Shape Phase Transitions in Molecular and Nuclear Structure

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Overview

Outline

Algebraic Approach Basic Steps

- Definition of the Spectrum Generating Algebra (SGA), aka Dynamical Algebra, for the system under study.

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- Consideration of the possible Dynamical Symmetries.
- 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.

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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.

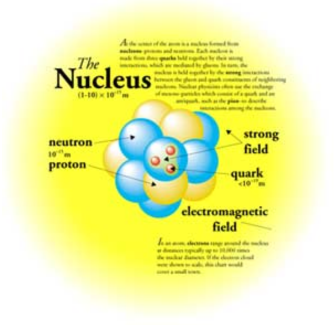
Algebraic Approach to Molecules and Nuclei

F. Iachello, *Contemp. Math.* 160 151 (1994)

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...



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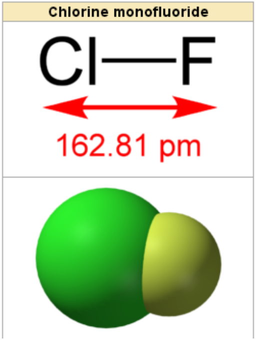
Study of N–dimensional systems $\Rightarrow U(N+1)$ SGA

Molecules

- Dipolar interaction: $N = 3$
- SGA: $U(4)$
- Vibron Model (VM)
- F. Iachello
  Chem. Phys. Lett. 78 581 (1981)
- 1D and 2D limits of the Vibron Model



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Simple Concepts on Classical Phase Transitions

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

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- Most stable phase is the one with the lowest thermodynamical potential (Φ) which is a function of variable parameters (F(T,V), F(T,B); G(T,p), G(T,M)).
- Φ is analogous to the potential energy, V(x), of a particle: systems like minimum energy states, in potential minima.

Transition Parameters and Classification

Control and Order Parameters

Control Parameters parameters of the thermodynamical potential Φ 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.

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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.

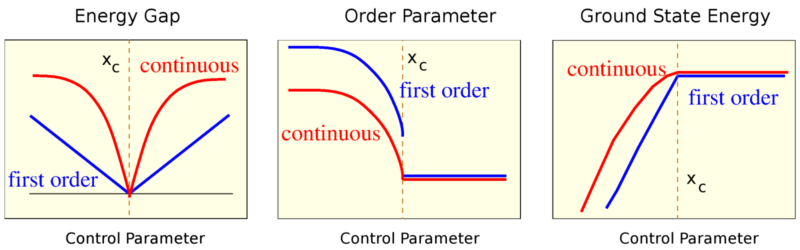
QPT occurs at some critical value (x_c) of the control parameter x, that controls an interaction strength in the system's Hamiltonian $H(x)$, is varied.

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

At the critical point:

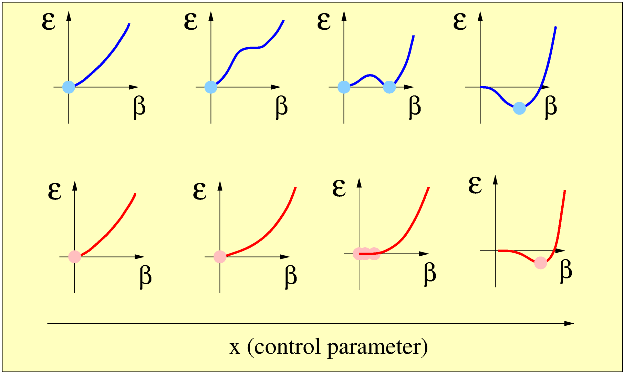
1. The ground state energy E_0 is nonanalytic.
2. The gap Δ between the first excited state and the ground state vanishes.

QPT Critical Point



Energy Surfaces

First order transitions (blue) and Continuous transitions (red)



First Order

Continuous

Shape Phase Transitions

Ground State Quantum Phase Transitions

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

P. Cejnar and J. Jolie. *Prog. Part. Nucl. Phys.* 62 210 (2009)

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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.

Shape Phase Transitions

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.

M.A. Caprio, P. Cejnar, F. Iachello. *Ann. Phys.* 323 1106 (2008).

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Outline

Molecular Spectroscopy: Water

Example: H_2O, $\tilde{X}$ electronic state, $\mathcal{C}_{2v}$ symmetry

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

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Rotational excitation: asymmetric rotor

H_2O: $J_{K_A K_C}, 1_{01} = 23.79$ cm^{-1}, $1_{10} = 42.37$ cm^{-1}
$\rightarrow E_{rot} \simeq 10$ cm^{-1} $\simeq 0.0012$ eV

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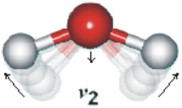
Vibrational excitation, water normal modes

H_2O, 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_2O, bending: A symm. $\nu_2 = 1594.746$ cm$^{-1} \rightarrow E_{bend} \simeq 0.1$ eV

Molecular bending vibrations

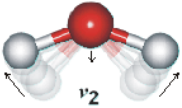


www1.lsbu.ac.uk/water

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.

Molecular bending vibrations



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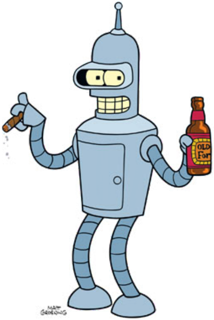

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The 2D Limit of the Vibron Model (2DVM)

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.

F. Iachello and S. Oss. *J. Chem. Phys.* 104 6956 (1996)

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

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

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

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Circular Bosons

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

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Generators of the $U(3)$ SGA

$$\{\hat{n}, \hat{n}_s, \hat{\ell}, \hat{Q}_\pm, \hat{R}_\pm, \hat{D}_\pm\}$$

FPB and F. Iachello. *Phys. Rev.* A77 032115 (2008)

2DVM Dynamical Symmetries and Hamiltonian

Dynamical Symmetries

$$\begin{array}{ccccccc} U(3) & \supset & U(2) & \supset & SO(2) & \text{Dyn. Symmetry (I)} \\ N & & n & & \ell & \\ U(3) & \supset & SO(3) & \supset & SO(2) & \text{Dyn. Symmetry (II)} \\ N & & w & & \ell & \end{array}$$

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\begin{array}{lll}
U(2) & \hat{C}_1[U(2)] = \hat{n} & \hat{C}_2[U(2)] = \hat{n}(\hat{n}+1) \\
SO(3) & \hat{C}_2[SO(3)] = \hat{W}^2 = \frac{\hat{D}_+\hat{D}_- + \hat{D}_-\hat{D}_+}{2} + \hat{\ell}^2 & \\
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General one- and two-body Hamiltonian operator

$$\hat{H} = \varepsilon\,\hat{n} + \alpha\,\hat{n}(\hat{n}+1) + \beta\,\hat{\ell}^2 + A\hat{P}$$

Cylindrical Oscillator Dynamical Symmetry

$$\begin{array}{ccccc} U(3) & \supset & U(2) & \supset & SO(2) \\ [N] & & n & & \ell \end{array}$$

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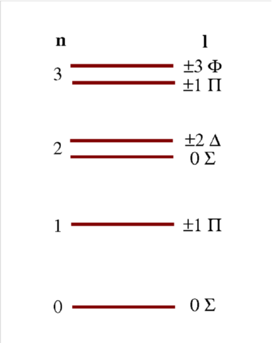

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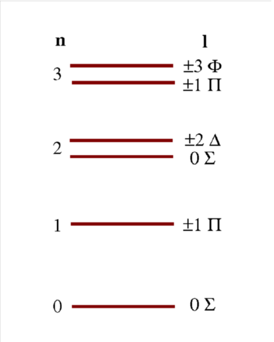

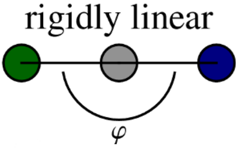

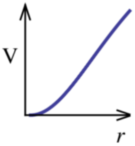

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$$\begin{aligned} \omega &= N, N-2, N-4, \ldots, 1(\text{or } 0) \\ \ell &= \pm\omega, \pm(\omega-1), \ldots, 0 \\ v &= \frac{N-\omega}{2} = 0, 1, \ldots, \frac{N-1}{2}(\text{or } \frac{N}{2}) \\ \ell &= 0, \pm 1, \pm 2, \ldots, \pm(N-2v) \end{aligned}$$

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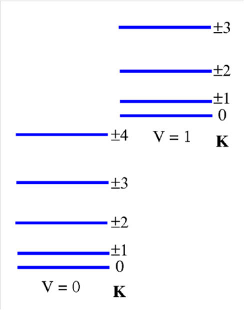

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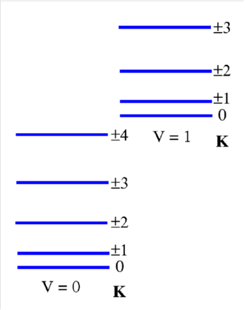

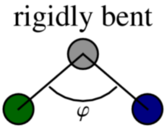

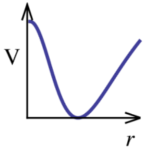

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Single Bender Model Hamiltonian

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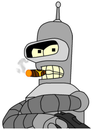
Single Bender Model Hamiltonian

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



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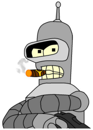

$$\hat{\mathcal{H}} = \varepsilon \left[(1-\xi)\hat{n} + \frac{\xi}{N-1}\hat{P} \right]$$

- ε: energy scale
- ξ: 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
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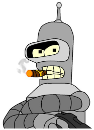

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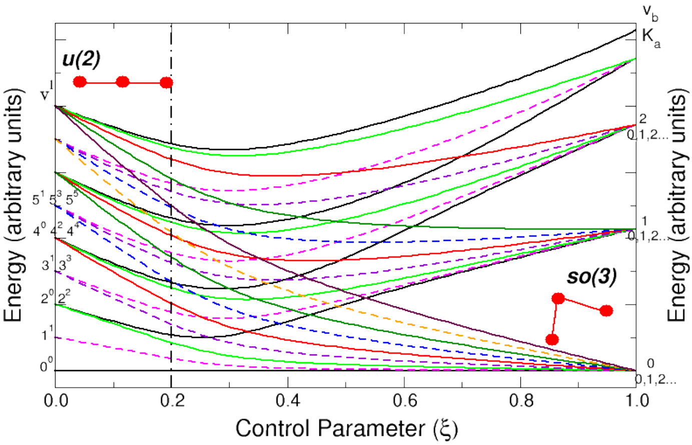
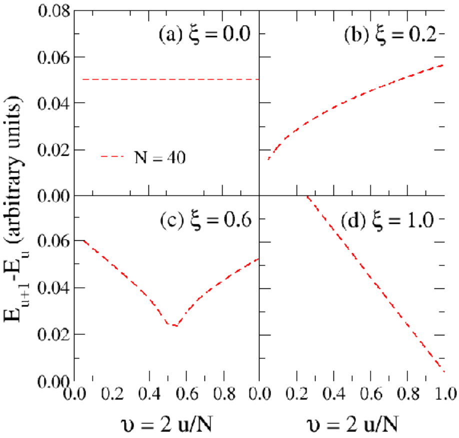
The system undergoes a second order QPT in $\xi_c = 0.2$.

Correlation Energy Diagram



Spectroscopig Signatures: Birge-Sponer Plot



R. N. Dixon *Trans. Faraday Soc.* 60 1363 (1964).

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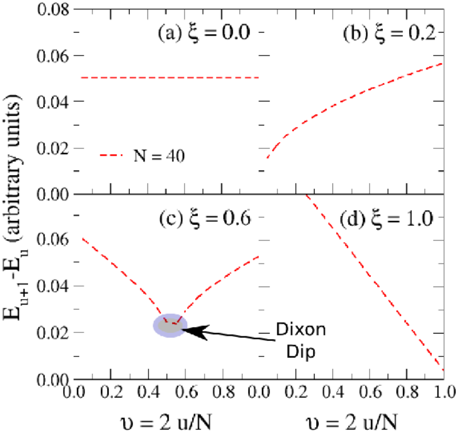

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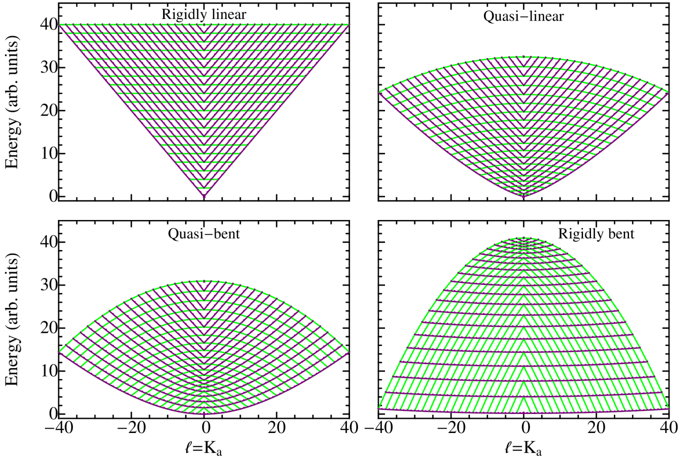
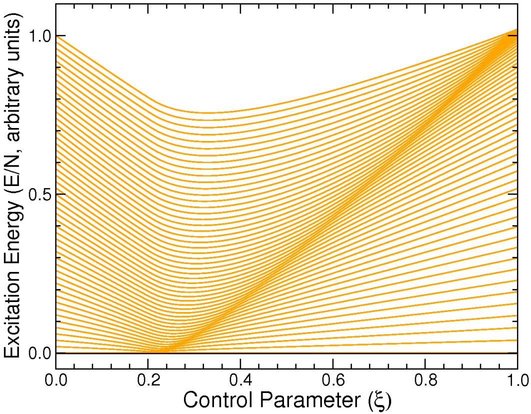
Spectroscopig Signatures: Quantum Monodromy Plot



ESQPT in the 2DVM

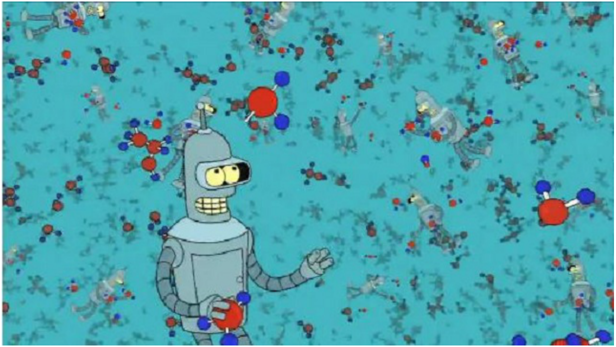


M.A. Caprio, P. Cejnar, F. Iachello. Ann. Phys. 323 1106 (2008).

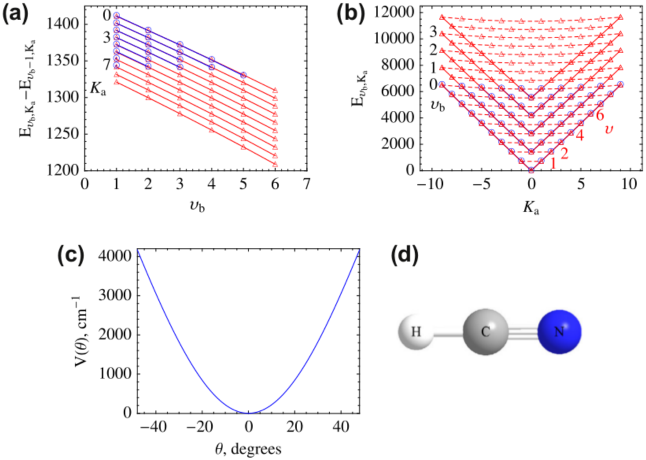
Outline

Application to Single Bender Molecular Species

- D. Larese and F. Iachello. *J. Mol. Struct.* 1006 611 (2011).
- D. Larese, FPB, and F. Iachello. *J. Mol. Struct.* 1051 310 (2013).



Dynamical Symmetry (I): HCN



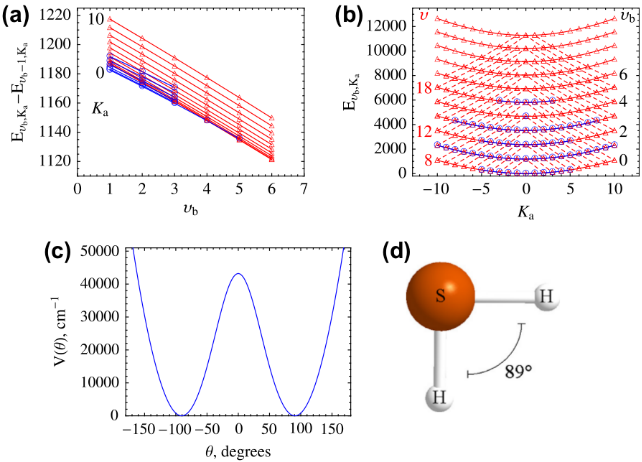
(a) Birge-Sponer Plot

(b) Monodromy Plot

(c) Bending Potential

(d) Molecule Model

Dynamical Symmetry (II): H_2S



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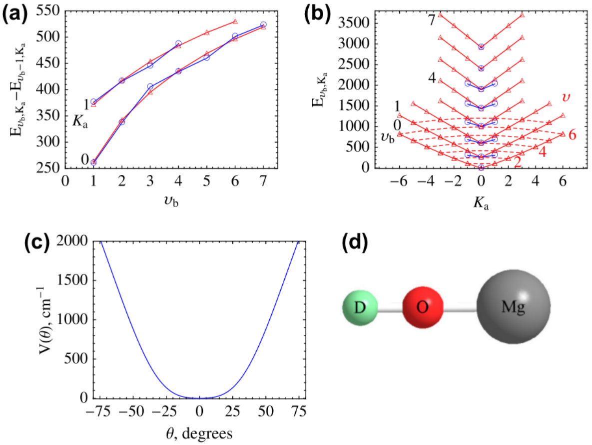

- (a) Birge-Sponer Plot
- (b) Monodromy Plot
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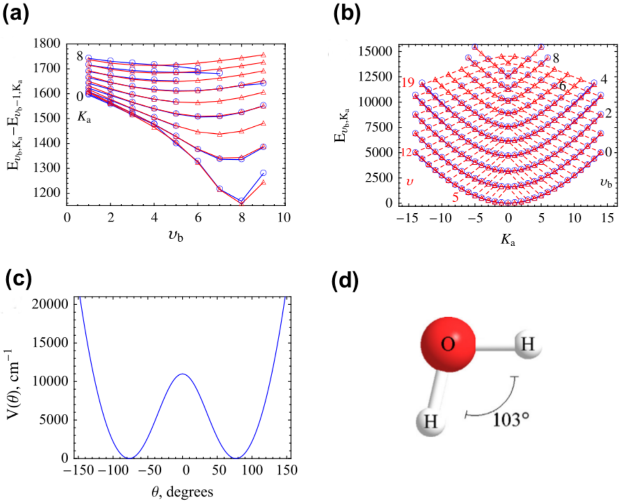
- (d) Molecule Model

Nonrigid Species: H_2O



(a) Birge-Sponer Plot
(b) Monodromy Plot
(c) Bending Potential
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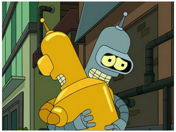
Outline

Algebraic approach to coupled benders

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

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



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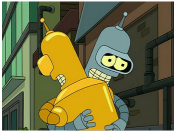

$$U_1(3) \otimes U_2(3) \supset U_1(2) \otimes U_2(2) \begin{array}{c} \nearrow SO_1(2) \otimes SO_2(2) \searrow \\ \searrow U_{12}(2) \nearrow \end{array} SO_{12}(2), \quad \begin{array}{c}(Ia)\\(Ib)\end{array}$$

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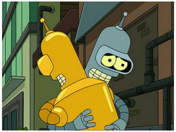

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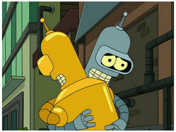

$$\begin{array}{ccccccccc}
 & & & & SO_1(2) \otimes SO_2(2) & & & & \text{(Ia)} \\
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F. Iachello and S. Oss, *J. Chem. Phys.* 104 6956 (1996).

Block Dimensions in the Coupled Benders Hamiltonian

Two-fluid model: huge increase in matrix dimensions.

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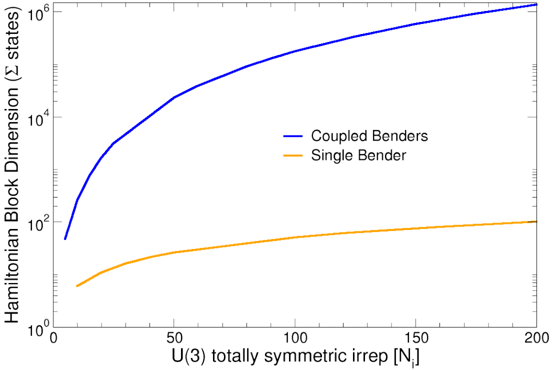

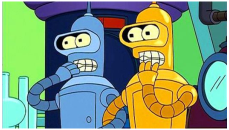

Coupled Benders Hamiltonian (ABBA molecules)

Model Hamiltonian (3 control parameters: $0 \leq \xi \leq 1$, η_1, and $\eta_2 < 0$)

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

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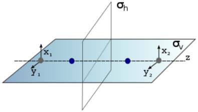
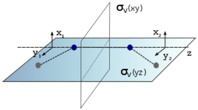
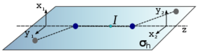
Linear, $\mathcal{D}_{\infty h}$
$r_1 = r_2 = 0$
(C_2H_2, $\tilde{X}$)



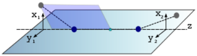
Cis, $\mathcal{C}_{2v}$
$r_1 r_2 > 0, \phi = 0$
(C_2H_2, *cis*-$\tilde{A}$)



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



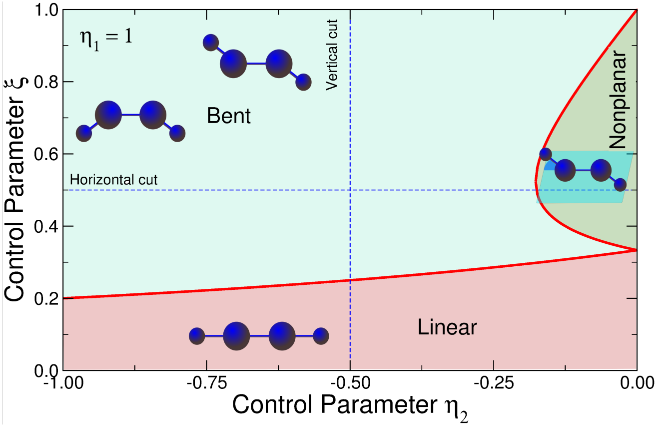
Non-planar, $\mathcal{C}_2$
$r_1 = r_2 \neq 0$
$0 < \phi \leq \frac{\pi}{2}$ (H_2O_2)



F. Iachello and FPB, *Mol. Phys.* 106 223 (2008); F. Iachello and FPB, *J. Phys. Chem. A* 113 13273 (2009);

FPB and L. Fortunato, *Phys. Lett. A* 376 236 (2012); D. Larese *et al.*, *J. Chem. Phys.* 140, 014304 (2014)

Coupled Benders Phase Diagram



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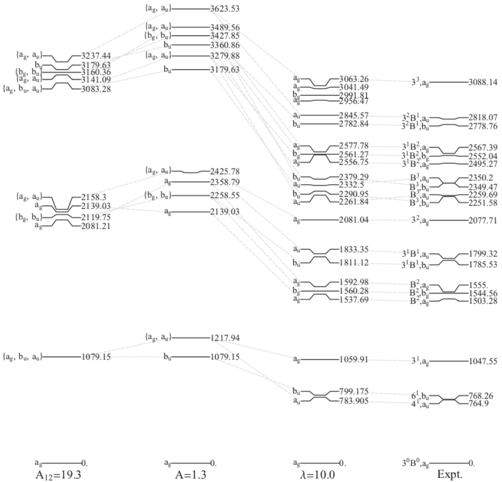
$\tilde{A}_1A_u$ trans-C_2H_2 spectrum: *J. Chem. Phys.* 140, 014304 (2014)



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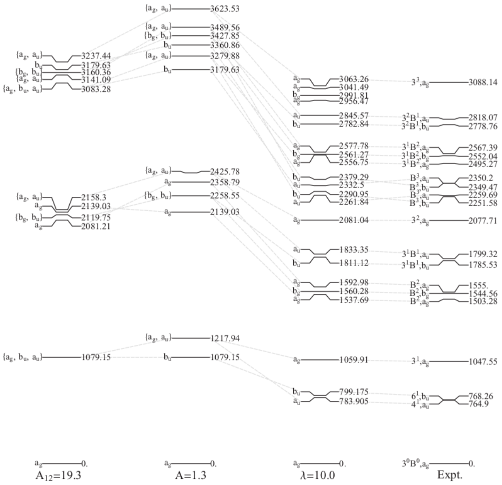
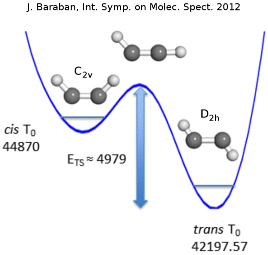


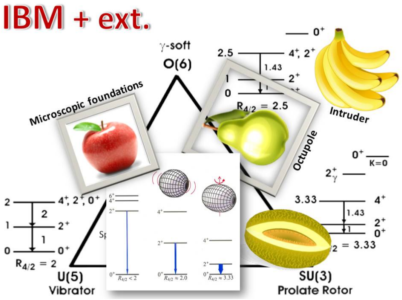


J. Baraban

Int. Symp. on Molec. Spect. 2012

Outline

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 ($\ell = 2$)
- A. Arima and F. Iachello. *Phys. Rev. Lett.* 35 1069 (1975)
- IBM-2, IBM-3, IBFM, SUSY in nuclei.

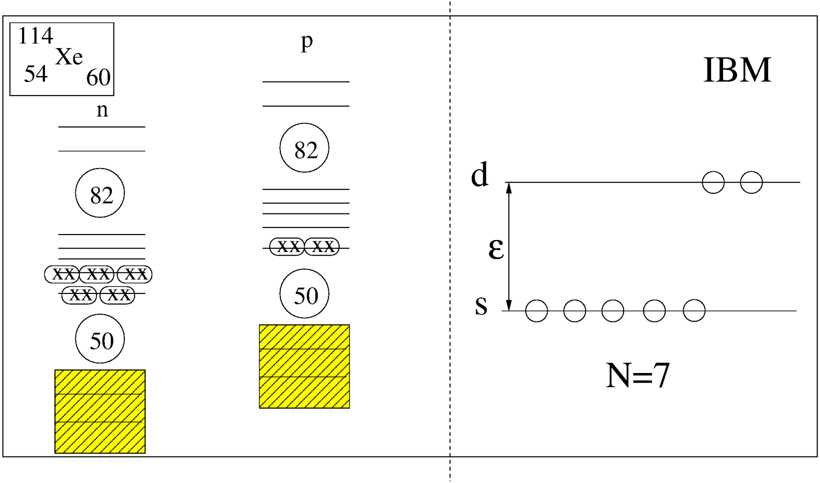
The IBM: Approximations

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:

$$\left[s, s^\dagger\right] = 1 \quad , \qquad \left[\tilde{d}_\mu, d^\dagger_{\mu\prime}\right] = \delta_{\mu,\mu'} \quad , \mu = \pm 2, \pm 1, 0$$

Structure: Definition of the N Value



IBM Dynamical Symmetries and Model Hamiltonian

Dynamical Symmetries

$U(6)$	$\supset$	$U(5)$		$\supset$	$SO(5)$	$\supset$	$SO(3)$	Vibrational
N		n			τ		$\delta\ell$	
$U(6)$	$\supset$		$SU(3)$		$\supset$		$SO(3)$	Rotational
N			(λ, μ)				$\kappa\ell$	
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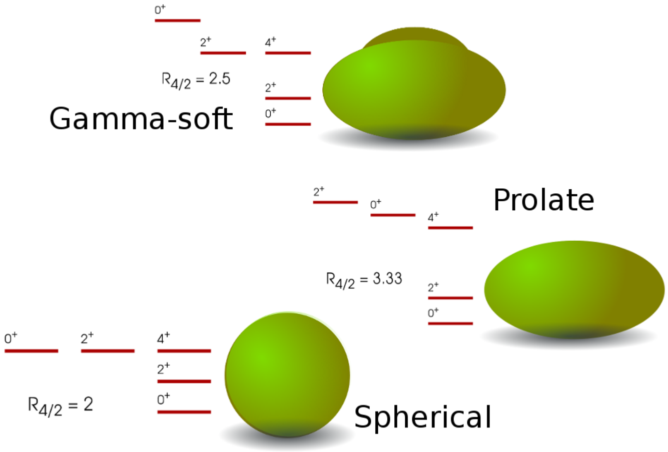
Model Hamiltonian

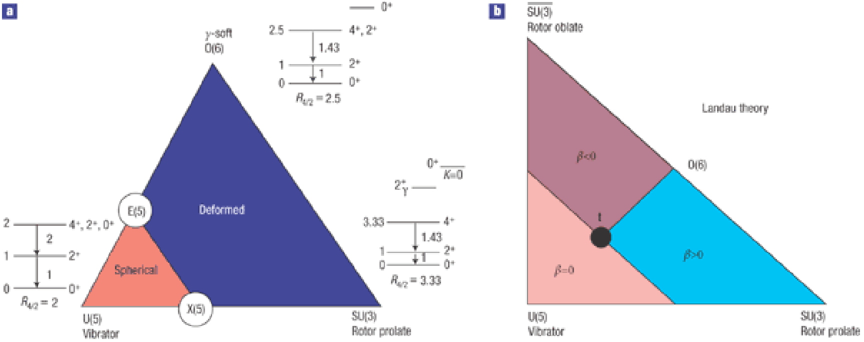
$$H_\chi(\eta) = a\left[\eta \hat{n}_d - \frac{1-\eta}{N}\hat{Q}_\chi \cdot \hat{Q}_\chi\right]$$

Nuclear Shapes and Spectra



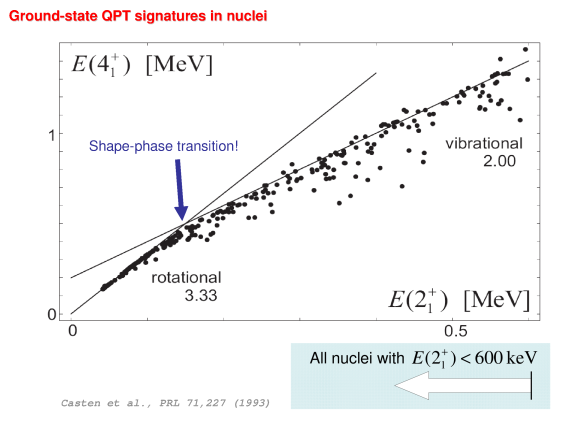
Interacting Boson Model Phase Diagram

R. F. Casten, *Nat. Phys.* 2 811 (2006)



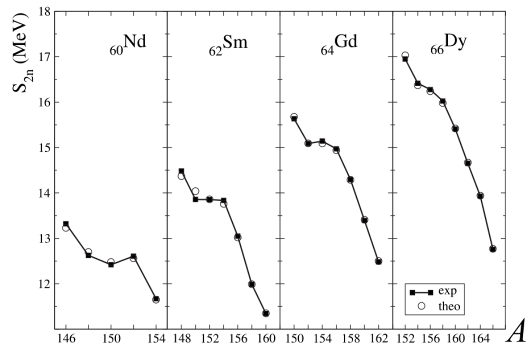
Fingerprints of Shape Phase Transitions in Nuclei

Energy Ratios



Signatures of First-Order Phase Transition

Two-Neutron Separation Energies



J. E. García-Ramos *et al.*, *Phys. Rev. C* 68 024307 (2003)

Concluding Remarks

Conclusions

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Thanks for your kind attention...

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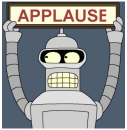

The Usual Suspects

- 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: C_2H_2, $\tilde{X}$ electronic state, $\mathcal{D}_{\infty h}$ symmetry

Rotational excitation: C_2H_2, $\tilde{X}$: rotational $\simeq 10$ cm$^{-1} \simeq 0.001$ eV

Vibrational excitation:

C_2H_2, $\tilde{X}$: stretching $\simeq 2000 - 3500$ cm$^{-1} \simeq 0.2 - 0.4$ eV

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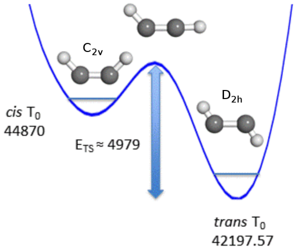
Electronic excitation

C_2H_2, $\tilde{A}$ state

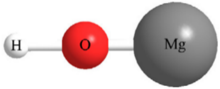
$\mathcal{D}_{2h}$ symmetry (non-linear *trans*)

Energy $\simeq 42000$ cm^{-1} $\simeq 5$ eV

J. Baraban, Int. Symp. on Molec. Spect. 2012



Quasilinear Species: MgOX



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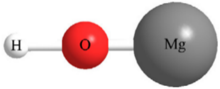

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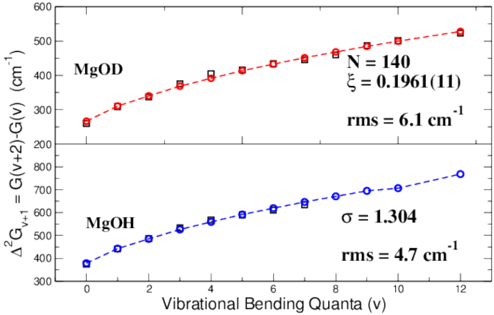
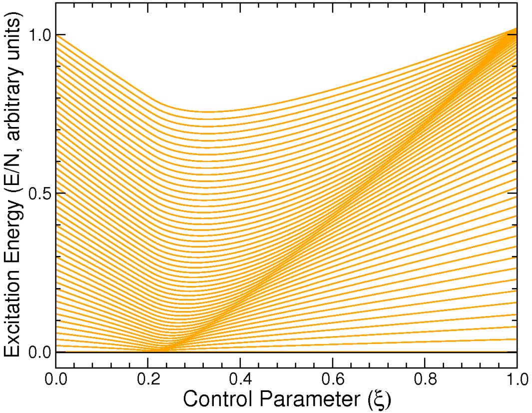
N_D 140	N_H 107
ϵ (cm^{-1}) 467.0(5)	A (cm^{-1}) 0.8194(13)
rms_D (cm^{-1}) 6.1	rms_H (cm^{-1}) 4.7

MgOH Data: P.R. Bunker *et al.*
Chem. Phys. Lett. 95 217 (1995).



ESQPT in the 2DVM



M.A. Caprio, P. Cejnar, F. Iachello. Ann. Phys. 323 1106 (2008).

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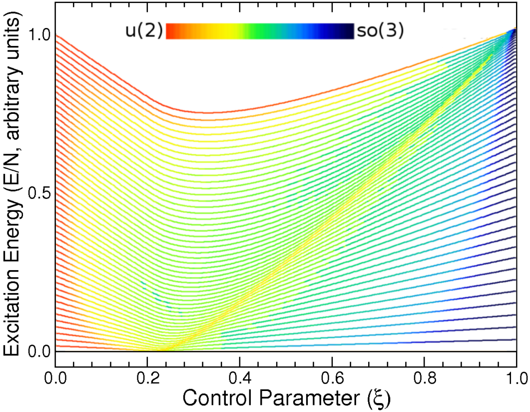

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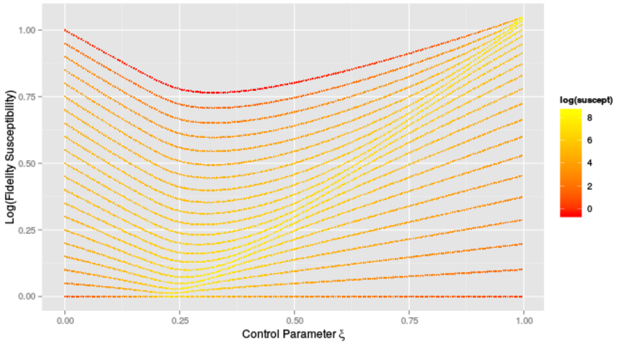

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N		σ		τ		$\delta\ell$	

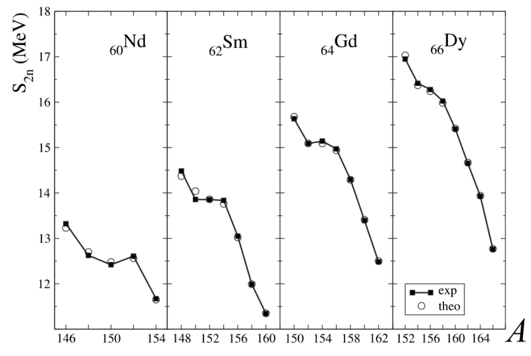
General one- and two-body Hamiltonian operator

$$H = \epsilon_s s^\dagger s + \epsilon_d d^\dagger \cdot \tilde{d} + u_0 \left(s^\dagger\right)^2 s^2 \quad (1)$$

$$+ u_2 s^\dagger d^\dagger \cdot \tilde{d} s + v_0 \left[d^\dagger \cdot d^\dagger s^2 + h.c.\right] \quad (2)$$

Signatures of First-Order Phase Transition

Two-Neutron Separation Energies



J. E. García-Ramos *et al.*, *Phys. Rev. C* 68 024307 (2003)

Signatures of First-Order Phase Transition

B(E2) for $2_1^+ \to 0_1^+$ and $4_1^+ \to 2_1^+$ *PRC* 68 024307 (2003)