EXCITED STATE QUANTUM PHASE TRANSITIONS AND MONODROMY

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QUANTUM PHASE TRANSITIONS (QPT)

QPT are phase transitions that occur as a function of a coupling constant, ξ, called control parameter, that appears in the quantum Hamiltonian, H, that describes the system

$$H = \varepsilon\left[(1-\xi)H_1 + \xi H_2\right] \qquad 0 \le \xi \le 1$$

Associated with phase transitions there are order parameters, the expectation values of suitably chosen operators that describe the state of the system <O>.
Introduced in the 1970's, they have become in recent years of great importance in a variety of systems.

[QPT are also called ground state phase transitions [§] and/or zero temperature phase transitions.]

[§] R. Gilmore, J. Math. Phys. 20,891 (1979).

EXCITED STATE QUANTUM PHASE TRANSITIONS (ESQPT)

ESQPT [§] are phase transitions that occur as a function of excitation energy, E_x , for fixed values of the control parameter, ξ.

ESQPT are intimately connected with quantum monodromy. In this presentation, this connection will be discussed.

ESQPT and quantum monodromy have been recently observed in molecular physics. This observation will also be discussed in this talk.

[§] M.A. Caprio, P. Cejnar and F. Iachello, Ann. Phys. (N.Y.) 323, 1106 (2008).

ALGEBRAIC MODELS ¶

QPT and ESQPT can be conveniently studied within the framework of algebraic models. For these models one can do both the semi-classical and the quantal analysis, and thus study both semi-classical and quantal monodromy. Also, in many-body systems, finite size scaling (1/N expansion) can be easily investigated. The latter point is particularly important in applications to finite systems: nuclei, molecules, finite polymers, photonic crystals, optical lattices, etc.
In this presentation, particular emphasis will be given to the semi-classical analysis of algebraic models.

¶ F. Iachello, *Lie Algebras and Applications*, 2nd ed., Springer-Verlag, Berlin (2015).

An algebraic model is an expansion of the Hamiltonian and other operators in terms of elements, $G_{\alpha\beta}$, of an algebra (often a Lie algebra, $G_{\alpha\beta} \in g$, or a contraction of it). The algebra g is called the spectrum generating algebra (SGA).

$$H = E_0 + \sum_{\alpha\beta} \varepsilon_{\alpha\beta} G_{\alpha\beta} + \sum_{\alpha\beta\gamma\delta} u_{\alpha\beta\gamma\delta} G_{\alpha\beta} G_{\gamma\delta} + \ldots$$

$$T = t_0 + \sum_{\alpha\beta} t_{\alpha\beta} G_{\alpha\beta} + \ldots$$

An interesting situation occurs when H does not contain all elements of g, but only the invariant (Casimir) operators of a chain of algebras $g \supset g' \supset g'' \supset \ldots$

$$H = E_0 + \alpha C(g) + \alpha' C(g') + \ldots$$

called a dynamic symmetry (DS). In this case the energy eigenvalues can be written explicitly in terms of quantum numbers labeling the representation of g

$$E = \langle H \rangle = E_0 + \alpha \langle C(g) \rangle + \alpha' \langle C(g') \rangle + \ldots$$

It is convenient to write the elements $G_{\alpha\beta} \in g$ as bilinear products of creation and annihilation operators (Jordan-Schwinger realization). For bosonic systems

$$G_{\alpha\beta} = b_\alpha^\dagger b_\beta \qquad \alpha, \beta = 1, \ldots, n$$

From $\left[b_\alpha, b_\beta^\dagger \right] = \delta_{\alpha\beta}$ $\qquad \left[b_\alpha, b_\beta \right] = \left[b_\alpha^\dagger, b_\beta^\dagger \right] = 0$

one obtains the commutation relations

$$\left[G_{\alpha\beta}, G_{\gamma\delta} \right] = \delta_{\beta\gamma} G_{\alpha\delta} - \delta_{\alpha\delta} G_{\gamma\beta}$$

which define the real form of g=u(n) [or gl(n)]

The basis upon which the elements act is the totally symmetric representation,

$$\left| N \right\rangle \equiv \square\square\ldots\square \qquad \left| N \right\rangle = \frac{1}{\sqrt{N!}} \left(b_\alpha^\dagger \right)^{n_\alpha} \left(b_{\alpha'}^\dagger \right)^{n_{\alpha'}} \ldots . \left| 0 \right\rangle$$

characterized by the total number of bosons N.

Fermionic systems can also be treated algebraically in terms of bilinear products of anti-commuting operators

$$G_{ij} = a_i^\dagger a_j \qquad\qquad i, j = 1,...,m$$

$$\left\{a_i, a_j^\dagger\right\} = \delta_{ij} \qquad\qquad \left\{a_i, a_j\right\} = \left\{a_i^\dagger, a_j^\dagger\right\} = 0$$

spanning the Lie algebra U(m).

Mixtures of bosonic and fermionic systems can be treated in terms of the realization

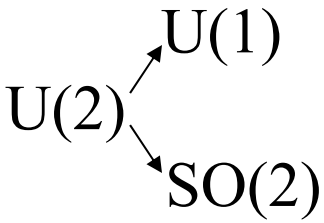
$$\begin{pmatrix} b_\alpha^\dagger b_\beta & b_\alpha^\dagger a_i \\ a_i^\dagger b_\alpha & a_i^\dagger a_j \end{pmatrix}$$

spanning the graded Lie algebra (also called superalgebra) u(n/m)

[Fermionic and mixed Bose-Fermi systems will not be discussed here]

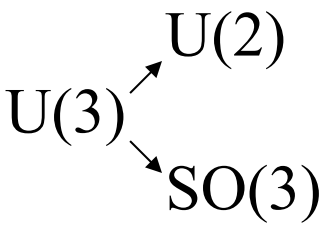
ALGEBRAIC MODELS (BOSONIC)

A list of algebraic bosonic models extensively investigated is given below. These provide a description of many-body problems with $f = n - 1$ degrees of freedom

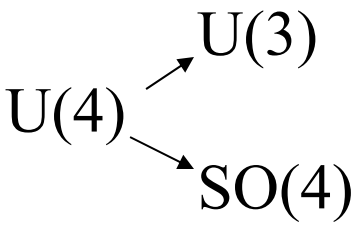


Lipkin: schematic model of many-body systems

1-dim vibron: Stretching vibrations of molecules

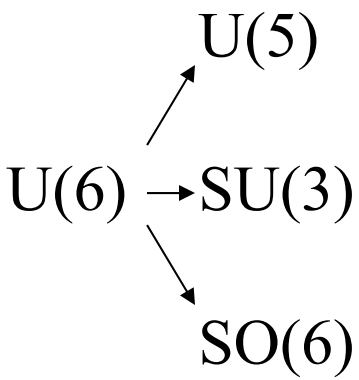


2-dim vibron: Bending vibrations of molecules



3-dim vibron[§] : Rotations-vibrations of molecules

List (cont.)



Interacting Boson Model (IBM)¶ :
Rotations-vibrations of atomic nuclei

A convenient realization of these models is with a scalar boson, called s, and another boson b_m with $f = 2\ell + 1$ components. The integer or half-integer number $\ell = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$ is called 'quasi-spin'. The use of both integer and half-integer allows one to treat problems in both odd and even dimensions.

¶ F. Iachello and A. Arima, *The Interacting Boson Model*, Cambridge University Press, Cambridge (1987).

§ F. Iachello and R.D. Levine, *Algebraic Theory of Molecules*, Oxford University Press, Oxford, (1995).

GEOMETRY OF ALGEBRAIC MODELS

Geometry can be associated to algebraic models with algebra g by constructing appropriate coset spaces, obtained by splitting g into

$$g = h \oplus p$$

(h: subalgebra of g=stability algebra; p: remainder) ← Cartan decomposition

For models with u(n) structure the appropriate coset space *(g/h)* is

$$u(n) / u(n-1) \oplus u(1)$$

($u(n-1)$: maximal stability algebra)

This space is a globally symmetric Riemannian space ¶ with dimension 2(n-1)

¶ F. Iachello, *Lie Algebras and Applications*, Springer, Berlin (2015), Ch. 5.

For bosonic models, the algebra *h* can be constructed by selecting one boson, b_1 , and choosing

$$h \doteq b_1^\dagger b_1, b_\alpha^\dagger b_\beta \qquad \alpha, \beta = 2, ..., n$$

$$p \doteq b_1^\dagger b_\alpha, b_\alpha^\dagger b_1 \qquad \alpha = 2, ..., n$$

Associated with the Cartan decomposition there are geometric variables η_i defined by

Extremal state

$$\left|\eta_i\right\rangle = \exp\left[\sum_i \eta_i p_i\right]\left|\Lambda_{ext}\right\rangle \qquad p_i \in p$$

For bosonic systems

$$\left|N;\eta_\alpha\right\rangle = \left[\exp\left(\eta_\alpha b_\alpha^\dagger b_1 - \eta^*{}_\alpha\, b_1^\dagger b_\alpha\right)\right]\frac{1}{\sqrt{N!}}\left(b_1^\dagger\right)^N\left|0\right\rangle$$

For systems with fixed value of N, it is convenient to introduce projective coherent states in terms of projective variables

$$\left|N;\vartheta_\alpha\right\rangle = \frac{1}{\sqrt{N!}}\left[b_1^\dagger + \vartheta_\alpha b_\alpha^\dagger\right]^N\left|0\right\rangle$$

For algebraic models written in terms of boson operators s, b_m it is convenient to rewrite the coherent state as

$$\left|N;\alpha\right\rangle = \frac{1}{\sqrt{N!}}\left(s^{\dagger} + \sum_m \alpha_m b_m^{\dagger}\right)^N \left|0\right\rangle$$

with normalization

$$\left\langle N;\alpha \,|\, N;\alpha\right\rangle = \left(1 + \sum_m \left|\alpha_m\right|^2\right)^N$$

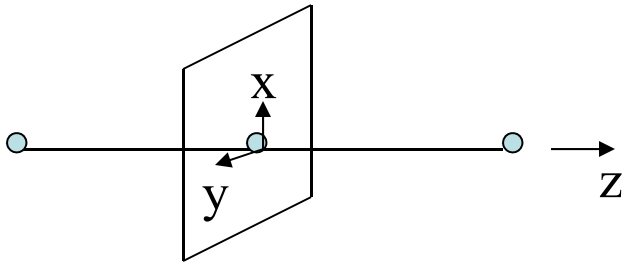
The semi-classical Hamiltonian associated with the quantum algebraic Hamiltonian is

$$H_{cl}(\alpha) = \frac{\left\langle N;\alpha\middle|H\middle|N;\alpha\right\rangle}{\left\langle N;\alpha \,|\, N;\alpha\right\rangle}$$

This Hamiltonian depends on the complex coordinate α_m which can be split into real coordinates and momenta

$$(q_m, p_m)$$

AN EXAMPLE. BENDING VIBRATIONS OF MOLECULES: A 2-DIM PROBLEM



QUANTUM DESCRIPTION ¶

Cartesian boson creation and annihilation operators $\tau_x^\dagger, \tau_y^\dagger, \tau_x, \tau_y$ plus a scalar $\sigma^\dagger, \sigma$ conveniently combined into circular bosons

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

Elements of U(3):

$$\hat{n} = \tau_+^\dagger \tau_+ + \tau_-^\dagger \tau_- \qquad \hat{D}_\pm = \sqrt{2}\left(\pm\tau_\pm^\dagger \sigma \mp \sigma^\dagger \tau_\mp\right)$$

$$\hat{n} = \sigma^\dagger \sigma \qquad \hat{Q}_\pm = \sqrt{2}\tau_\pm^\dagger \tau_\mp$$

$$\hat{\ell} = \tau_+^\dagger \tau_+ - \tau_-^\dagger \tau_- \qquad \hat{R}_\pm = \sqrt{2}\left(\tau_\pm^\dagger \sigma + \sigma^\dagger \tau_\mp\right)$$

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

Dynamical symmetries

$$U(3) \begin{cases} \nearrow U(2) \supset SO(2) & \text{(I)} \\ \searrow SO(3) \supset SO(2) & \text{(II)} \end{cases}$$

Labeling of states (quantum numbers)

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

$$n = N, N-1, \ldots, 1, 0$$

$$\ell = n, n-2, \ldots, 1 \text{ or } 0$$

(n=odd or even)

$$\left| \begin{array}{ccccc} U(3) & \supset & SO(3) & \supset & SO(2) \\ \downarrow & & \downarrow & & \downarrow \\ [N] & & v & & \ell \end{array} \right\rangle$$

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

(N=odd or even)

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

Algebraic Hamiltonian

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

with

$$\hat{P} = N(N+1) - \left[\frac{1}{2}\left(\hat{D}_{+}\hat{D}_{-} + \hat{D}_{+}\hat{D}_{-}\right) + \hat{\ell}^2\right]$$

Solutions

Vibrational behavior

$$E^{(I)}(n) = E_0 + \varepsilon n$$

ξ=0 U(2) symmetry (I)

ξ=1 SO(3) symmetry (II)

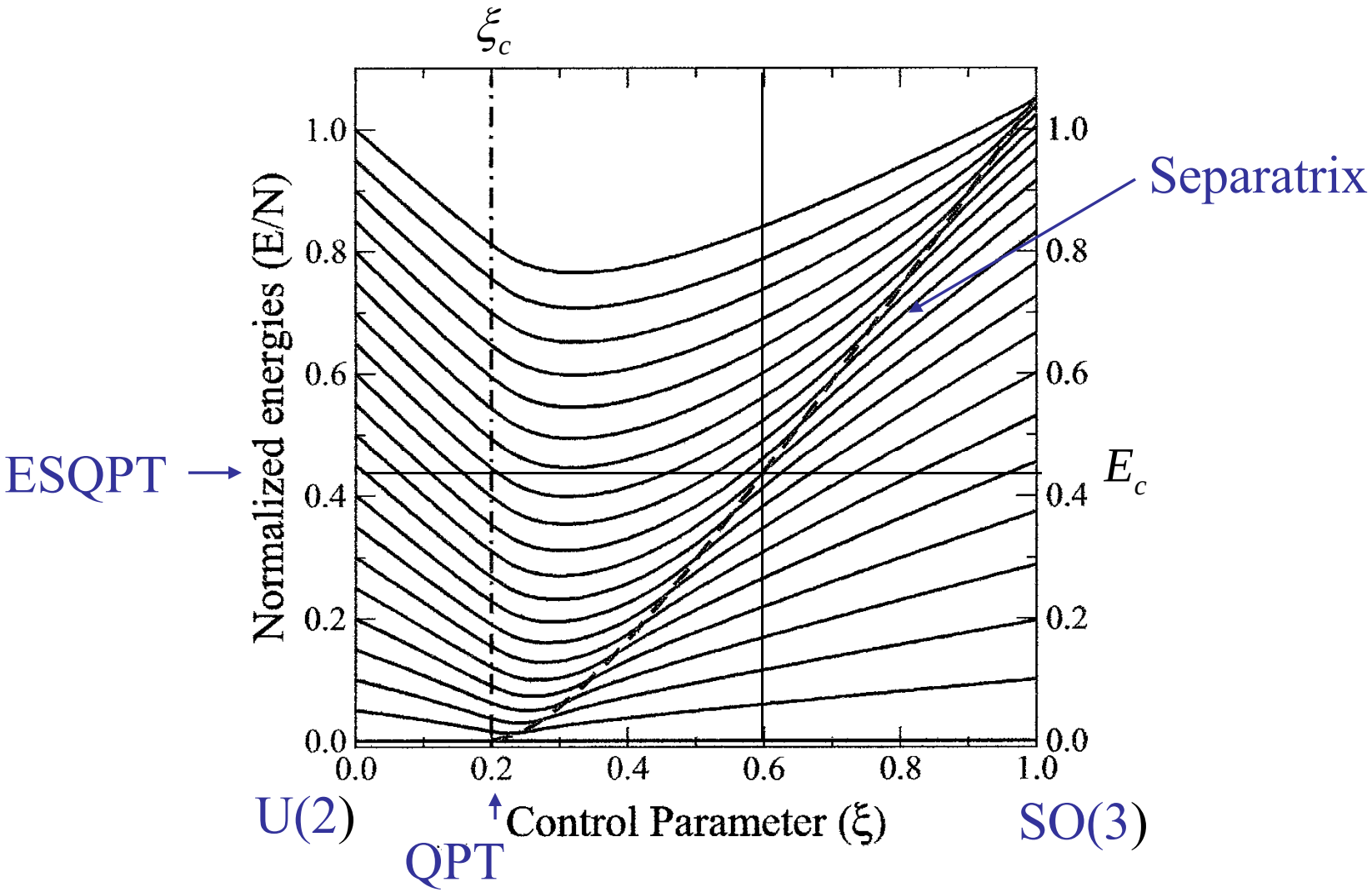
$$E^{(II)}(v) = E'_0 + \varepsilon\left[v - \frac{1}{N}v^2\right]$$

Different quantum number!

A single global quantum number cannot be globally defined, due to the different dynamic symmetries of the two phases.

CORRELATION DIAGRAM ¶

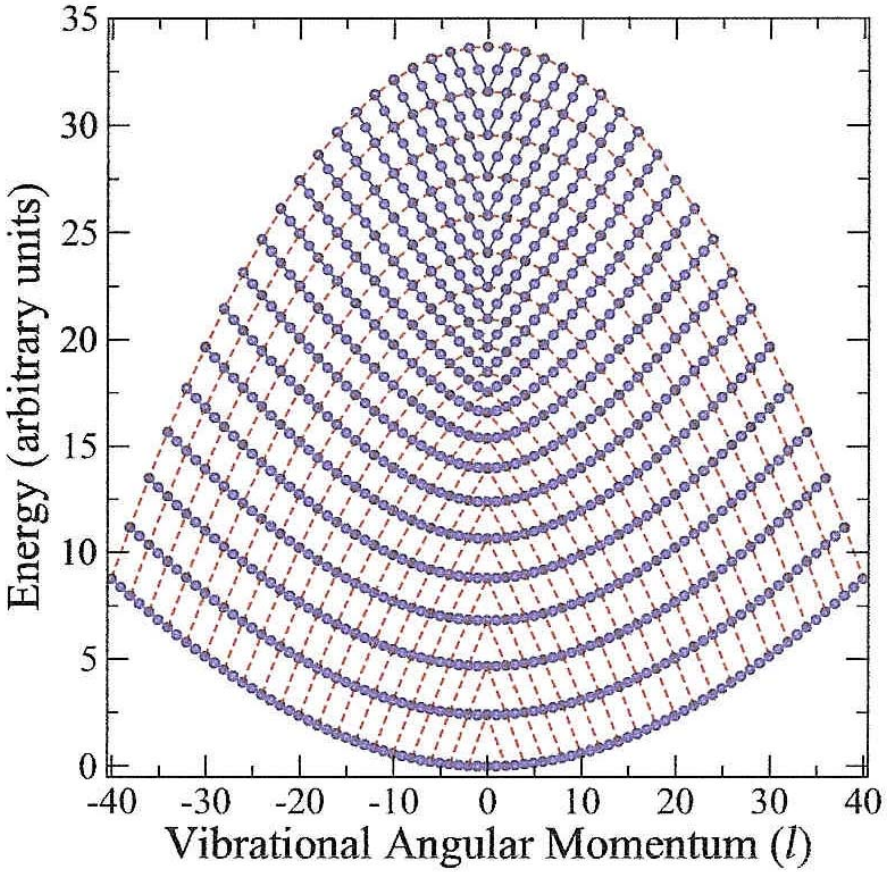
Energy spectrum for N=40 and $\ell = 0$



¶ F. Perez-Bernal and F. Iachello, Phys. Rev. A 77, 032115 (2008)

QUANTUM MONODROMY DIAGRAM

Energy spectrum for N=40 and ξ=0.6



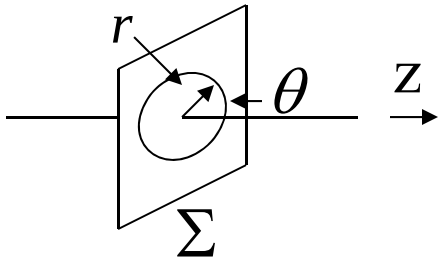
Rotational behavior	$E(l) = E_0 + al^2$	$u < u_c$	SO(3)
	$E(l) = E_0 + bl$	$u > u_c$	U(2)

[u_c value of u (numbering of states) at which the separatrix is crossed]

SEMI-CLASSICAL DESCRIPTION

Coordinates: Cartesian x, y ; Polar r, θ

Momenta: p_x, p_y p_r, p_θ



Coherent state (putting all momenta equal to zero)

$$\left|[N];r,\theta\right\rangle$$

Effective potential

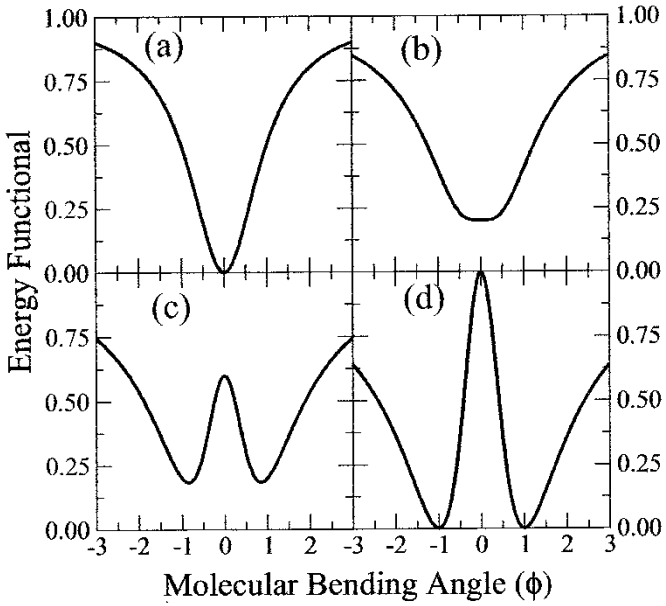
$$V(r,\theta)=\frac{\left\langle[N];r,\theta\left|H\right|[N];r,\theta\right\rangle}{\left\langle[N];r,\theta\,|\,[N];r,\theta\right\rangle}$$

For H given above

$$V(r)=\varepsilon\left[(1-\xi)\frac{r^2}{1+r^2}+\xi\left(\frac{1-r^2}{1+r^2}\right)^2\right]$$

Shape of the potential as a function of ξ

$\xi = 0$ $\xi = 0.2$



$\xi = 0.6$ $\xi = 1$

Quadratic-quartic potential $V(r) = ar^2 + br^4$

called a "sombrero potential" or a "champagne bottle potential" ¶

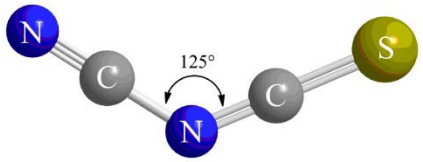
¶ M.S. Child, J. Phys. A: Math. Gen. 31, 657 (1998).

ESQPT AND MONODROMY IN MOLECULES

QPTs and ESQPTs have been recently observed in molecules ¶ .

Hamiltonian

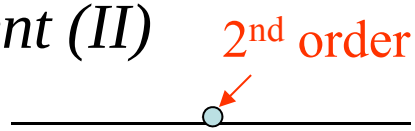
$$H = \varepsilon\left[(1-\xi)\hat{n} + \frac{\xi}{N}\hat{P}\right]$$



There is in this case only one control parameter and two phases.

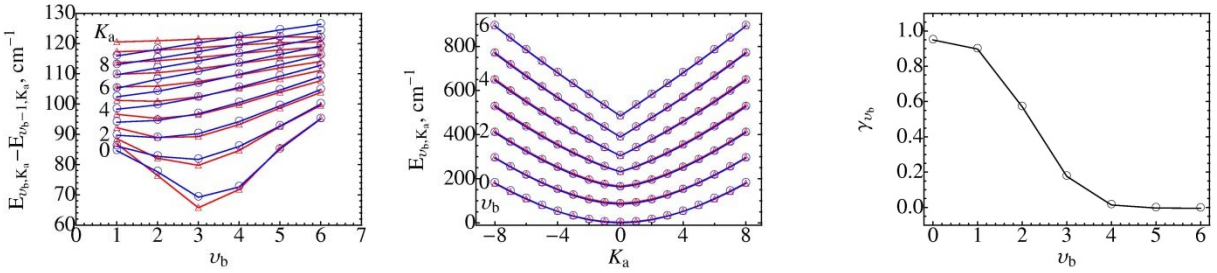
U(3) ⟨ U(2) *Linear (I)*
SO(3) *Bent (II)*

The phase diagram is a line



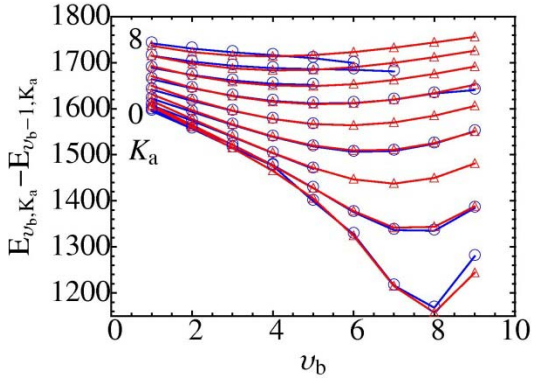
Particularly important has been the observation of ESQPT (the only known example so far).

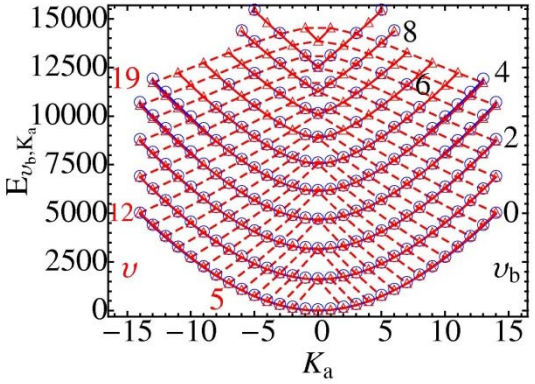
Monodromy Diagram of NCNCS

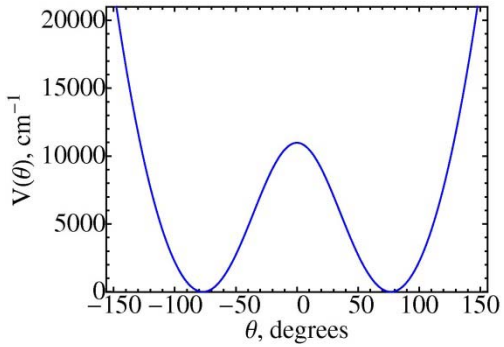


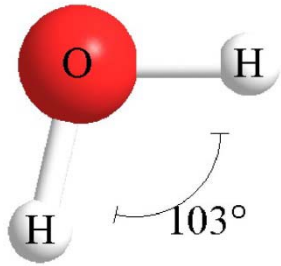
¶ D. Larese and F. Iachello, J. Mol. Struct. 1006, 611 (2011).

One of the best examples of ESQPT and monodromy is provided by the water molecule, H_2O, which is bent in the ground state and becomes linear at E_x~11,000cm^{-1}.









¶ D. Larese, F. Perez-Bernal and F. Iachello, J. Mol. Struct. 1051, 310 (2013)

DYNAMICS OF ALGEBRAIC MODELS ¶

Semi-Classical Hamiltonian obtained from the group coherent state

$$H = \frac{1}{2N^2}\left(1-\xi+2\xi r^2\right)\left[p_r^2+\frac{p_\theta^2}{r^2}\right]+\frac{1-5\xi}{2}r^2+\xi r^4$$

radial momentum — angular momentum — radial coordinate

where $\left\langle p_\theta^2 \right\rangle = \ell^2$ (conserved angular momentum) and $0 \le r \le \sqrt{2}$ (bound domain). H can be rewritten as

$$H_{cl} = \frac{\hbar^2}{2m(r)}\left[p_r^2+\frac{p_\theta^2}{r^2}\right]+V(r)$$

with $N^{-1} \to \hbar$

$$m(r) = \frac{1}{1-\xi+2\xi r^2}$$

Coordinate dependent mass

$$V(r) = \frac{1-5\xi}{2}r^2+\xi r^4$$

¶ O.S. van Roosmalen, Ph.D. Thesis, Rijksuniversiteit Groningen, 1982.
R.L. Hatch and S. Levit, Phys. Rev. C25, 614 (1982).
M.A. Caprio, P. Cejnar and F. Iachello, Ann. Phys. (N.Y), 323, 1106 (2008).

SEMI-CLASSICAL SPECTRUM $\ell = 0$

Semi-classical action

$$S(\xi;E) = 2\int_{r_1(E)}^{r_2(E)} dr\left[2m(r)\left[E - V(r)\right]\right]^{1/2}$$

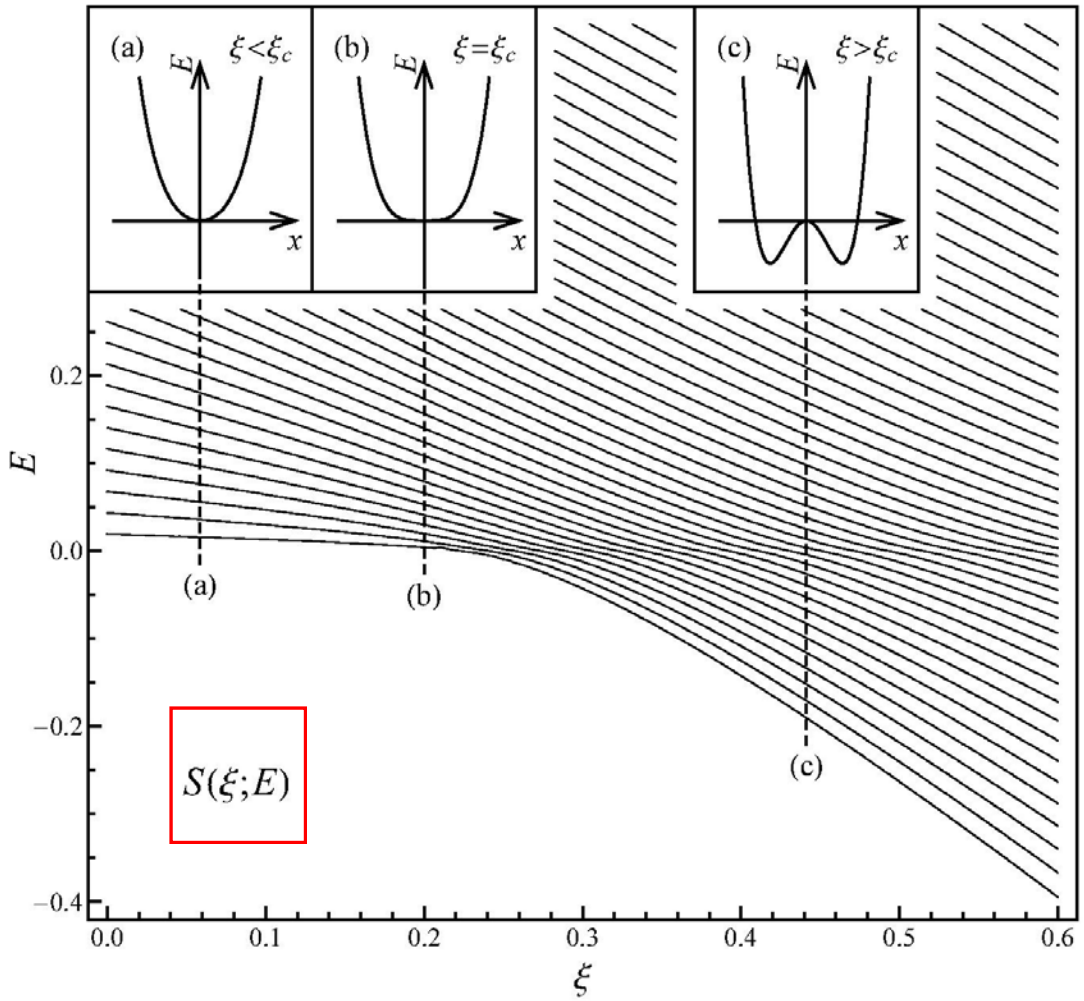
WKB quantization condition

$$S(\xi;E) = \left(k + \frac{1}{2}\right)2\pi N^{-1} \qquad k = 0,1,\ldots$$

Semi-classical energy levels $E_k(\xi)$

⟹ Contours of S(ξ;E) in the ξ-E plane

Contours calculated numerically ¶



¶ M.A. Caprio *et al.*, *Loc. Cit.*

PROPERTIES OF THE SEMI-CLASSICAL SPECTRUM

The derivative $\frac{dE_k}{d\xi}$ along a single contour undergoes a singularity in which $\frac{dE_k}{d\xi} \to 0, \frac{d^2E_k}{d\xi^2} \to \pm\infty$ at a critical value $\xi = \xi_c^{ex}$

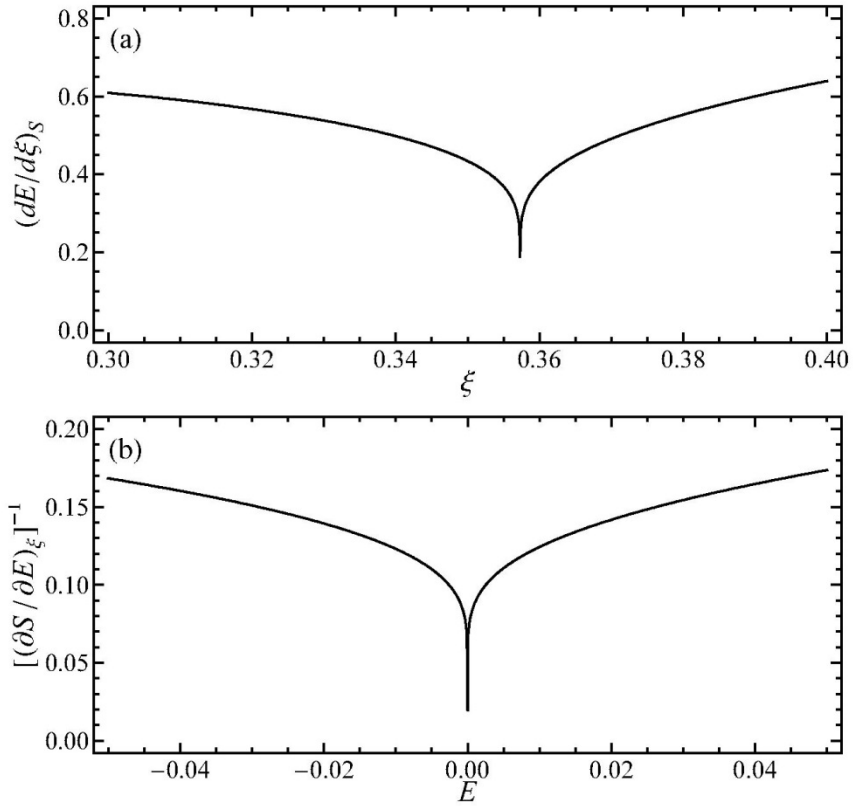
The gap between adjacent levels $\Delta = \frac{dE_k}{dk}$ vanishes at E=0.

The gap can be written as $\Delta(E) = \frac{2\pi}{N}\left(\frac{\partial S}{\partial E}\right)^{-1}$ or $\Delta(E) = 2\pi N^{-1}\tau^{-1}$

Therefore, the period τ becomes infinite at E=0.

So does the level density $\rho \propto \frac{1}{\Delta}$

Singularities in the derivatives of the classical action



For non-zero angular momentum, the origin is classically forbidden. This mitigates the effects just described. The phenomena associated with the ESQPT are suppressed at sufficiently large ℓ at a given value of N.

EXPLICIT FORM OF THE SPECTRUM NEAR THE SINGULARITY ¶

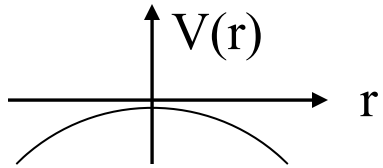
Near the top of the barrier, for E → 0, the barrier can be treated as an inverted oscillator $V(r) = -Ar^2$. Also the position dependent kinetic term $\propto r^2 p^2$ becomes irrelevant.

The action can be written as $\hbar S(E) = \frac{1}{\hbar\omega}(-E\log E + \alpha_0 + \alpha E + \ldots)$

where $\hbar\omega = 2\left[\hbar^2(2m)\right]^{1/2} A^{1/2}$

By imposing the WKB quantization condition and retaining only terms linear in E

$$-E\log E + \alpha E = 2\pi\hbar\omega\left(k - k_c\right)$$



one obtains

$$E(k) = \frac{-2\pi\hbar\omega(k - k_c)}{W\left[-e^{-\alpha}2\pi\hbar\omega(k - k_c)\right]}$$

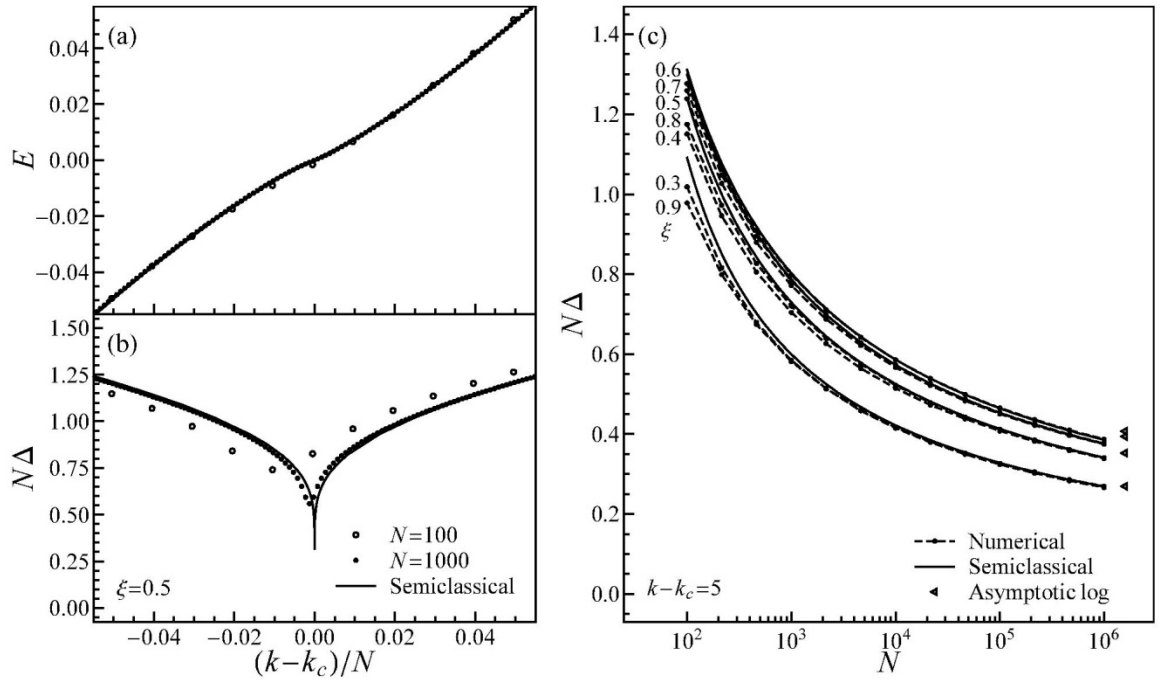
Lambert function

¶ M.A. Caprio *et al.*, *loc.cit.*

For the algebraic Hamiltonian, introducing $\Xi(\xi) \equiv (1-\xi)(1-5\xi)$ one has the semi-classical estimates

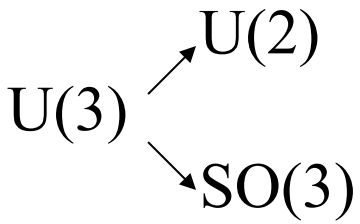
$$E(N,\xi,k) = -\frac{2\pi\Xi(\xi)^{1/2}(k-k_c)/N}{W\left[-e^{-\alpha}2\pi\Xi(\xi)^{1/2}(k-k_c)/N\right]}$$

$$\Delta(N,\xi,k) = -\frac{2\pi\Xi(\xi)^{1/2}/N}{W\left[-e^{-\alpha}2\pi\Xi(\xi)^{1/2}(k-k_c)/N\right]+1}$$



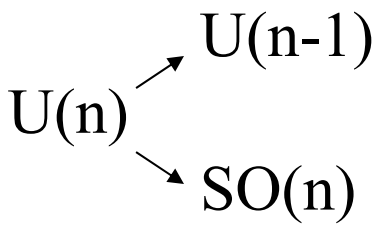
SUMMARY AND CONCLUSIONS

QPT, ESQPT and Monodromy have been studied in algebraic models of many-body systems both quantally and semi-classically.
The case



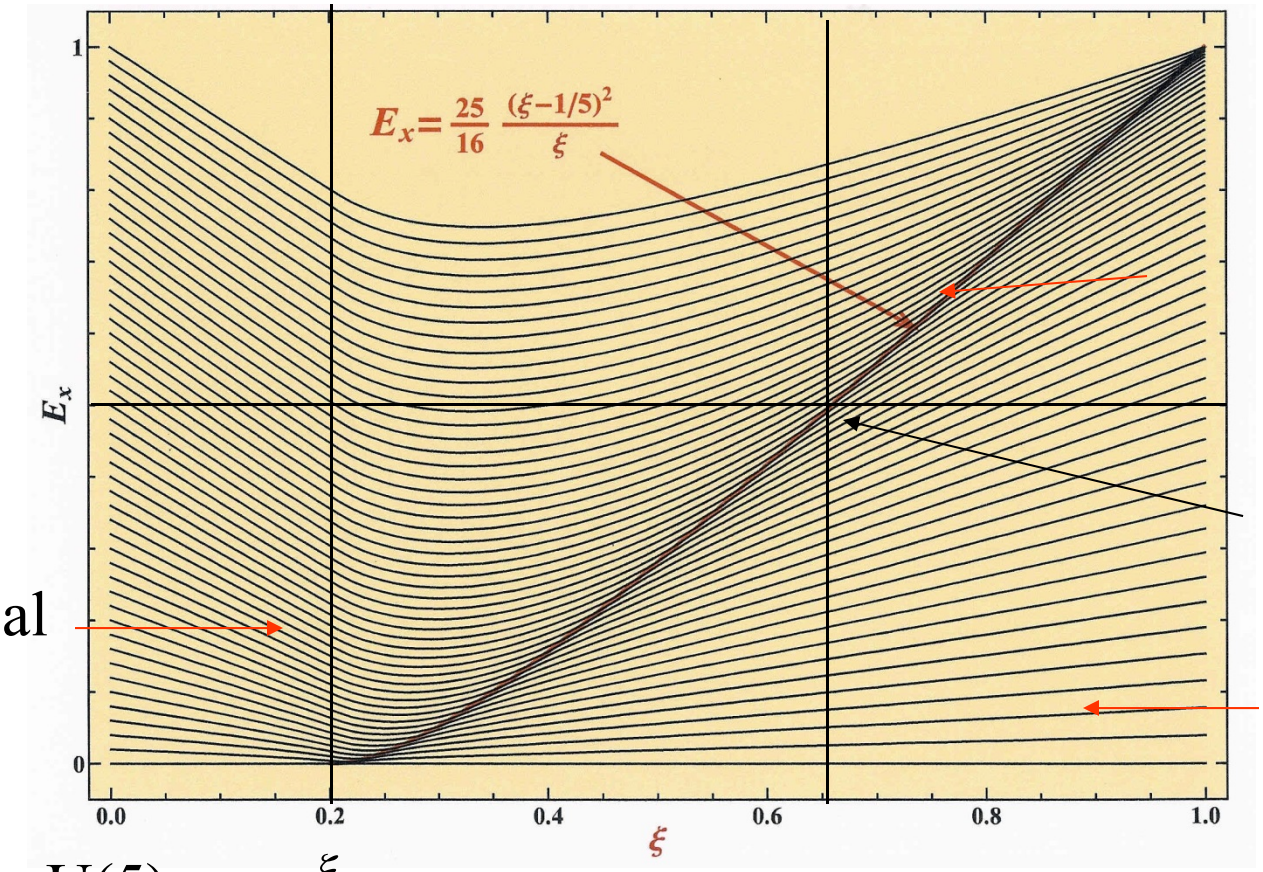
has been shown. Experimental evidence for ESQPT and Quantum Monodromy in the bending vibrations of the water molecule, H_2O, has been presented.

ESQPT and Monodromy are related to properties of the potential. The analysis presented here for U(3) applies equally well to all problems of type



which have a 2nd order phase transition U(n-1)-SO(n). These transitions have been investigated extensively and have the same universal behavior.

STRUCTURE OF THE SPECTRUM FOR 2nd ORDER QPT



Separatrix

E_{xc}

ESQPT

Spherical

Deformed

U(5)

ξ_c

SO(6)

QPT

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

For algebraic models that support 1st order transitions, the structure of the spectrum and its semi-classical analysis is much more complex, since it involves several control parameters and several order parameters.

The potential now depends on several coordinates. An example is the Interacting Boson Model (IBM) that describes rotations and vibrations of a liquid drop with ellipsoidal shape.

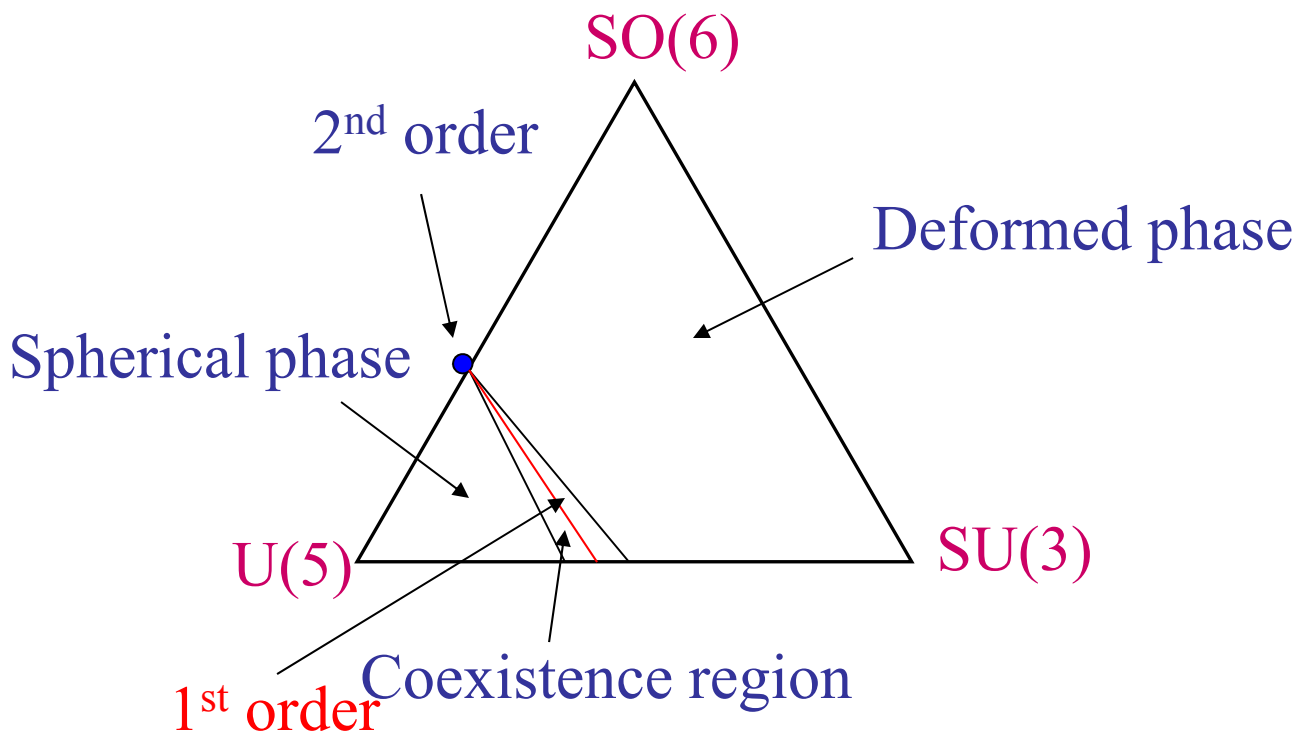
This model has two control parameters and three phases

The potential depends on two intrinsic variables (β,γ)

[Quantum monodromy of IBM has some similarities with that of ellipsoidal billiards ¶]

¶ H. Waalkens and H.R. Dullin, Ann. Phys. 295, 81 (2002).

PHASE DIAGRAM OF THE INTERACTING BOSON MODEL



A complete analysis of classical and quantum monodromy for algebraic structures that support 1st order transitions is currently being done, but it will not be reported here.

This talk is dedicated to the memory of Hilbrand Johannes Groenewold, whose work on quantum-classical correspondence inspired some aspects of the work discussed here on quantum-classical correspondence in algebraic models, published with Groningen affiliation:

A.E.L. Dieperink, O. Scholten and F. Iachello, *Kernfysisch Versneller Instituut, Rijksuniversiteit Groningen*, Classical limit of the Interacting Boson Model, Phys. Rev. Lett. 44, 1747 (1980).