Shape Phase Transitions in Molecular and Nuclear Structure

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Overview

1. **Introduction**
   - A Primer on the Algebraic Approach
   - A Pedestrian Primer on QPTs

2. **Molecular Structure: Bending Dynamics**
   - Some Considerations on Molecular Spectroscopy
   - Single Bender: The 2DVM
   - Phase Diagram of the 2DVM
   - Comparison with Experimental Data

3. **More Complex Systems**
   - Coupled Molecular Benders
   - Nuclear Structure: the Interacting Boson Model

4. **Concluding Remarks**
Outline

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4 Concluding Remarks
Algebraic Approach Basic Steps

- Definition of the **Spectrum Generating Algebra (SGA)**, aka **Dynamical Algebra**, for the system under study.
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- Every operator is expressed in terms of the SGA generators.
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- Dynamical symmetries’ branching rules and Casimir operators eigenvalues.
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- Dynamical symmetries’ branching rules and Casimir operators eigenvalues.
- Phenomenological Approach: find parameter values that optimize the agreement with experimental data.
Definitions: Spectrum Generating Algebra (SGA)

Definition

The **Spectrum Generating Algebra (SGA)** is such that its generators allow to connect the eigenstates of the system’s Hamiltonian. Thus, the system’s Hilbert space carries an irreducible representation (irrep) of the SGA. The Hamiltonian and every other operator of interest are written in terms of the SGA generators.
Definitions: Symmetry Algebra & Dynamical Symmetry

**Definition**

The *Symmetry Algebra (SA)* is a subalgebra of the SGA containing the SGA generators that commute with the Hamiltonian operator. Degenerate eigenstates carry SA irreps.
Definitions: Symmetry Algebra & Dynamical Symmetry

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**Definition**

**Dynamical Symmetries (DS)** are subalgebra chains starting in the SGA and ending in the SA. They represent limiting physical situations that are analytically solvable. Each DS provides a basis to carry out the calculations.
Algebraic Approach to Molecules and Nuclei


Study of $N$-dimensional systems $\Rightarrow U(N + 1)$ SGA

**Nuclei**

- Quadrupole degree of freedom: $N = 5$
- SGA: $U(6)$
- Interacting Boson Model IBM
- A. Arima y F. Iachello
  *Phys. Rev. Lett.* **35** 1069 (1975)
- IBM-2, IBM-3, IBFM, SUSY...
Algebraic Approach to Molecules and Nuclei


Study of $N$–dimensional systems $\Rightarrow U(N + 1)$ SGA

Molecules

- Dipolar interaction: $N = 3$
- SGA: $U(4)$
- Vibron Model (VM)
- F. Iachello
- 1D and 2D limits of the Vibron Model

Chlorine monofluoride

162.81 pm
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Simple Concepts on Classical Phase Transitions

Phase and Phase Transition

Phase state of matter that is uniform throughout, both in its chemical composition and its physical properties.

Phase Transition marked by an abrupt change in one or more properties of the system.

Most stable phase is the one with the lowest thermodynamic potential ($\Phi$) which is a function of variable parameters ($F(T,V)\), $F(T,B)$, $G(T,p)$, $G(T,M)$).

$\Phi$ is analogous to the potential energy, $V(x)$, of a particle: systems like minimum energy states, in potential minima.
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Transition Parameters and Classification

Control and Order Parameters

Control Parameters parameters of the thermodynamical potential $\Phi$ that can be changed arbitrarily and smoothly (e.g. $T$, $p$, external $B$).

Order Parameters observables that are changing as the control parameters are varied. Typically they are zero in one phase and different from zero in the other one.
## Transition Parameters and Classification

### Control and Order Parameters

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**Order Parameters** observables that are changing as the control parameters are varied. Typically they are zero in one phase and different from zero in the other one.

### Classification

- **First Order** Involve latent heat.
- **Continuous** Does not involve latent heat.
Quantum Phase Transitions

Let’s consider a system that is composed by two parts, having each one a different symmetry: $G_1$ and $G_2$.

QPT occurs at some critical value $(x_c)$ of the control parameter $x$, that controls an interaction strength in the system’s Hamiltonian $H(x)$, is varied.

$$\hat{H} = x\hat{H}_1 + (1-x)\hat{H}_2$$

At the critical point:

1. The ground state energy $E_0$ is nonanalytic.
2. The gap $\Delta$ between the first excited state and the ground state vanishes.
QPT Critical Point

Energy Gap

Order Parameter

Ground State Energy

Control Parameter

Control Parameter

Control Parameter

$\chi_c$

continuous

first order

continuous

first order

continuous

first order

$\chi_c$
First order transitions (blue) and Continuous transitions (red)
Shape Phase Transitions

Ground State Quantum Phase Transitions

Singlarities in the evolution of the system’s ground state properties (shape phase transitions) as a control parameter is varied (aka zero-temperature phase transitions).

Shape Phase Transitions

**Ground State Quantum Phase Transitions**

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Shape phase transitions strictly take place at the thermodynamic limit (large $N$): importance of precursors for mesoscopic systems and the scaling behavior of the relevant quantities.
Excited State Quantum Phase Transitions

Is this behavior extensible to states throughout the excitation spectrum? Yes

ESQPT are universal to two-level pairing many-body models for both bosonic and fermionic constituents.


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Molecular Spectroscopy: Water

Example: H$_2$O, $\tilde{X}$ electronic state, $C_{2v}$ symmetry

Modern spectroscopy techniques allow the precise measurement of highly-excited rovibrational molecular states (approx. $10^5$ experimental term energies).
Molecular Spectroscopy: Water

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Rotational excitation: asymmetric rotor

H₂O: $J_{K_A K_C}$, $1_{01} = 23.79 \text{ cm}^{-1}$, $1_{10} = 42.37 \text{ cm}^{-1}$

$\rightarrow E_{rot} \simeq 10 \text{ cm}^{-1} \simeq 0.0012 \text{ eV}$
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Vibrational excitation, water normal modes

H$_2$O, stretching: A symm. $\nu_1 = 3657.053$ cm$^{-1}$;
B symm. $\nu_3 = 3755.029$ cm$^{-1}$ $\rightarrow E_{str} \simeq 0.4$ eV
H$_2$O, bending: A symm. $\nu_2 = 1594.746$ cm$^{-1}$ $\rightarrow E_{bend} \simeq 0.1$ eV
Molecular bending vibrations

Different experimental techniques to access different energy scales involved.

Many experimental energy levels.

Experimental errors $\leq 1/1000$.

Highly-excited bending overtones at reach.
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QPTs in Molecular and Nuclear Structure
The 2D Limit of the Vibron Model (2DVM)

The 2D limit of the vibron model is the simplest two-level model which still retains a non-trivial angular momentum quantum number.

It has been successfully applied to the modeling of the bending vibrational dynamics of several molecular species.

The 2D limit of the vibron model (2DVM)

Boson Operators: \( \{ \tau_{\alpha}^{\dagger}, \tau_{\alpha}, \sigma^{\dagger}, \sigma \}; \alpha = x, y \)

\[
\left[ \tau_i, \tau_j^{\dagger} \right] = \delta_{i,j}; \; i, j = x, y \quad \left[ \sigma, \sigma^{\dagger} \right] = 1
\]
The 2D limit of the vibron model (2DVM)

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\left[ \tau_i, \tau^{\dagger}_j \right] = \delta_{i,j} \quad ; \quad i, j = x, y \quad \quad \quad [\sigma, \sigma^{\dagger}] = 1
\]

Circular Bosons

\[
\tau^{\dagger}_{\pm} = \mp \frac{\tau^{\dagger}_x \pm i \tau^{\dagger}_y}{\sqrt{2}} \quad , \quad \tau_{\pm} = \mp \frac{\tau_x \mp i \tau_y}{\sqrt{2}}
\]
The 2D limit of the vibron model (2DVM)

Boson Operators: \( \{ \tau_{\alpha}^\dagger, \tau_{\alpha}, \sigma^\dagger, \sigma \}; \alpha = x, y \)

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\left[ \sigma, \sigma^\dagger \right] &= 1
\end{align*}
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Circular Bosons

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\tau_{\pm}^\dagger = \mp \frac{\tau_x^\dagger \pm i\tau_y^\dagger}{\sqrt{2}}, \quad \tau_{\pm} = \mp \frac{\tau_x \mp i\tau_y}{\sqrt{2}}
\]

Generators of the \( U(3) \) SGA

\[
\{ \hat{n}, \hat{n}_s, \hat{l}, \hat{Q}_{\pm}, \hat{R}_{\pm}, \hat{D}_{\pm} \}
\]

2DVM Dynamical Symmetries and Hamiltonian

Dynamical Symmetries

\[ U(3) \supset U(2) \supset SO(2) \quad \text{Dyn. Symmetry (I)} \]
\[ N \quad n \quad \ell \]

\[ U(3) \supset SO(3) \supset SO(2) \quad \text{Dyn. Symmetry (II)} \]
\[ N \quad w \quad \ell \]
2DVM Dynamical Symmetries and Hamiltonian

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\[
\begin{align*}
U(2) & \quad \hat{C}_1[U(2)] = \hat{n} & \hat{C}_2[U(2)] = \hat{n}(\hat{n} + 1) \\
SO(3) & \quad \hat{C}_2[SO(3)] = \hat{W}^2 = \frac{\hat{D}_+\hat{D}_- + \hat{D}_-\hat{D}_+}{2} + \hat{\ell}^2 \\
SO(2) & \quad \hat{C}_1[SO(2)] = \hat{\ell} & \hat{C}_2[SO(2)] = \hat{\ell}^2
\end{align*}
\]
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SO(3) \quad \hat{C}_2[SO(3)] = \hat{W}^2 = \frac{\hat{D}_+ \hat{D}_- + \hat{D}_- \hat{D}_+}{2} + \hat{l}^2
\]

\[
SO(2) \quad \hat{C}_1[SO(2)] = \hat{l} \quad \hat{C}_2[SO(2)] = \hat{l}^2
\]

General one- and two-body Hamiltonian operator

\[
\hat{H} = \varepsilon \hat{n} + \alpha \hat{n}(\hat{n} + 1) + \beta \hat{l}^2 + A\hat{P}
\]
Cylindrical Oscillator Dynamical Symmetry

\[ U(3) \supset U(2) \supset SO(2) \]

\[
\begin{align*}
[N] & \quad n \quad \ell \\
N & = N, N-1, N-2, \ldots, 0 \\
\ell & = \pm n, \pm (n-2), \ldots, 1 \text{(or 0)}
\end{align*}
\]
Cylindrical Oscillator Dynamical Symmetry

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\[ \ell = \pm n, \pm(n-2), \ldots, 1 \text{(or 0)} \]

rigidly linear
Displaced Oscillator Dynamical Symmetry

\[
U(3) \supset SO(3) \supset SO(2)
\]

\[
\begin{align*}
\omega &= N, N - 2, N - 4, \ldots, 1 \text{ (or 0)} \\
\ell &= \pm \omega, \pm (\omega - 1), \ldots, 0 \\
\nu &= \frac{N - \omega}{2} = 0, 1, \ldots, \frac{N - 1}{2} \text{ (or } \frac{N}{2} \text{)} \\
\ell' &= 0, \pm 1, \pm 2, \ldots, \pm (N - 2\nu)
\end{align*}
\]
Displaced Oscillator Dynamical Symmetry

\[ U(3) \supset SO(3) \supset SO(2) \]

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N & \quad \omega \\
\omega & = N, N - 2, N - 4, \ldots, 1 (\text{or } 0) \\
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$$U(3) \supset SO(3) \supset SO(2)$$

$$\omega = N, N - 2, N - 4, \ldots, 1(\text{or } 0)$$

$$\ell = \pm \omega, \pm (\omega - 1), \ldots, 0$$

$$v = \frac{N - \omega}{2} = 0, 1, \ldots, \frac{N - 1}{2} (\text{or } \frac{N}{2})$$

$$\ell = 0, \pm 1, \pm 2, \ldots, \pm (N - 2v)$$

rigidly bent

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Single Bender Model Hamiltonian

\[ U(3) \supset U(2) \supset SO(2) \quad \text{Dynamical Symmetry (I)} \]
\[ U(3) \supset SO(3) \supset SO(2) \quad \text{Dynamical Symmetry (II)} \]
Single Bender Model Hamiltonian

\[ \hat{H} = \varepsilon \left[ (1 - \xi)\hat{n} + \frac{\xi}{N - 1} \hat{P} \right] \]

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The system undergoes a second order QPT in \( \xi_c = 0 \).
**Single Bender Model Hamiltonian**

\[ \hat{H} = \varepsilon \left[ (1 - \xi) \hat{n} + \frac{\xi}{N - 1} \hat{P} \right] \]

- \( \varepsilon \): energy scale
- \( \xi \): control parameter: \( \xi \in [0, 1] \)
  - \( \xi = 0.0 \) rigidly-linear
  - \( 0.0 < \xi \leq 0.2 \) quasilinear
  - \( 0.2 < \xi < 1.0 \) non-rigid
  - \( \xi = 1.0 \) rigidly-bent

**Dynamical Symmetry (I)**

\[ U(3) \supset U(2) \supset SO(2) \]

**Dynamical Symmetry (II)**

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Single Bender Model Hamiltonian

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The system undergoes a second order QPT in \(\xi_c = 0.2\).
Correlation Energy Diagram

The diagram shows the energy as a function of the control parameter ($\xi$) for different energy levels. The labels $u(2)$ and $so(3)$ indicate specific energy levels or states. The energy is plotted in arbitrary units on both the y-axes and x-axes, with energy levels ranging from 0 to 1 and control parameter ranging from 0 to 1.
Spectroscopic Signatures: Birge-Sponer Plot

\[ B_{u+1} - B_u \text{ (arbitrary units)} \]

\[ \nu = 2 \frac{u}{N} \]

Spectroscopic Signatures: Birge-Sponer Plot

Spectroscopig Signatures: Quantum Monodromy Plot

![Energy vs. Angular Momentum](image-url)
ESQPT in the 2DVM

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Application to Single Bender Molecular Species

Dynamical Symmetry (I): HCN

(a) Birge-Sponer Plot
(b) Monodromy Plot
(c) Bending Potential
(d) Molecule Model
Dynamical Symmetry (II): H$_2$S

(a) Birge-Sponer Plot  
(b) Monodromy Plot  
(c) Bending Potential  
(d) Molecule Model
Quasilinear Species: MgOD

(a) Birge-Sponer Plot
(b) Monodromy Plot
(c) Bending Potential
(d) Molecule Model
Nonrigid Species: $\text{H}_2\text{O}$

(a) Birge-Sponer Plot
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Algebraic approach to coupled benders

Dynamical Algebra: $U_1(3) \times U_2(3)$

$$\sigma_j , \quad \tau_{j,\pm} = \mp \frac{\tau_{j,x} \pm i \tau_{j,y}}{\sqrt{2}} \quad , \quad j = 1, 2.$$
Algebraic approach to coupled benders

Dynamical Algebra: $U_1(3) \times U_2(3)$

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$$\sigma j, \quad \tau^\dagger_j, \pm = \mp \frac{\tau^\dagger_j, x \pm i \tau^\dagger_j, y}{\sqrt{2}}, \quad j = 1, 2.$$  

\[
\begin{array}{ccc}
U_1(3) \otimes U_2(3) & \supset & U_1(2) \otimes U_2(2) \\
\supset & \supset & \supset \quad \supset \\
SO_1(2) \otimes SO_2(2) & \supset & SO_{12}(2), \\
\supset & \supset & \supset \quad \supset \quad \supset \\
SO_1(2) \otimes SO_2(2) & \supset & SO_{12}(2), \\
\supset & \supset & \supset \quad \supset \\
SO_{12}(3) & \supset & SO_{12}(2), \\
\supset & \supset & \supset \quad \supset \\
U_{12}(2) & \supset & SO_{12}(2), \\
\supset & \supset & \supset \quad \supset \\
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\supset & \supset & \supset \quad \supset \\
U_{12}(3) & \supset & SO_{12}(2), \\
\end{array}
\]

Block Dimensions in the Coupled Benders Hamiltonian

Two-fluid model: huge increase in matrix dimensions.
**Block Dimensions in the Coupled Benders Hamiltonian**

Two-fluid model: huge increase in matrix dimensions.

![Graph showing Hamiltonian Block Dimension vs. U(3) totally symmetric irrep [N]](image-url)
Coupled Benders Hamiltonian (ABBA molecules)

**Model Hamiltonian** (3 control parameters: \(0 \leq \xi \leq 1\), \(\eta_1\), and \(\eta_2 < 0\))

\[
\hat{H} = \varepsilon \left\{ (1 - \xi) \left[ \hat{n}_1 + \hat{n}_2 + \frac{\eta_1}{N} \hat{Q}_1 \cdot \hat{Q}_2 \right] + \frac{\xi}{N} \left[ \hat{P}_1 + \hat{P}_2 + 2\eta_2 \hat{W}_1 \cdot \hat{W}_2 \right] \right\}
\]
Coupled Benders Hamiltonian (ABBA molecules)

Model Hamiltonian (3 control parameters: $0 \leq \xi \leq 1$, $\eta_1$, and $\eta_2 < 0$)

$$\hat{H} = \varepsilon \left\{ (1 - \xi) \left[ \hat{n}_1 + \hat{n}_2 + \frac{\eta_1}{N} \hat{Q}_1 \cdot \hat{Q}_2 \right] + \frac{\xi}{N} \left[ \hat{P}_1 + \hat{P}_2 + 2\eta_2 \hat{W}_1 \cdot \hat{W}_2 \right] \right\}$$

Linear, $D_{\infty h}$
- $r_1 = r_2 = 0$
- $(C_2H_2, \tilde{X})$

Cis, $C_{2v}$
- $r_1 r_2 > 0$, $\phi = 0$
- $(C_2H_2, cis-\tilde{A})$

Trans, $C_{2h}$
- $r_1 r_2 < 0$, $\phi = 0$
- $(C_2H_2, trans-\tilde{A})$

Non-planar, $C_2$
- $r_1 = r_2 \neq 0$
- $0 < \phi \leq \frac{\pi}{2}$ (H$_2$O$_2$)

Coupled Benders Phase Diagram

$\tilde{A}_1A_u$ trans-$\text{C}_2\text{H}_2$ spectrum: \textit{J. Chem. Phys.} \textbf{140}, 014304 (2014)
$\tilde{A}_1A_u$ trans-$C_2H_2$ spectrum: *J. Chem. Phys.* **140**, 014304 (2014)


Int. Symp. on Molec. Spect. 2012
The Interacting Boson Model and his Kin

**Interacting Boson Model (IBM)**

- Low-lying States Medium-Heavy Even–Even Nuclei
- Dynamical Algebra: $U(6)$
- Boson operators: $s$ ($\ell = 0$) and $d$ ($\ell = 2$)
- IBM-2, IBM-3, IBFM, SUSY in nuclei.
The IBM: Approximations

1. Only valence nucleons determine the dynamics of the low-lying collective levels in nuclei.
2. These nucleons are paired to angular momenta $L = 0$ or $L = 2$.
3. Fermion pairs are treated as bosons: $s$ and $d$ Commutation relations:

\[
\begin{align*}
[s, s^\dagger] &= 1, \\
[\tilde{d}_\mu, d_{\mu'}^\dagger] &= \delta_{\mu,\mu'}, \quad \mu = \pm 2, \pm 1, 0
\end{align*}
\]
Structure: Definition of the $N$ Value

$^{114}\text{Xe}$

$p$

IBM

$d$

$\varepsilon$

$s$

$N=7$
IBM Dynamical Symmetries and Model Hamiltonian

Dynamical Symmetries

\[ \begin{align*}
U(6) & \supset U(5) \supset SO(5) \supset SO(3) \quad \text{Vibrational} \\
N & \quad n \\
U(6) & \supset SU(3) \supset SO(3) \quad \text{Rotational} \\
N & \quad (\lambda, \mu) \\
U(6) & \supset SO(6) \supset SO(5) \quad \text{Gamma Soft} \\
N & \quad \sigma
\end{align*} \]
IBM Dynamical Symmetries and Model Hamiltonian

### Dynamical Symmetries

<table>
<thead>
<tr>
<th>U(6)</th>
<th>U(5)</th>
<th>SO(5)</th>
<th>SO(3)</th>
<th>Vibrational</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>n</td>
<td>τ</td>
<td>δℓ</td>
<td></td>
</tr>
<tr>
<td>U(6)</td>
<td>SU(3)</td>
<td>SO(3)</td>
<td></td>
<td>Rotational</td>
</tr>
<tr>
<td>N</td>
<td>(λ, μ)</td>
<td></td>
<td>κℓ</td>
<td></td>
</tr>
<tr>
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<td>SO(3)</td>
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<td>σ</td>
<td>τ</td>
<td>δℓ</td>
<td></td>
</tr>
</tbody>
</table>

### Model Hamiltonian

\[
H_\chi(\eta) = a \left[ \eta \hat{n}_d - \frac{1 - \eta}{N} \hat{Q}_\chi \cdot \hat{Q}_\chi \right]
\]
Nuclear Shapes and Spectra

Gamma-soft

\( R_{4/2} = 2.5 \)

\( 0^+ \)

\( 2^+ \)

\( 4^+ \)

Prolate

\( R_{4/2} = 3.33 \)

\( 0^+ \)

\( 2^+ \)

\( 4^+ \)

Spherical

\( R_{4/2} = 2 \)

\( 0^+ \)

\( 2^+ \)

\( 4^+ \)

Curro Pérez Bernal

QPTs in Molecular and Nuclear Structure
Interacting Boson Model Phase Diagram

Fingerprints of Shape Phase Transitions in Nuclei

Energy Ratios

Ground-state QPT signatures in nuclei

\[ E(4_i^+) \] vs. \[ E(2_i^+) \] [MeV]

- Shape-phase transition!
- Vibrational 2.00
- Rotational 3.33

All nuclei with \( E(2_i^+) < 600 \text{ keV} \)

Casten et al., PRL 71, 227 (1993)
Signatures of First-Order Phase Transition

Two-Neutron Separation Energies

Concluding Remarks

Conclusions

- Algebraic models useful probe of origins and fundamental properties of QPTs in many-body systems.
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Thanks for your kind attention...
Algebraic models useful probe of origins and fundamental properties of QPTs in many-body systems.

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Open questions and problems: connection with Quantum Optics and Spin Chains, ESQPT in coupled systems, normal-local transitions in benders. Some clues in Pedro Pérez’s talk on Thursday...

Thanks for your kind attention...
The Usual Suspects

- Francesco Iachello, Danielle Larese, Patrick H. Vaccaro (Yale University, USA)
- Andrea Vitturi, Lorenzo Fortunato (Padova University, Italy)
- Jorge Dukelsky and Armando Relaño (IEM-CSIC, Spain)
- Pavel Cejnar (Charles University, Czech Republic)
- Piet van Isacker (GANIL, France)
- Manuel Calixto and Elvira Romera (University of Granada, Spain)
- Octavio Castaños, Renato Lemus, Alejandro Frank (ICN-UNAM, Mexico)
- José Miguel Arias, Miguel Carvajal, José E. García-Ramos, FPB, Pedro Pérez-Fernández (US-UHU, Spain)
Molecular Spectroscopy: Acetylene

Example: $\text{C}_2\text{H}_2$, $\tilde{X}$ electronic state, $\mathcal{D}_{\infty h}$ symmetry

**Rotational excitation:** $\text{C}_2\text{H}_2$, $\tilde{X}$: rotational $\simeq 10 \text{ cm}^{-1} \simeq 0.001 \text{ eV}$

**Vibrational excitation:**
- $\text{C}_2\text{H}_2$, $\tilde{X}$: stretching $\simeq 2000 - 3500 \text{ cm}^{-1} \simeq 0.2 - 0.4 \text{ eV}$
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Electronic excitation
- $\text{C}_2\text{H}_2$, $\tilde{A}$ state
  - $D_{2h}$ symmetry (non-linear trans)
  - Energy $\simeq 42000 \text{ cm}^{-1} \simeq 5 \text{ eV}$

Quasilinear Species: MgOX

Model Hamiltonian

\[ \hat{H} = E_0' + \varepsilon \hat{n} + A\hat{P} \]
Quasilinear Species: MgOX

Model Hamiltonian
\[ \hat{H} = E_0' + \varepsilon \hat{n} + A \hat{P} \]

<table>
<thead>
<tr>
<th>$N_D$</th>
<th>$N_H$</th>
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</thead>
<tbody>
<tr>
<td>140</td>
<td>107</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>$\epsilon$ (cm$^{-1}$)</th>
<th>$A$ (cm$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>467.0(5)</td>
<td>0.8194(13)</td>
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</tbody>
</table>

$rms_D$ (cm$^{-1}$) | $rms_H$ (cm$^{-1}$) |
<table>
<thead>
<tr>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>6.1</td>
<td>4.7</td>
</tr>
</tbody>
</table>

ESQPT in the 2DVM

ESQPT in the 2DVM

- **Excitation Energy (E/N, arbitrary units)**
- **Control Parameter (\(\xi\))**

Legend:
- \(u(2)\)
- \(so(3)\)
ESQPT in the 2DVM

Log(Fidelity Susceptibility) vs Control Parameter $\zeta$
# IBM Dynamical Symmetries and Hamiltonian

**Dynamical Symmetries**

<table>
<thead>
<tr>
<th>$U(6)$</th>
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<tbody>
<tr>
<td>$N$</td>
<td>$n$</td>
<td>$\tau$</td>
<td>$\delta \ell$</td>
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<tr>
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<tr>
<td>$N$</td>
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<th>$U(6)$</th>
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<tr>
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</table>

General one- and two-body Hamiltonian operator:

$$H = \epsilon_s s_s^\dagger + \epsilon_d d_d^\dagger \cdot \tilde{d} + u_0 (s_s^\dagger)^2 s_s^2(1) + u_2 s_s^\dagger d_d^\dagger \cdot \tilde{d} ds + v_0 \left[ d_d^\dagger \cdot d_d^\dagger s_s^2 + h.c. \right](2) + v_2 \left[ (d_d^\dagger \times d_d^\dagger)^2 \cdot \tilde{d} ds + h.c. \right](3) + \sum_{L=0,2,4} C_L (d_d^\dagger \times d_d^\dagger) (L) \cdot (\tilde{d} \times \tilde{d}) (L) (4)$$
IBM Dynamical Symmetries and Hamiltonian

### Dynamical Symmetries

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Group</th>
<th>Subgroup</th>
<th>Subgroup</th>
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### General one- and two-body Hamiltonian operator

\[
H = \epsilon_s s^\dagger s + \epsilon_d d^\dagger \cdot \tilde{d} + u_0 \left( s^\dagger \right)^2 s^2
\]  
\[
+ u_2 s^\dagger d^\dagger \cdot \tilde{d}s + v_0 \left[ d^\dagger \cdot d^\dagger s^2 + h.c. \right]
\]
Signatures of First-Order Phase Transition

Two-Neutron Separation Energies

Signatures of First-Order Phase Transition

\[ B(E2) \text{ for } 2^+_1 \rightarrow 0^+_1 \text{ and } 4^+_1 \rightarrow 2^+_1 \quad \text{PRC 68 024307 (2003)} \]