{cccccc} g = 1 & r_{1..4} & 180^\circ & \rho_{xyz} & 90^\circ & R_{xyz} & 180^\circ \\ \hline A_1 & 1 & 1 & 1 & 1 & 1 & 1 \\ A_2 & 1 & 1 & 1 & -1 & -1 & -1 \\ E & 2 & -1 & 2 & 0 & 0 & 0 \\ T_1 & 3 & 0 & -1 & 1 & -1 & -1 \\ T_2 & 3 & 0 & -1 & -1 & 1 & 1 \\ \end{array}$$

$1, R_{z+90^\circ}, \rho_{z180^\circ}, R_{z-90^\circ}$

$A_1(O) \downarrow C_4 = 1, \ 1, \ 1, \ 1. = (0)4$

$A_2(O) \downarrow C_4 = 1, -1, 1, -1. = (2)4$

$E(O) \downarrow C_4 = 2, 0, 2, 0. = (0)4 \oplus (2)4$

$T_1(O) \downarrow C_4 = 3, 1, -1, 1. = (0)4 \oplus (1)4 \oplus (3)4$

$T_2(O) \downarrow C_4 = 3, -1, -1, -1. = (2)4 \oplus (1)4 \oplus (3)4$

$O \downarrow C_4$ subduction

$$\begin{array}{cccccccc} O \downarrow C_4 & 0_4 & 1_4 & 2_4 & 3_4 & = \bar{T}_4 \\ \hline A_1 & 1 & . & . & . \\ A_2 & . & . & 1 & . \\ E & 1 & . & 1 & . \\ T_1 & 1 & 1 & 1 & 1 \\ T_2 & . & 1 & 1 & 1 \\ \end{array}$$

Octahedral $O \supseteq C_3$ subgroup correlations

$$\chi^\mu_g(O) \begin{array}{cccccc} g = 1 & r_{1..4} & \rho_{xyz} & R_{xyz} & i_{1..6} \\ \hline A_1 & 1 & 1 & 1 & 1 & 1 \\ A_2 & 1 & 1 & 1 & -1 & -1 \\ E & 2 & -1 & 2 & 0 & 0 \\ T_1 & 3 & 0 & -1 & 1 & -1 \\ T_2 & 3 & 0 & -1 & -1 & 1 \\ \end{array}$$

$1, r_{z+120^\circ}, r_{z-120^\circ}, R_{z-90^\circ}$

$A_1(O) \downarrow C_3 = 1, 1, 1. = (0)3$

$A_2(O) \downarrow C_3 = 1, 1, 1. = (0)3$

$E(O) \downarrow C_3 = 2, -1, -1. = (1)3 \oplus (3)3$

$T_1(O) \downarrow C_3 = 3, 0, 0. = (0)3 \oplus (1)3 \oplus (3)3$

$T_2(O) \downarrow C_3 = 3, 0, 0. = (0)3 \oplus (1)3 \oplus (3)3$

$O \downarrow C_3$ subduction

$$\begin{array}{cccccccc} O \downarrow C_3 & 0_3 & 1_3 & 2_3 & = \bar{T}_3 \\ \hline A_1 & 1 & . & . \\ A_2 & 1 & . & . \\ E & . & 1 & 1 \\ T_1 & 1 & 1 & 1 \\ T_2 & 1 & 1 & 1 \\ \end{array}$$
Review: Spherical rotor levels and RES plots
Spectral fine structure of $\text{SF}_6$, $\text{SiF}_4$, $\text{C}_8\text{H}_8$, ...
$O \supset C_4$ and $O \supset C_3$ symmetry correlation
Some more examples of $J=30$ levels (including $T^{[6]}$ vs $T^{[4]}$ effects)
Angular Momentum Cones and **Quantum** Polar Angles

\[ \Theta^J_m = \arccos\left( \frac{m}{\sqrt{J(J+1)}} \right) \]

**J=30**

\[ K_{100}=30 \]

[Cubane \( \text{C}_8\text{H}_8 \upsilon_{11} \text{P}(30) \)]


**J=30 Eigenstates of** \( \mathbf{H} = \mathbf{B} \mathbf{J}^2 + \mathbf{T}^{[4]} \)
Eigenvalues of $H = BJ^2 + \cos \phi T^4 + \sin \phi T^6$ vs. mix angle $\phi$: $0 < \phi < \pi$

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**Fig. 6** p. 742 and **Fig. 29** p. 791

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After: *Int. J. Molecular Science 14*(2013) Fig. 6 p. 742 and Fig. 29 p. 791
Details of $P(88) \nu_4 SF_6$ and $P(88) \nu_4 CF_4$ spectral structure and implications

Outline of rovibronic Hamiltonian theory

- Coriolis scalar interaction
- Rovibronic nomograms and PQR structure
- Rovibronic energy surfaces (RES) and cone geometry
- Spin symmetry correlation, tunneling, and entanglement
- Hyperfine vs. superfine structure (Case 1. vs Case 2.)
- Spin-0 nuclei give Bose Exclusion
- The spin-symmetry species mixing problem
- Analogy between PE surface dynamics and RES
- Rotational Energy Eigenvalue Surfaces (REES)
Symmetry-level-cluster effects in $\text{SF}_6$, $\text{SiF}_4$, $\text{CH}_4$, $\text{CF}_4$

Graphical approach to rotation-vibration-spin Hamiltonian

$$<H> \sim v_{\text{vib}} + BJ(J+1) + <H_{\text{Scalar Coriolis}} > + <H_{\text{Tensor Centrifugal}} > + <H_{\text{Nuclear Spin}} > + <H_{\text{Tensor Coriolis}} > + ...$$

to help understand complex rotational spectra and dynamics.

OUTLINE

Introductory review

- Rovibronic nomograms and PQR structure
  - Example(s)
    - $v_3$ and $v_4$ $\text{SF}_6$
  - Rotational Energy Surfaces ($\text{RES}$) and $\Theta^J_K$-cones
    - Example(s)
      - $v_4$ P(88) $\text{SF}_6$
  - Spin symmetry correlation tunneling and entanglement
    - Example(s)
      - $\text{SF}_6$

Recent developments

- Analogy between PE surface and RES dynamics
  - Example(s)
    - $v_3$ $\text{SF}_6$
    - $v_3/2v_4$

- Rotational Energy Eigenvalue Surfaces ($\text{REES}$)
Details of \( P(88) v_4 \) \( SF_6 \) and \( P(88) v_4 \) \( CF_4 \) spectral structure and implications

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\[ <H> \sim \nu_{\text{vib}} + BJ(J+1) + \langle H^{\text{Scalar Coriolis}} \rangle + \langle H^{\text{Tensor Centrifugal}} \rangle + \langle H^{\text{Nuclear Spin}} \rangle + \langle H^{\text{Tensor Coriolis}} \rangle + \ldots \]

OUTLINE

Introductory review

- **Rovibronic nomograms and PQR structure**
  - Rotational Energy Surfaces (RES) and $\Theta^K$-cones
  - Spin symmetry correlation tunneling and entanglement

Recent developments

- Analogy between PE surface and RES dynamics
- Rotational Energy Eigenvalue Surfaces (REES)

Example(s)

- $\nu_3$ and $\nu_4$ SF$_6$
- $\nu_4$ P(88) SF$_6$
PQR structure due to Coriolis scalar interaction between vibrational angular momentum $\ell$
and total momentum $\mathbf{J} = \ell + \mathbf{N}$ of rotating nuclei
\[
\langle H \rangle \sim \nu_{\text{vib}} + B J(J+1) + \langle H_{\text{Scalar Coriolis}} \rangle + \langle H_{\text{Tensor Centrifugal}} \rangle + \langle H_{\text{Tensor Coriolis}} \rangle + \langle H_{\text{Nuclear Spin}} \rangle + \ldots
\]

\[
\begin{cases}
N+1 & \text{for } J = N+1 \\
0 & \text{for } J = N \\
N & \text{for } J = N-1
\end{cases}
\]

\[
\begin{align*}
H_{\text{Scalar Coriolis}} &= -B \zeta 2J_{\text{Total}} \cdot \ell_{\text{vibe}} \\
&= -B \zeta [ J^2 - (J-\ell)^2 + \ell^2] \\
&= -B \zeta [ J^2 - N^2 + \ell^2] \\
&= -B \zeta [ J(J+1) - N(N+1) + \ell(\ell+1)]
\end{align*}
\]

**Involves:**
- angular momentum \( \ell \) of vibration “orbits”
- angular momentum \( N \) (or \( R \)) of rotating nuclei
- total momentum \( J = \ell + N \) of whole molecule.

\[
\begin{align*}
J = 3 & : N = 2 \\
J = 2 & : N = 3 \\
J = 1 & : N = 4 \\
J = 0 & : N \text{ varies from 0 to 4}
\end{align*}
\]

**Rotation-polarized mode**
- \( |x> + i|y> \)
- mostly goes left handed

Let: \( N = J - \ell \), and: \( N^2 = J^2 - 2J \cdot \ell + \ell^2 \)

or: \( 2J \cdot \ell = J^2 - N^2 + \ell^2 \)

\( \zeta = -0.22 \)

\( v_4 \) \( \text{SF}_6 \)

\( \text{Thursday, April 17, 2014} \)
\[ \langle H \rangle \sim v_{\text{vib}} + BJ(J+1) + \langle H^{\text{Scalar Coriolis}} \rangle + \langle H^{\text{Tensor Centrifugal}} \rangle + \langle H^{\text{Tensor Coriolis}} \rangle + \langle H^{\text{Nuclear Spin}} \rangle + \ldots \]

\[ \langle H \rangle \sim v_{\text{vib}} + B N(N+1) + 2B(1-\zeta) \cdot \begin{cases} N+1 & \text{for} : J=N+1 \\ 0 & \text{for} : J=N \\ N & \text{for} : J=N+1 \end{cases} \]

\[ H^{\text{Scalar Coriolis}} = -B \zeta 2J^{\text{Total}} \cdot \ell_{\text{vibe}} \]

\[ = -B \zeta [ J^2 - (J-\ell)^2 + \ell^2 ] \]

\[ = -B \zeta [ J^2 - N^2 + \ell^2 ] \]

\[ = -B \zeta [ J(J+1) - N(N+1) + \ell(\ell+1) ] \]

\[ \sim 10 \mu m \]

\[ v_3 \text{ SF}_6 \]

mostly goes right handed

\[ v_4 \text{ SF}_6 \]

mostly goes left handed

\[ \zeta_3 = 0.69 \]

\[ \zeta_4 = -0.22 \]
Details of $P(88) \nu_4 SF_6$ and $P(88) \nu_4 CF_4$ spectral structure and implications

Outline of rovibronic Hamiltonian theory

Coriolis scalar interaction

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Analogy between PE surface dynamics and RES

Rotational Energy Eigenvalue Surfaces (REES)
\[ \langle H \rangle \sim v_{\text{vib}} + B J(J+1) + \langle H_{\text{Scalar Coriolis}} \rangle + \langle H_{\text{Tensor Centrifugal}} \rangle + \langle H_{\text{Tensor Coriolis}} \rangle + \langle H_{\text{Nuclear Spin}} \rangle + \ldots \]

\[ \begin{align*}
\langle H \rangle \sim v_{\text{vib}} + B N(N+1) + 2B(1-\zeta) \cdot \begin{cases} 
N+1 & \text{for } J=N+1 \\
0 & \text{for } J=N \\
N & \text{for } J=N-1
\end{cases} 
\end{align*} \]

\[ H_{\text{Scalar Coriolis}} = -B \zeta 2 J_{\text{Total}} \cdot \mathbf{\ell}_{\text{vibe}} \]
\[ = -B \zeta [ J^2 - (J-\ell)^2 + \ell^2 ] \]
\[ = -B \zeta [ J^2 - N^2 + \ell^2 ] \]
\[ = -B \zeta [ J(J+1) - N(N+1) + \ell(\ell+1) ] \]

\[ \nabla v_4 \text{SF}_6 \]
mostly goes left handed

\[ \zeta_4 = -0.22 \]
Summary of low-J (PQR) ro-vibe structure

(Using rovib. nomogram)
Details of $P(88) v_4 SF_6$ and $P(88) v_4 CF_4$ spectral structure and implications

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Rotational Energy Eigenvalue Surfaces (REES)
PQR structure due to Coriolis scalar interaction between vibrational angular momentum $\ell$ and total momentum $J = \ell + N$ of rotating nuclei

$P(N)=P(88)$ structure due to tensor centrifugal/Coriolis due to vibrational $\ell$ and total momentum $J = \ell + N$
Graphical approach to rotation-vibration-spin Hamiltonian

\[ \langle H \rangle \sim \nu_{\text{vib}} + B J(J+1) + \langle H^{\text{Scalar Coriolis}} \rangle + \langle H^{\text{Tensor Centrifugal}} \rangle + \langle H^{\text{Nuclear Spin}} \rangle + \langle H^{\text{Tensor Coriolis}} \rangle + \ldots \]

**OUTLINE**

- Introductory review
- **Rovibronic nomograms and PQR structure**
- **Rotational Energy Surfaces (RES) and \( \theta'_K \)-cones**
- Spin symmetry correlation tunneling and entanglement
- Recent developments
- Analogy between PE surface and RES dynamics
- Rotational Energy Eigenvalue Surfaces (REES)

Example(s)
- \( \nu_3 \) and \( \nu_4 \) \( \text{SF}_6 \)
- \( \nu_4 \) \( \text{P}(88) \) \( \text{SF}_6 \)
- \( \nu_3 \) \( \text{SF}_6 \)
$\text{SF}_6$ Spectra of $O_h$ Ro-vibronic Hamiltonian described by RE Tensor Topography

\begin{equation}
H = B \left( J_x^2 + J_y^2 + J_z^2 \right) + t_{440} \left( J_x^4 + J_y^4 + J_z^4 - \frac{3}{5} J^4 \right) + \cdots
\end{equation}

\begin{align*}
H &= BJ^2 + t_{440} \left( T_0^4 + \sqrt{\frac{5}{14}} \left( T_4^4 + T_{-4}^4 \right) \right) + \cdots
\end{align*}

Rovibronic Energy (RE) Tensor Surface

precessing $J$ vector

Herzberg rules still apply near separatrices or saddle points

Saddle Point

\[ \Theta_m = \arccos \left( \frac{K}{\sqrt{J(J+1)}} \right) \]

\[ \sqrt{J(J+1)} \sim J + \frac{1}{2} \]
SF$_6$ $\nu_4$ rovib FT spectra $\sim 615\text{cm}^{-1}$

McDowell et al. LosAlamos

Saddle Point

Herzberg rules still apply near separatrices or saddle points
Primary AET species mixing increases with distance from "separatrix"

PQR structure due to Coriolis scalar interaction between vibrational angular momentum \( \ell \) and total momentum \( J = \ell + N \) of rotating nuclei

\[ P(N) = P(88) \] structure due to tensor centrifugal/Coriolis due to vibrational \( \ell \) and total momentum \( J = \ell + N \)

Superfine structure modeled by \( J \)-tunneling in body frame (Underlying F-spin-permutation symmetry is involved, too.)
Primary AET species mixing increases with distance from “separatrix”

4-fold (100)-clusters $C_4$ symmetry

Internal 3-fold axial quanta label $C_3$-CLUSTERS

Cubic Octahedral symmetry $O$

\[
\begin{array}{c|ccc}
A_1 & 1 & \cdot & \cdot \\
A_2 & \cdot & \cdot & 1 \\
E & 1 & 1 & 1 \\
T_1 & 1 & 1 & \cdot \\
T_2 & \cdot & 1 & 1 \\
\end{array}
\]

\[3 \text{ modulo } 4 \text{ equals -1 modulo } 4 \ (\text{and } 83 \text{ mod } 4)\]

\[83 = 84 - 1\]

\[K_3 = \ldots 81 82 83 84 85 86 87 88\]

pure $A_1 T_1 E T_2 A_2$ species

\[\begin{array}{c|ccc}
A_1 & 1 & \cdot & \cdot \\
A_2 & 1 & \cdot & \cdot \\
E & \cdot & 1 & 1 \\
T_1 & 1 & 1 & 1 \\
T_2 & 1 & 1 & 1 \\
\end{array}\]

(2 modulo 3 equals -1 modulo 3 and 86 mod 3)

\[86 = 88 - 1\]
$\langle H \rangle \sim \nu_{\text{vib}} + B J(J+1) + H^{\text{Scalar Coriolis}} + H^{\text{Tensor Centrifugal}} + H^{\text{Tensor Coriolis}} + H^{\text{Nuclear Spin}} + \ldots$

**$O_h$ or $T_d$ Spherical Top:** (Hecht CH$_4$ Hamiltonian 1960)

$$H = B \left( J_x^2 + J_y^2 + J_z^2 \right) + t_{440} \left( J_x^4 + J_y^4 + J_z^4 - \frac{3}{5} J^4 \right) + \ldots$$

$$= B J^2 + t_{440} \left( T_0^4 + \sqrt{\frac{5}{14}} \left[ T_4 + T_{-4}^4 \right] \right) + \ldots$$

$J = 88$

RE Surface topo-lines track precessing semi-classical $J$ vector

$\theta^J_K = \acos \left[ \frac{K}{\sqrt{J(J+1)}} \right]$
Duality: The “Flip Side” of Symmetry Analysis. LAB versus BODY, STATE versus PARTICLE, boils down to:

OUTSIDE versus INSIDE

Example:
Cubic-Octahedral O reduced to Tetragonal $C_4$

\[
\begin{array}{cccc}
C_4 & 0 & 14 & 24 & 34 \\
A_1 & 1 & . & . & . \\
A_2 & . & . & 1 & . \\
E & 1 & . & 1 & . \\
T_1 & 1 & 1 & . & 1 \\
T_2 & . & 1 & 1 & 1 \\
\end{array}
\]

INSIDE or BODY
Symmetry reduction results in Level or Spectral UN-SPLITTING (“clustering”)

Internal $J$ gets “stuck” on RES axes Must “tunnel” axis-to-axis at rate $s$

\[
\begin{array}{cccccc}
|U> & |D> & |E> & |W> & |N> & |S> \\
H & 0 & s & s & s & s \\
0 & H & s & s & s & s \\
s & s & H & 0 & s & s \\
s & s & 0 & H & s & s \\
s & s & s & s & H & 0 \\
s & s & s & s & 0 & H \\
\end{array}
\]
Duality: The “Flip Side” of Symmetry Analysis.

LAB versus BODY,
STATE versus PARTICLE,
boils down to:

OUTSIDE versus INSIDE

Example:
Cubic-Octahedral O
reduced to Tetragonal $C_4$

Internal $J$ gets “stuck” on RES axes
Must “tunnel” axis-to-axis at rate $s$
OUTSIDE or LAB
Symmetry reduction results in
Level or Spectral SPLITTING
External B-field does Zeeman splitting

Duality: The “Flip Side” of Symmetry Analysis.
LAB versus BODY, STATE versus PARTICLE,
boils down to:
OUTSIDE versus INSIDE

Example:
Cubic-Octahedral O reduced to Tetragonal C₄

INSIDE or BODY
Symmetry reduction results in
Level or Spectral UN-SPLITTING (“clustering”)

Internal J gets “stuck” on RES axes
Must “tunnel” axis-to-axis at rate s

Tunneling (s) between axes splits the 0₄ cluster as shown on following pages

Thursday, April 17, 2014
Internal $J$ gets “stuck” on RES axes
Must “tunnel” axis-to-axis at rate $s$

Tunneling $s=-S$ is negative here

\[
\begin{array}{cccccccc}
H & 0 & s & s & s & s & & & \\
0 & H & s & s & s & s & & & +2 \\
s & s & H & 0 & s & s & & & +1 \\
s & s & 0 & H & s & s & & & +1 \\
s & s & s & s & H & 0 & & & +1 \\
s & s & s & s & 0 & H & & & +1 \\
\end{array}
\]

\[
\begin{array}{cccccccc}
H & 0 & s & s & s & s & & & \\
0 & H & s & s & s & s & & & +2 \\
s & s & H & 0 & s & s & & & +2 \\
s & s & 0 & H & s & s & & & +2 \\
s & s & s & s & H & 0 & & & +2 \\
s & s & s & s & 0 & H & & & +2 \\
\end{array}
\]

\[
\begin{array}{cccccccc}
H & 0 & s & s & s & s & & & \\
0 & H & s & s & s & s & & & +1 \\
s & s & H & 0 & s & s & & & -1 \\
s & s & 0 & H & s & s & & & -1 \\
s & s & s & s & H & 0 & & & -1 \\
s & s & s & s & 0 & H & & & -1 \\
\end{array}
\]
Duality: The “Flip Side” of Symmetry Analysis.

LAB versus BODY, STATE versus PARTICLE,
boils down to:

OUTSIDE versus INSIDE

Example:
Cubic-Octahedral $O$
reduced to Tetragonal $C_4$

Internal J gets “stuck” on RES axes
Must “tunnel” axis-to-axis at rate $s$

INSIDE or BODY
Symmetry reduction results in
Level or Spectral UN-SPLITTING
 (“clustering”)

OUTSIDE or LAB
Symmetry reduction results in
Level or Spectral SPLITTING
External B-field does Zeeman splitting

“Coerced” Symmetry Breaking

“Spontaneous” Symmetry Breaking

Stronger $C_4$

higher $\vert B \vert$

lower $\vert s \vert$

$tunneling$ $matrix$ $eigenvalues$
Details of \( P(88) \nu_4 SF_6 \) and \( P(88) \nu_4 CF_4 \) spectral structure and implications

Outline of rovibronic Hamiltonian theory

Coriolis scalar interaction

Rovibronic nomograms and PQR structure

Rovibronic energy surfaces (RES) and cone geometry

Spin symmetry correlation, tunneling, and entanglement

Hyperfine vs. superfine structure (Case 1. vs Case 2.)

Spin-0 nuclei give Bose Exclusion

The spin-symmetry species mixing problem

Analogy between PE surface dynamics and RES

Rotational Energy Eigenvalue Surfaces (REES)
Borde', et al.
PRL 45,14 (1980)
Primary AET species mixing increases with distance from "separatrix"

CASE 1  Unmixed primary $A_1 T_1 E T_2 A_2$ species

CASE 2  Extreme mixing
Primary AET species mixing increases with distance from "separatrix"

CASE 1 Unmixed primary $A_1 T_1 E T_2 A_2$ species

CASE 2$_4$ Extreme mixing in tight $C_4$-CLUSTERS

CASE 2$_3$- Major mixing in lowest two $C_3$-CLUSTERS
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\[ \langle H \rangle \sim v_{\text{vib}} + BJ(J+1) + \langle H^{\text{Scalar Coriolis}} \rangle \]
\[ + \langle H^{\text{Tensor Centrifugal}} \rangle \]
\[ + \langle H^{\text{Nuclear Spin}} \rangle \]
\[ + \langle H^{\text{Tensor Coriolis}} \rangle \]
\[ + \ldots \]

OUTLINE

Introductory review

• Rovibronic nomograms and PQR structure
  - Example(s)
    - \( v_3 \) and \( v_4 \) SF\(_6\)

• Rotational Energy Surfaces (RES) and \( \theta^j_K \)-cones
  - Example(s)
    - \( v_4 \) P(88) SF\(_6\)

Recent developments

• Analogy between PE surface and RES dynamics
  - Example(s)
    - \( v_3 \) SF\(_6\)

• Rotational Energy Eigenvalue Surfaces (REES)
Primary AET species mixing increases with distance from "separatrix".

4-fold (100)-clusters $C_4$ symmetry

Internal 3-fold axial quanta label $C_3$-CLUSTERS mixed

pure $A_1, T_1, E, T_2, A_2$ species
Primary AET species mixing increases with distance from "separatrix".

(a) SF₆ υ₁ Rotational Structure

(b) P(88) Fine Structure (Rotational anisotropy effects)

(c) Superfine Structure (Rotational axis tunneling)

4-fold (100)-clusters C₄ symmetry

Cubic Octahedral symmetry O

A₁ 1 1 1 1
A₂ • • • 1
E 1 1 1 1
T₁ 1 1 1 1
T₂ • 1 1 1

3 modulo 4 equals -1 modulo 4 (and 83 mod 4)
83 = 84 - 1

(2 modulo 3 equals -1 modulo 3 and 86 mod 3)

86 = 88 - 1
Entanglement!

How F-nuclei become distinguished
(but not distinguishable)
in SF₆.

If rotation is not too stuck on C₄ axis
all six ○ nuclei are equivalent

Spin-Permutation to Octahedral Correlations

Species Spin Weights

Greatly simplified sketches of ultra high resolution IR SF₆ spectroscopy of Christian Borde’, C. Saloman, and Oliver Pfister who did SiF₄, too.
DISentanglement!

How F-nuclei become distinguished
(but not distinguishable)
in SF₆.

If rotation is not too stuck on C₄ axis
all six nuclei are equivalent

With rotation stuck on C₄ axis
polar nuclei are “left out in the cold”

“Brrrr it’s cold!”

“We’re HOT!”

If polar nuclei have a greater B-field

Spin-Permutation to Octahedral Correlations

Species Spin Weights

Greatly simplified sketches of ultra high resolution IR SF₆ spectroscopy of Christian Borde‘, C. Saloman, and Oliver Pfister who did SiF₄, too.
Primary AET species mixing increases with distance from "separatrix".

CASE 1 - Unmixed primary $A_1, T_1, E, T_2, A_2$ species

CASE 2 - Extreme mixing in tight $C_4$-CLUSTERS

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For a zero-spin $X^{16}O_6$ molecule, hundreds of lines would vanish! Just eight $A_1$ singlets remain.

Without nuclear spin: Forget all this stuff!

Goodbye clusters!  (Goodbye Columbus)
Some examples of Bose Exclusion

Spherical Top Molecules with Spin-0 Nuclei

OsO₄

Only 1 hyperfine state: \( I=0 \)

Spherical Top Molecules with Spin-1/2 Nuclei

\( \text{CF}_4, \text{SiF}_4 \ldots \)

\( 2^4 = 16 \) hyperfine states: \( I=0-2 \)

\( \text{SF}_6 \ldots \)

\( 2^6 = 64 \) hyperfine states: \( I=0-3 \)

\( 12\text{C}_{60} \)

\( 2^{60} = 1.15 \times 10^{18} \) hyperfine states: \( I=0-30 \)

Example of extreme symmetry exclusion

\( Y_h \) Symmetry reduced to \( C_V \) by a single neutron

(in \( ^{13}\text{C} \))

... (and partial recovery)

Some examples of Fermi (non) Exclusion

\( ^{12}\text{C}_{60} \)

\( ^{13}\text{C}^{12}\text{C}_{59} \)

\( J=50 \)

2 levels allowed by Pauli Exclusion

\( J=50 \)

202 levels allowed

Question: Where did those 200 levels go?

Better Question: Where did those 1.15 octillion levels go?
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CONSERVATION OF ROVIBRONIC SPECIES - Two Views:

Old
(1939, 1945, and 1966)

"...transitions between...species (A₁...E...T₂)...
...are very strictly forbidden..."

...for diatomic molecules...I p. 150
...for D₂ asymmetric tops...II p.468
...for Dₙ symmetric tops...II p.415
...for O-T₄ spherical tops...II p.441-453

...during transitions involving...
...rotational states,...III p.246
...vibrational states,...” ”
...electronic states,...” ”
...collisional states...” ”

versus

New (1978-present)

Nuclear Spin Conversion in Molecules
Jon T. Hougen and Takeshi Oka

Molecules with identical nuclei having nonzero spin can exist in different states called nuclear spin modifications by most researchers and nuclear spin isomers by some. Once prepared, a para-H₂ sample can be preserved for months as initially shown by Bonhoeffer and Harteeck in 1929 (3). Once prepared, a para-H₂ sample can be preserved for months

[review of C₃H₄ study:
Sun, Takagi, Matsushima,
Science 310, 1938(2005)]

Strictly versus NOT!
Conservation and preservation?

To conserve vs. To convert
To preserve vs. To pervert

No Way! versus WAY!
Conversion, perversion or transition?

Widespread and extreme mixing of species reported in CF₄, SiF₄ and SF₆:
HOW CONSERVED IS ROVIBRONIC-SPIN SYMMETRY?

What preserves it? versus What messes it up?

$A_{2u}^1$

No Way!

...because nuclear moments...
...are so very slight...

$perturbation \sim \left| (A_{1g}^3 \text{spin-rovib.}|E_{2g}^5) \right|^2$

$E_{A_{1g}}^3 - E_{E_{2g}}^5$

...too darn small ($\sim$kHz)...
How conserved is rovibronic-spin symmetry? What preserves it? versus What mixes it up?

No Way!

"...because nuclear moments... ...are so very slight..."

E_{2g}^{5} → (A_{1g}^{3}| spin-rovib. | E_{2g}^{5}) \quad \text{perturbation ~} | \quad (A_{1g}^{3}| spin-rovib. | E_{2g}^{5}) |^{2}

E_{A_{1g}}^{3} - E_{E_{2g}}^{5}

...too darn small (~kHz)... ...too darn big (like 10MHz)... ...exponentially tiny! (like $10^{-50}$Hz)

"Accidental" degeneracy
Lea, Leask & Wolf JPCSol.23, 1381(1962)

Level-clustering
Dorney and Watson JMS 42,135(1972)
Harter and Patterson PRL38,224(1977) JCP 66,4872(1977)
RE Surface precession vs. tunneling
Harter and Patterson JMP 20,1453(1979) JCP 80,4241(1984)

RE Superhyperfine transitions
Hyperfine effects may rule! $A_{1} \quad T_{1} \quad E \quad T_{2} \quad A_{2}$ get seriously mixed up.

Harter, Patterson, and daPaixao, Rev.Mod.Phys. 50, 37(1978)
Harter and Patterson, Phys. Rev. A19,2277(1979) (CF_{4})
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- Spin symmetry correlation tunneling and entanglement

Recent developments

- Analogy between PE surface and RES dynamics
- Rotational Energy Eigenvalue Surfaces (REES)

Example(s)

- \( \nu_3 \) and \( \nu_4 \) SF\(_6\)
- \( \nu_4 \) P(88) SF\(_6\)
- SF\(_6\)

- \( \nu_3 \) SF\(_6\)
Potential Energy Surface (PES) Dynamics

Inter-PES electronic transitions

Vibrational Franck-Condon effects

- Frequency mismatch of PES

Rotation Energy Surface (RES) Dynamics

Inter-PES electronic transitions

Rotational “Franck-Condon” effects

- Frequency mismatch of RES

Analogy between

Vibronic and Rovibronic

- Shape or position mismatch of PES

Duschinsky rotation or translation

- Shape or position mismatch of RES
Non-Born-Oppenheimer Surfaces
Strong vibration-electronic mixing
Jahn-Teller-Renner effects
• Multiple and variable conformer minima

Rotation Energy Eigen-Surfaces (REES)
Inter-PES electronic transitions
Rotational JTR effects
• Multiple and variable J-axes

Analogy between Vibronic and Rovibronic

Example for 2-state vibronic-rotor coupling
Avoided crossings
Recall scalar Coriolis

$PQR$ plots vs. $B\zeta$

Here is a $J=60$ piece of it:

$N=59 = J-1$

$N=60 = J$

$N=61 = J+1$

$-0.5 \quad B\zeta = 0 \quad +0.5$

Now consider this plot with tensor Coriolis, too

(Just 4\textsuperscript{th}-rank $[2x2]^4$ tensor here.

See next talk \textbf{RJ06} and a 4PM talk \textbf{RI09}

by \textit{Mitchell et. al.} and \textit{Boudon et. al.} who will pull much higher rank!)
How to display such monstrous avoided cluster crossings: REES: *Rotational Energy Eigenvalue Surfaces*

Vibration (or vibronic) momentum $\ell$ retains its quantum representaion(s).

For $\ell=1$ that is the usual 3-by-3 matrices.

Rotational momentum $J$ is treated semi-classically. $|J| = \sqrt{J(J+1)}$

Usually $\mathbf{J}$ is written in Euler coordinates: $J_x = |J|\cos\gamma \sin\beta$, etc.

Plot resulting H-matrix eigenvalues vs. classical variables.

( $\ell=1$) 3-by-3 H-matrix e-values are polar plotted vs. azimuth $\gamma$ and polar $\beta$. 
Body-$\Sigma\Pi\pm$-Basis

$$<\text{H}>= (\nu_3 + B|J|^2)
\begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
\end{pmatrix} + 2B\zeta |J|
\begin{pmatrix}
\cos\beta & \frac{1}{\sqrt{2}}e^{-i\gamma}\sin\beta & 0 \\
\frac{1}{\sqrt{2}}e^{i\gamma}\sin\beta & 0 & \frac{1}{\sqrt{2}}e^{-i\gamma}\sin\beta \\
0 & \frac{1}{\sqrt{2}}e^{i\gamma}\sin\beta & -\cos\beta \\
\end{pmatrix}

+ 2t_{224}|J|^2
\begin{pmatrix}
3\cos^2\beta - 1 & -\sqrt{8}e^{-i\gamma}\sin\beta\cos\beta & \sin^2\beta(6\cos2\gamma + i4\sin2\gamma) \\
-\sqrt{8}e^{i\gamma}\sin\beta\cos\beta & 0 & -6\cos^2\beta + 2 \sqrt{8}e^{i\gamma}\sin\beta\cos\beta \\
\sin^2\beta(6\cos2\gamma - i4\sin2\gamma) & \sqrt{8}e^{i\gamma}\sin\beta\cos\beta & 3\cos^2\beta - 1 \\
\end{pmatrix}$$

Lab-PQR-Basis

$$<\text{H}>= (\nu_3 + B|J|^2)
\begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
\end{pmatrix} + 2B\zeta |J|
\begin{pmatrix}
+1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & -1 \\
\end{pmatrix}$$

(Either basis should give same REES)

$$H_{pp} = (35\cos^4\beta - 30\cos^2\beta + 5\sin^2\beta\sin4\gamma + 5)/4 = H_{RR}$$

$$H_{pq} = 5\sin\beta(7\cos^2\beta - 3\cos\beta - \sin^2\beta(\cos\beta\cos4\gamma + i\sin4\gamma))/\sqrt{8} = H_{QR}$$

$$H_{pq} = 5(-7\cos^4\beta + 8\cos^2\beta + (1 - \cos^2\beta)\cos4\gamma + 2i\cos\beta\sin^2\beta\sin4\gamma - 1)/4$$
$v_3$ REES
New geometric approach to rotational eigenstates and spectra

Introduction to Rotational Energy Surfaces (RES) and multipole tensor expansion

Rank-2 tensors from $D^2$-matrix

Building Hamiltonian $H = A J_x^2 + B J_y^2 + C J_z^2$ out of scalar and tensor operators

Comparing quantum and semi-classical calculations

Symmetric rotor levels and RES plots
Asymmetric rotor levels and RES plots
Spherical rotor levels and RES plots

$\text{SF}_6$ spectral fine structure
$\text{CF}_4$ spectral fine structure
Example of frequency hierarchy for 16µm spectra of CF₄ (Freon-14)
W.G.Harter
Ch. 31
Atomic, Molecular, & Optical Physics Handbook
Am. Int. of Physics
Gordon Drake Editor (1996)
Example of frequency hierarchy for 16μm spectra of CF₄ (Freon-14)

W.G. Harter

Fig. 32.7

Springer Handbook of Atomic, Molecular, & Optical Physics

Gordon Drake Editor (2005)
As of April 3, 2014

**Links to the current Harter-Soft LearnIt web apps for Physics**

*Bold links have default redirect pages. *Italics* are not yet meant for production.*Red*: the final stages of testing.

List of *production* Harter-Soft Web Apps & Textbooks (For public)

- **Classical Mechanics with a Bang!** - URL is "http://www.uark.edu/ua/modphys/markup/CMwBangWeb.html"
- **Quantum Theory for the Computer Age** - URL is "http://www.uark.edu/ua/modphys/markup/QTCAWeb.html"
- **LearnIt Web Applications** - URL is "http://www.uark.edu/ua/modphys/markup/LearnItWeb.html"

Individual web-apps for current classes:

- **BohrIt** - Production; URL is "http://www.uark.edu/ua/modphys/markup/BohrItWeb.html"
- **BounceIt** - Production; URL is "http://www.uark.edu/ua/modphys/markup/BounceItWeb.html"
- **BoxIt** - Production; URL is "http://www.uark.edu/ua/modphys/markup/BoxItWeb.html"
- **CoulIt** - Production; URL is "http://www.uark.edu/ua/modphys/markup/CoulItWeb.html"
- **Cycloidulum** - Production; URL is "http://www.uark.edu/ua/modphys/markup/CycloidulumWeb.html"
- **JerkIt** - Production; URL is "http://www.uark.edu/ua/modphys/markup/JerkItWeb.html"
- **MolVibes** - Production; URL is "http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html"
- **Pendulum** - Production; URL is "http://www.uark.edu/ua/modphys/markup/PendulumWeb.html"
- **QuantIt** - Production; URL is "http://www.uark.edu/ua/modphys/markup/QuantItWeb.html"

The old relativity website (2005):

- **Relativity - Pirelli Entrant** - Production; URL is "http://www.uark.edu/ua/pirelli" or "http://www.uark.edu/ua/pirelli/html/default.html"

Newer relativity web-apps currently being developed (2013-)

- **RelativIt** Production; URL is "http://www.uark.edu/ua/modphys/markup/RelativItWeb.html"
- **RelaWavity** Production; URL is "http://www.uark.edu/ua/modphys/markup/RelaWavityWeb.html"

Additional classical web-apps:

- **Trebuchet** Production; URL is "http://www.uark.edu/ua/modphys/markup/TrebuchetWeb.html"
- **WaveIt** Production; URL is "http://www.uark.edu/ua/modphys/markup/WaveItWeb.html"

Link to master list of all Harter-Soft Web Apps & Textbooks (Prod, Testing, & Development)

[http://www.uark.edu/ua/modphys/testing/markup/Harter-SoftWebApps.html](http://www.uark.edu/ua/modphys/testing/markup/Harter-SoftWebApps.html)