Algebraic Models and Squeezed Coherent States of Anharmonic Oscillators

Maia Angelova

Mathematical Modelling Research Lab

Northumbria University,

Newcastle upon Tyne UK

“Beauty in Physics” Cocoyoc May 2012

Collaborators:

Véronique Hussin and Anaelle Hertz

Département de Mathématique et Statistique et CRM, Université de Montréal, Canada

Alejandro Frank

Instituto de Ciencias Nucleares, UNAM, Mexico

Outline

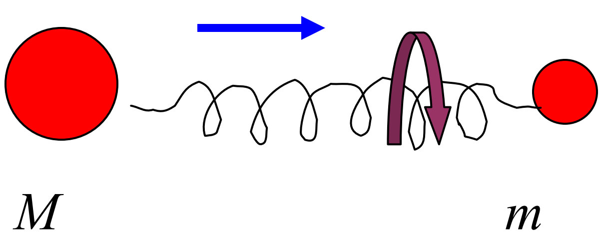
- Motivation
- Algebraic model of the Morse oscillator
- *q*-bosons and quantum deformations
- Algebraic model of the Dunham expansion
- Ladder operators
- Squeezed coherent states of the Morse quantum system
- Applications to diatomic molecules
- Discussion

1. Motivation

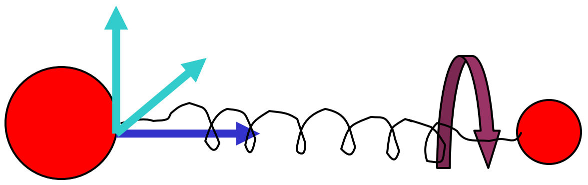
Vibrations in Molecules: Vibron Model F. Iachello et al

- **Diatomic molecules**,

H_2, $^{1}H^{35}Cl$,

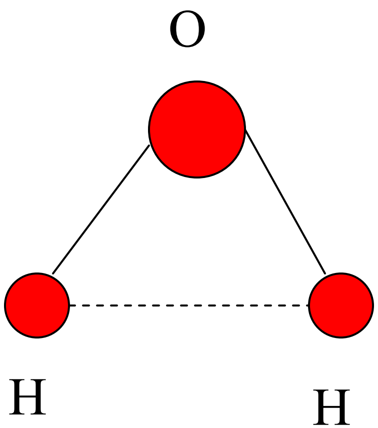


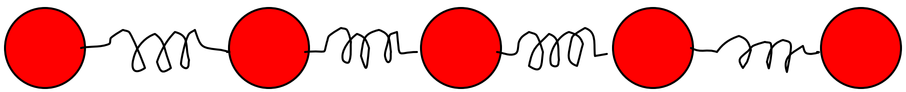
1-*D* harmonic oscillator *su(2)*



2-*D* and 3-*D* harmonic oscillators

•Polyatomic molecules and linear chains (polymers)



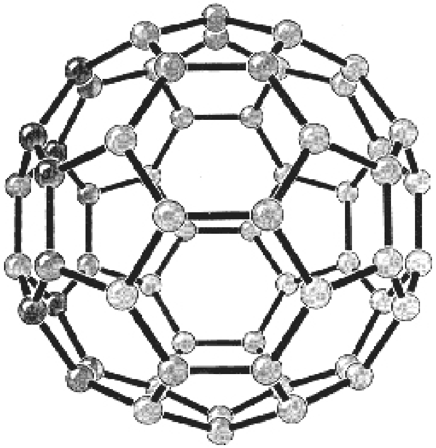


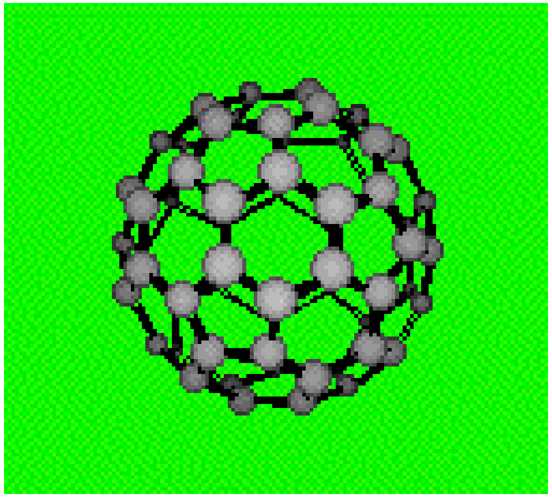
Carbon nanotube

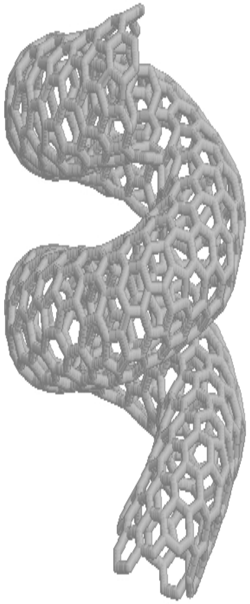
Solid Fullerene

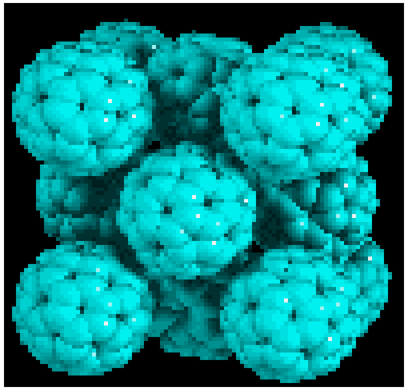
(Cubic *m3m*)

C_{60} (truncated Icosahedron I_h)





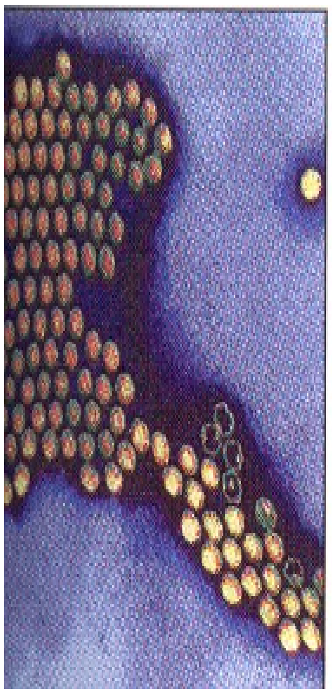


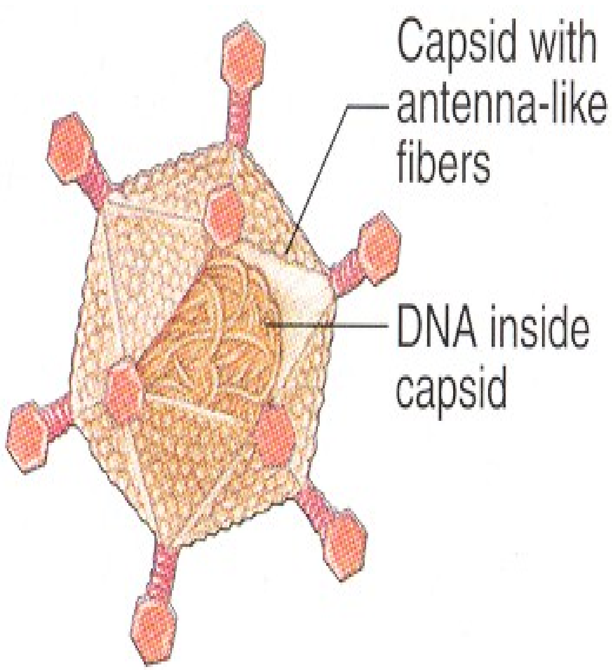


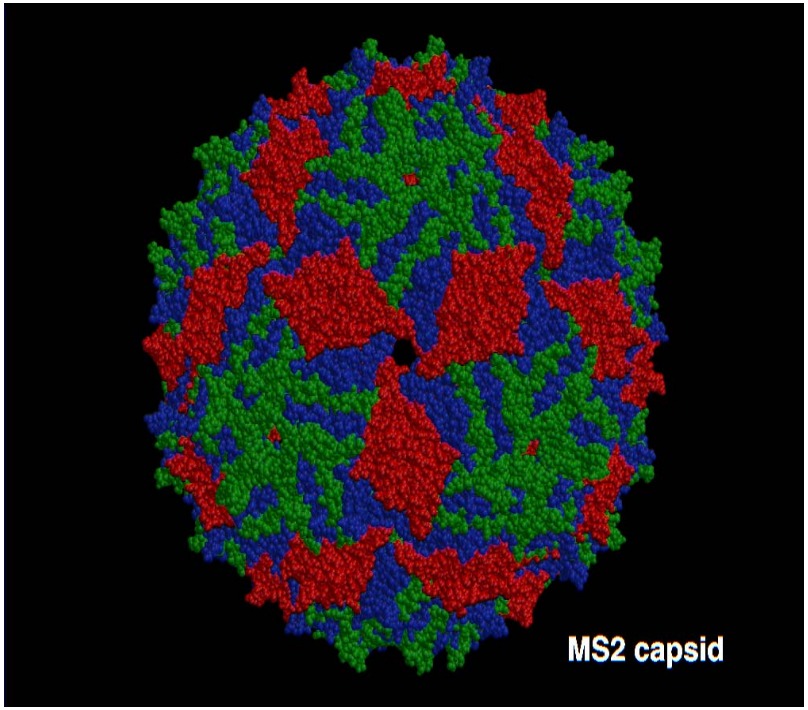
- **Living organisms : viruses, icosahedral viral capsids**

Icosahedron *I*

HIV Rev-RRE & TAR-Tat

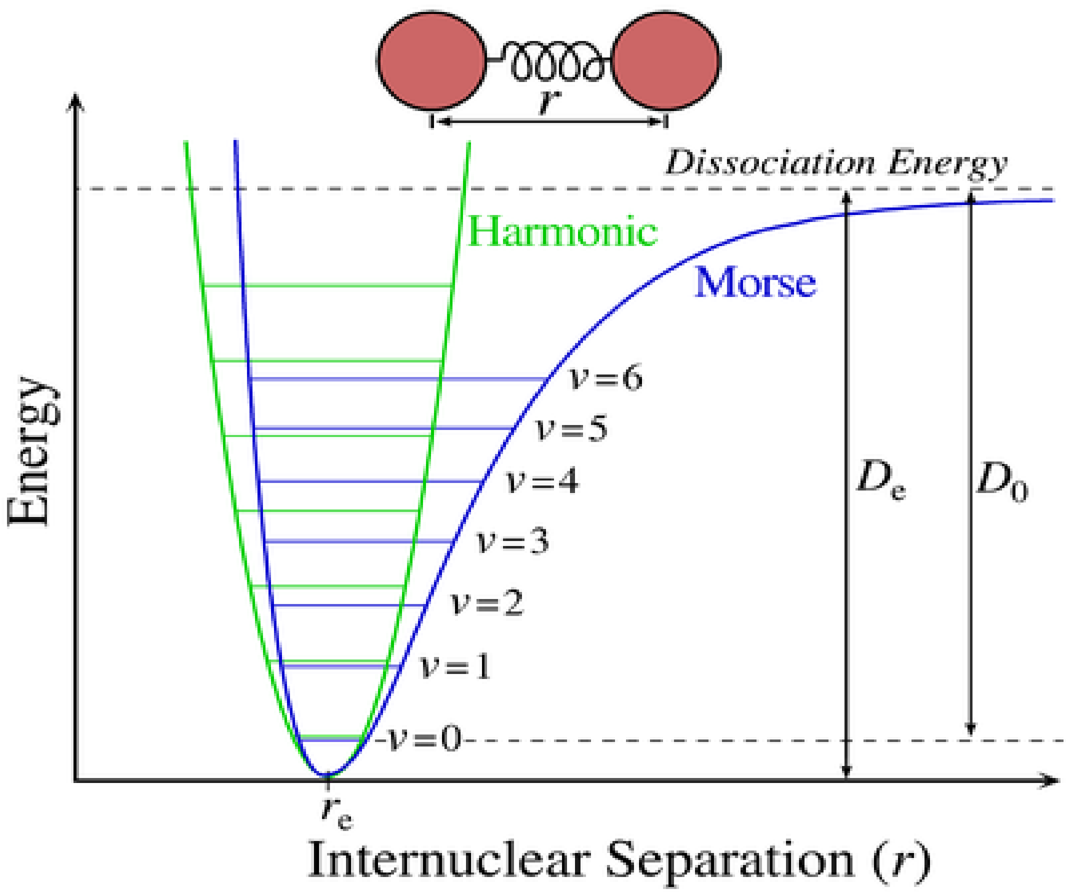






2. Algebraic Model of Morse Potential

- **Morse Potential**



$$V_r = D_e(1 - e^{-\beta(r-r_e)})^2$$

$$\beta = \sqrt{\frac{k_e}{2D_e}} = \sqrt{\frac{4\pi c}{\hbar}\mu\omega_e x_e}$$

$$D_e = \frac{\omega_e}{4x_e}, \qquad \omega_e = \frac{\beta}{c}\sqrt{\frac{2D_e}{\mu}},$$

$$x_e = \frac{\hbar\beta}{4\pi\sqrt{2\mu D_e}}$$

$$E_v^M = hc\omega_e\left\{\left(v+\frac{1}{2}\right) - x_e\left(v+\frac{1}{2}\right)^2\right\}$$

D_e – depth (defined relative to dissociate atoms), k_e – force constant of the minimum well, ω_e, x_e – molecular constants (Herzberg 1950)

• Algebraic Model

Algebraic methods combine Lie algebraic techniques, describing the interatomic interactions, with discrete symmetry technique, associated with the global symmetry of the atoms and molecules in complex compounds. The **interacting boson model** (Iachello & Arima) was applied very successfully to nuclei and particles and lately to describe stretching and bending modes in molecules **vibron model** (Iachello 81, Iachello & Levine 82,95, Alhassid et al 83, Frank & Van Isacker 94).

In the framework of the anharmonic model (Frank &Van Isacker 94), the anharmonic effects of the local interactions are described by a Morse-like potential. The Morse potential is associated with the *su(2)* algebra and leads to a deformation of this algebra.

$$H_M = \frac{A}{4}\left(\hat{N}^2 - 4\hat{J}_z^2\right) = \frac{A}{2}\left(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+ - \hat{N}\right) \qquad (1)$$

A is a constant, J_+, J_- are the raising and lowering operators, $\hat{N}$ is the number operator and N is the total number of bosons fixed by the potential shape.

$$N + 1 = \left(\frac{8\mu D_e d^2}{\hbar^2}\right)^{1/2} \qquad (2)$$

The eigenstates, $|[N], v\rangle$, correspond to the $u(2) \supset su(2)$ symmetry-adapted basis, where *v* is the number of quanta in the oscillator, $v=1,2,\ldots,[N/2]$.

Anharmonic boson operators :

$$\hat{b} = \frac{\hat{J}_+}{\sqrt{N}}, \qquad \hat{b}^* = \frac{\hat{J}_-}{\sqrt{N}}, \qquad \hat{v} = \frac{\hat{N}}{2} - \hat{J}_z, \qquad v = 1,2,\ldots,v_m, \qquad v_m = \frac{1}{2}\left(\frac{1}{x_e} - 1\right) \tag{3}$$

Commutation relations: $$\left[\hat{b}, \hat{v}\right] = \hat{b}, \qquad \left[\hat{b}^*, \hat{v}\right] = -\hat{b}^*, \qquad \left[\hat{b}, \hat{b}^*\right] = 1 - \frac{2\hat{v}}{N}, \tag{4}$$

Morse Hamiltonian: $$H_M \approx \frac{1}{2}\left(\hat{b}\,\hat{b}^* + \hat{b}^*\hat{b}\right) \tag{5}$$

Eigenvalues: $$\mathrm{E}_v^M = \hbar\omega_e\left(v + \frac{1}{2} - \frac{v^2}{N}\right), \qquad N \to \infty, \qquad \mathrm{E}_v^M \to \hbar\omega_e\left(v + \frac{1}{2}\right)$$

• Anharmonic *q*-bosons

Heisenberg-Weyl *q*-algebra HW_q commutation relations (Biedenharn 89, Macfarlane 89)

$$\left[\hat{a},\hat{a}^*\right]=q^{\hat{n}},\qquad \left[\hat{n},\hat{a}\right]=-a,\qquad \left[\hat{n},\hat{a}^*\right]=\hat{a}^* \qquad (6)$$

Deformation parameter q is in general a complex number, when $q\to 1$, the boson commutation relations for harmonic oscillator are recovered.

Casimir operator for HW_q:

$$\hat{C}=\hat{a}\hat{a}^*+\hat{a}^*\hat{a}-\frac{q^{\hat{n}+1}+q^{n}-2}{q-1},\qquad \left[\hat{C},\hat{a}]\right]=\left[\hat{C},\hat{a}^*\right]=\left[\hat{C},\hat{n}\right]=0$$

Possible Hamiltonian (Angelova, Dobrev&Frank 01):

$$H = \frac{1}{2}\left(\hat{a}\hat{a}^* + \hat{a}^*\hat{a}\right) = \frac{1}{2}C + \frac{1}{2}\frac{\hat{q}^{\hat{n}+1} + \hat{q}^{\hat{n}} - 2}{q-1} \qquad (7)$$

Anharmonic bosons are obtained when q is real, $q<1$:

$$p \equiv \frac{1}{1-q}, \qquad q = 1 - \frac{1}{p}, \qquad q^{\hat{n}} = \left(1 - \frac{1}{p}\right)^{\hat{n}}$$

Harmonic limit: $p \to \infty$. Assuming $1/p \ll 1$, neglecting terms of order $1/p^2$ and higher,

$$q^{\hat{n}} = 1 - \frac{\hat{n}}{p} \qquad (8)$$

Substituting (8) in commutation relation (6) and identifying the parameter p with $N/2$, n with v and the creation and anihilation operators a, a^* with b, b^*, we recover the $su(2)$ anharmonic relations (4).

• Physical interpretation of the deformation parameter (Angelova 04)

The form (4) of commutation relations of *su(2)*

$$\left[\hat{b},\hat{v}\right]=\hat{b}, \qquad \left[\hat{b}^*,\hat{v}\right]=-\hat{b}, \qquad \left[\hat{b},\hat{b}^*\right]=1-\frac{2\hat{v}}{N}, \qquad (4)$$

can be considered as a deformation of the harmonic oscillator relations with deformation parameter $N=2p$.

$$q^{\hat{n}} = 1 - \frac{\hat{n}}{p} \qquad (8)$$

The form of (8) and (4) indicates that for the low-lying levels of the Hamiltonian (7) the spectrum corresponds to the Morse eigenvalues. More generally, the parametrisation (7) means that up to order $1/p$, the HW_q algebra contracts to *su(2)*. This gives a possible physical interpretation for p or q in terms of N, *i.e.* the finite number of bosons in the potential well.

• Example:

$$^{1}H\,^{35}Cl$$

$N=55, \quad v_m=27, \quad p=27, \quad q=1-1/27=26/27.$

3. Algebraic Model with Quantum Deformations of the Dunham Expansion

- **Dunham expansion** (Dunham 1932)

Phenomenological description of the vibrational energy of diatomic molecules in a given electronic state:

$$\mathrm{E}_v^D = hc\omega_e\left(v+\frac{1}{2}\right) - hc\omega_e x_e\left(v+\frac{1}{2}\right)^2 + hc\omega_e y_e\left(v+\frac{1}{2}\right)^3 + \ldots \qquad (9)$$

where ω_e, x_e and y_e are the molecular constants, the numerical values of which are obtained by fitting the potential curve to the experimental spectral data (Herzberg 50, latest edition of CRM Spectroscopy).

If (9) is truncated to the quadratic term, one obtains the discrete spectrum of the Morse potential. It is convenient to re-write the energies in the form,

$$\mathrm{E}_v^{D'} = \mathrm{E}/hc\omega_e = \left(v+\frac{1}{2}\right) - x_e\left(v+\frac{1}{2}\right)^2 + y_e\left(v+\frac{1}{2}\right)^3 + \ldots \qquad (10)$$

• The Hamiltonian (Angelova, Dobrev&Frank 04)

Aim: to incorporate in different approximations both the Morse energy and the Dunham expansion.

$$H = \alpha\left(\hat{J}_{+}\hat{J}_{-} + \hat{J}_{-}\hat{J}_{+}\right) \qquad (10)$$

where α is a constant that we choose appropriately, $\hat{J}_{+}, \hat{J}_{-}$ are the raising and lowering generators of $U_q(su(2))$, deformation parameter q is a complex number.

The q-bosons algebra (HW_q) is defined by:

$$\hat{a}\hat{a}^{*} - q^{-1}\hat{a}^{*}\hat{a} = q^{\hat{n}}, \qquad [\hat{n},\hat{a}] = -\hat{a}, \qquad [\hat{n},\hat{a}^{*}] = \hat{a}^{*} \qquad (11)$$

where $\hat{a}^{*}$ is q-boson creation operator, $\hat{a}$ is q-boson annihilation operator, $\hat{n}$ is the boson number operator, and the boson commutation relations of the harmonic oscillator may be recovered for the value $q=1$.

Realization of $U_q(su(2))$ (Ganchev&Petkova 89):

$$\hat{J}_{+} = \hat{a}^{*}\left[2\hat{j} - \hat{n}\right]_q, \qquad \hat{J}_{-} = \hat{a}, \qquad \hat{J}_0 = \hat{n} - \hat{j}, \qquad [z]_q \equiv \frac{q^{z} - q^{-z}}{q - q^{-1}}, \qquad q-number$$

Morse: *q~1,* $\alpha = hc\omega_e / 4j$

$$\frac{1}{x_e} = 2j + 1$$

Dunham: *q*-real, new parameter *p'* $q = e^{-1/p'} = 1 - \frac{1}{p'} + \frac{1}{p'^2} + \ldots$

$$p' = \sqrt{\frac{2}{3y_e}}, \qquad j = \frac{1}{2}\left\{\sqrt{\frac{2}{3y_e}} arcthan\left(\sqrt{\frac{3y_e}{2x_e}}\right) - 1\right\}$$

Condition: $\frac{y_e}{x_e^2} < \frac{2}{3}$

Number of bound states: $\upsilon = \frac{1}{2}\left[\frac{\omega_e}{\omega_e x_e} - 1\right]$: Morse

$$n_- = \left[\frac{x_e}{3y_e}\left(1 - \sqrt{1 - \frac{3y_e}{x_e^2}}\right) - \frac{1}{2}\right]: \text{ Dunham}$$

HCl: Number of bound states Dunham: 29, Morse: 28,

4. Application to Diatomic Molecules

- The model was applied to 161 electronic states of all diatomic molecules for which values of the molecular constants are known.

- The values of the independent parameters p' and j are calculated in terms of the experimental constants x_e and y_e.

- p' - quantum deformation parameter is directly related to the coefficient y_e in the cubic term of Dunham expansion

- j - related to the coefficients x_e and y_e.

- The number of bound vibrational states generated by the electronic states of the diatomic molecule is estimated.

- The model fits well with all experimental data except for 30 states for which the values of x_e and y_e do not satisfy the conditions.

$^{1}H\ ^{35}Cl$ Statistical thermodynamics (Angelova&Frank 05)

ground state:

$p' = 188.66$ quantum deformation

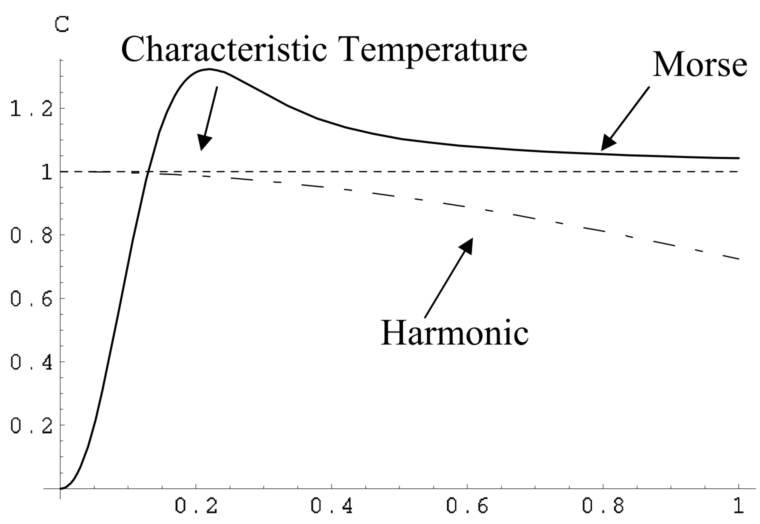
$j = 29.16$

Bound states: Dunham: 29, Morse: 28,

New experimental data: bound states Morse: 27, Dunham:28,

observed 23 lines (rovibrational)

Specific heat as a function of Θ/T, T- temperature, $\Theta = \frac{h\omega_e}{2k_B}$



4. Coherent States of the Morse Potential

Coherent states: In quantum mechanics a coherent state is a state of a quantum harmonic oscillator with dynamics that closely resembles the behaviour of classic harmonic oscillator. It is known as single harmonic oscillator prototype of the coherent state of the oscillating electromagnetic field.

Coherent states of **anharmonic** potentials:

- vibrations in molecules and solids
- quantum information and quantum computing
- quantum control

Morse potential is a good model for studying quantum information and quantum control as it gives a finite number of bound states. Thus the design of control is limited to a finite regime.

Generalised coherent states and Gaussian coherent states of Morse potential (Angelova&Hussin, 08).

Coherent states constructions:

Coherent states: (Schrodinger 1926)
Squeezed states: (Kennard 1927)

Definitions:

- Displacement operator method
- Ladder (annihilation) operator method
- Minimum uncertainty method

Many important papers:
Bargmann, Glauber, Klauder, Perelomov, Gilmore, Iachello, Man'ko.....
and many books Klauder &Skagerstam , Perelomov, Dodonov&Man'ko, Gazeau, Rand, ...

Klauder's construction of coherent states **CS** [Klauder, Phys Rev 2001],

$$\psi(z) = \frac{1}{\sqrt{N\left(|z|^2\right)}} \sum_{n \in I} \frac{z^n}{\sqrt{\rho_n}} |\psi_n\rangle$$

where $|\psi_n\rangle$ is a discrete set of energy eigenstates.
The sum is over the number of energy states and N is a normalisation factor.

Harmonic oscillator set I is infinite, Morse oscillator set I is finite.

For a quantum system with infinite spectrum,

$$A^-|\psi_n\rangle = \sqrt{k(n)}|\psi_{n-1}\rangle, \qquad A^+|\psi_n\rangle = \sqrt{k(n+1)}|\psi_{n+1}\rangle$$

Coherent states are defined as eigenstates of A^-,

$$\rho_n = \prod_{i=1} k(i), \qquad \rho_0 = 1.$$

Morse potential: $$V_M = D_e\left(e^{-2\beta x} - 2e^{-\beta x}\right)$$

Energy levels:

$$E_n = -\frac{\hbar^2}{2m_r}\beta^2\varepsilon_n^2, \qquad \varepsilon_n = \frac{\upsilon - 1}{2} - n = p - n, \qquad n = 0,1,2,\ldots,[p]$$

$$e(n) = \varepsilon_0^2 - \varepsilon_n^2 = n(2p - n),$$ shifted energies

$$y = \upsilon e^{-\beta x}$$ change of variable

$$\psi_{\mathrm{n}}^{\upsilon}(x) \approx e^{-\frac{y}{2}} y^{\varepsilon_n} L_n^{2\varepsilon_n}(y),$$ Eigenfunctions,

$L_n^{2\varepsilon_n}$ associated Laguerre polynomials

$$\upsilon = \sqrt{\frac{8m_r D_e}{\hbar^2\beta^2}}$$ physical parameter, $$p = \frac{\upsilon - 1}{2}$$

Squeezed Coherent States [Angelova, Hertz, Hussin 12]

$$\left(A^{-} + \gamma A^{+}\right)\psi(z,\gamma) \approx z\,\psi(z,\gamma),$$

z – coherent parameter, γ – squeezing parameter

$$\psi(\gamma, z, x) = \frac{1}{\sqrt{N^{\upsilon}(z,\gamma)}} \sum_{n=0}^{[p]-1} \frac{Z(z,\gamma,n)}{\sqrt{\rho_n}} \psi_n^{\upsilon}(x)$$

$$N^{\upsilon}(z,\gamma) = \sum_{n=0}^{[p]-1} \frac{\left|Z(z,\gamma,n)\right|^2}{\rho_n}$$

Ladder Operators, $y = \upsilon e^{-\beta x}$

$$A^{-} = -\left[\frac{d}{dy}(\upsilon - 2N) - \frac{(\upsilon - 2N - 1)(\upsilon - 2N)}{2y} + \frac{\upsilon}{2}\right]\sqrt{K(N)}$$

$$A^{+} = \left(\sqrt{K(N)}\right)^{-1}\left[\frac{d}{dy}(\upsilon - 2N - 2) + \frac{(\upsilon - 2N - 1)(\upsilon - 2N - 2)}{2y} - \frac{\upsilon}{2}\right]$$

$$k(n) = \frac{n(\upsilon - n)(\upsilon - 2n - 1)}{\upsilon - 2n + 1} K(n)$$

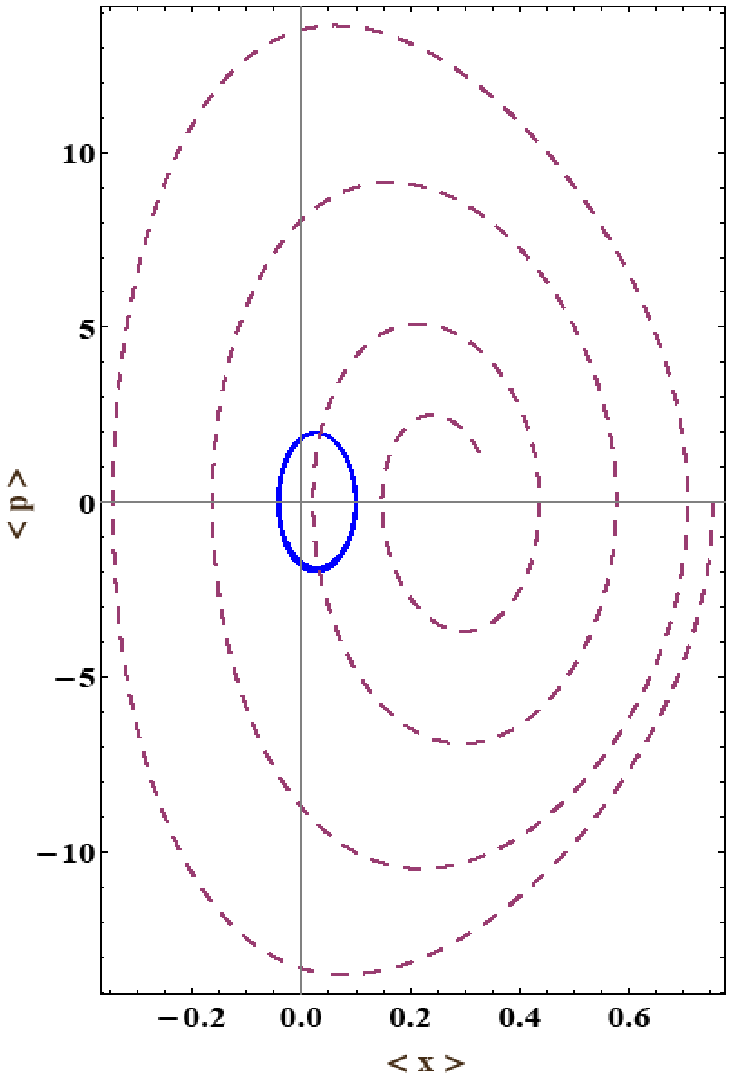
We introduce two types of states:

- Oscillator-like (*o*-type) –ladder operators: *h(2)* algebra

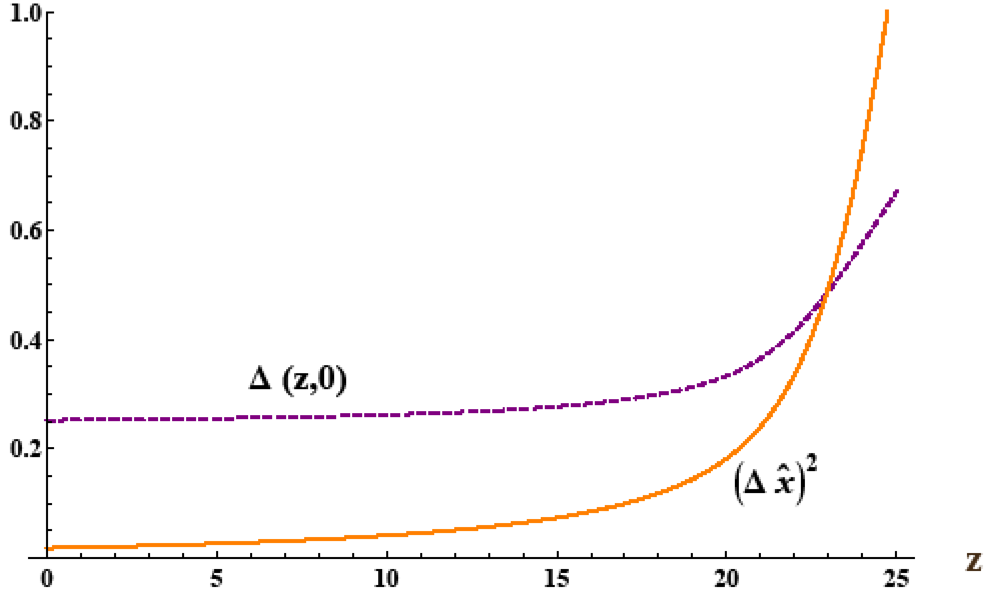
$$k(n)=n, \qquad \rho_n = n!, \qquad K_o(n)=\frac{\upsilon-2n+1}{(\upsilon-n)(\upsilon-2n-1)}$$

- Energy-like (*e*-type) –ladder operators: *su(1,1)* algebra

$$k(n)=e(n), \qquad K_e(n)=K_o(n)(\upsilon-1-n)$$



Phase-space trajectories for *o*-type (dashed) and *e*-type (solid) coherent states, $z=2$, $\gamma = 0$, t is [0,1].



Minimum uncertainty, z<20:

$$\Delta(z,0) = (\Delta x)^2 (\Delta p)^2 \approx \frac{1}{4}$$

good localisation in *x*

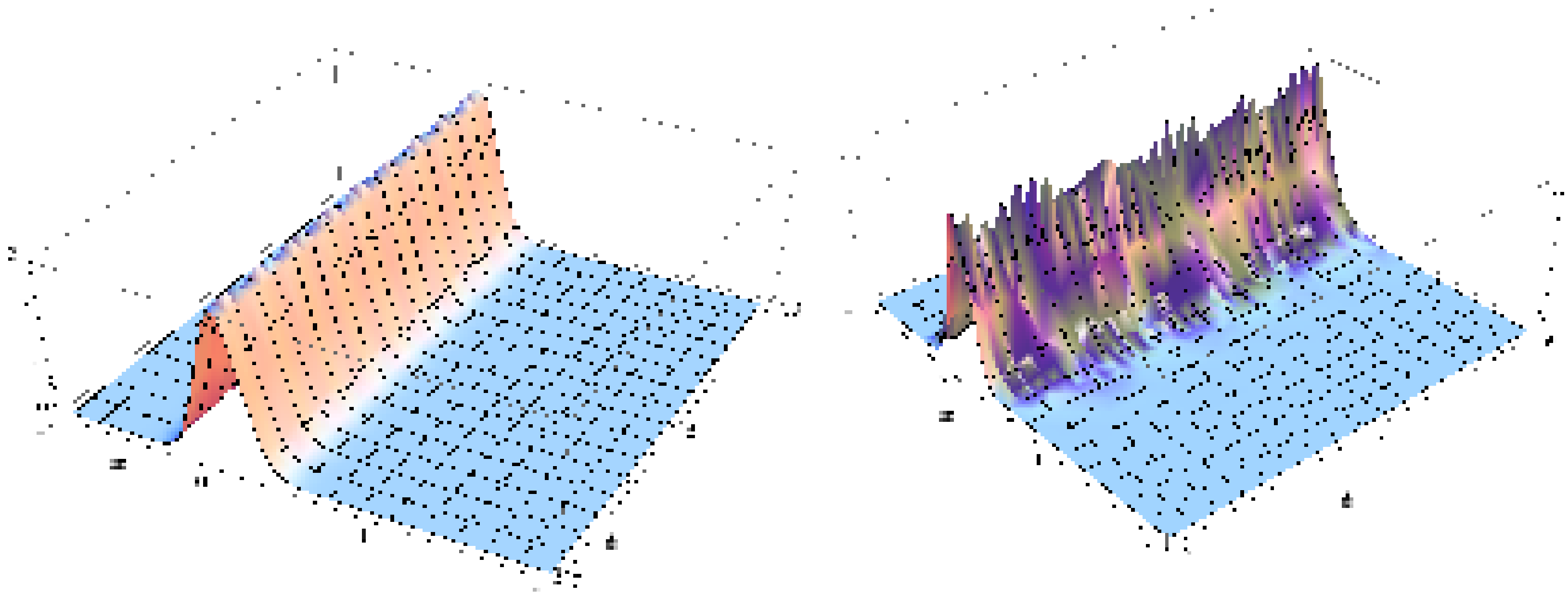
Fig: Uncertainty and dispersion for *e*-type at γ=0

Total noise

$$T = (\Delta x)^2 + (\Delta p)^2 = -1 + \frac{2}{1-\gamma^2}$$

Time Evolution :

$$\psi_{\upsilon}(z,\gamma,x,t)=\frac{1}{\sqrt{N^{\upsilon}(z,\gamma)}}\sum_{n=0}^{[p]-1}\frac{Z(z,\gamma,n)}{\sqrt{\rho_n}}e^{-\frac{iE_n t}{\hbar}}\psi_n^{\upsilon}(x)$$



(a) (b)

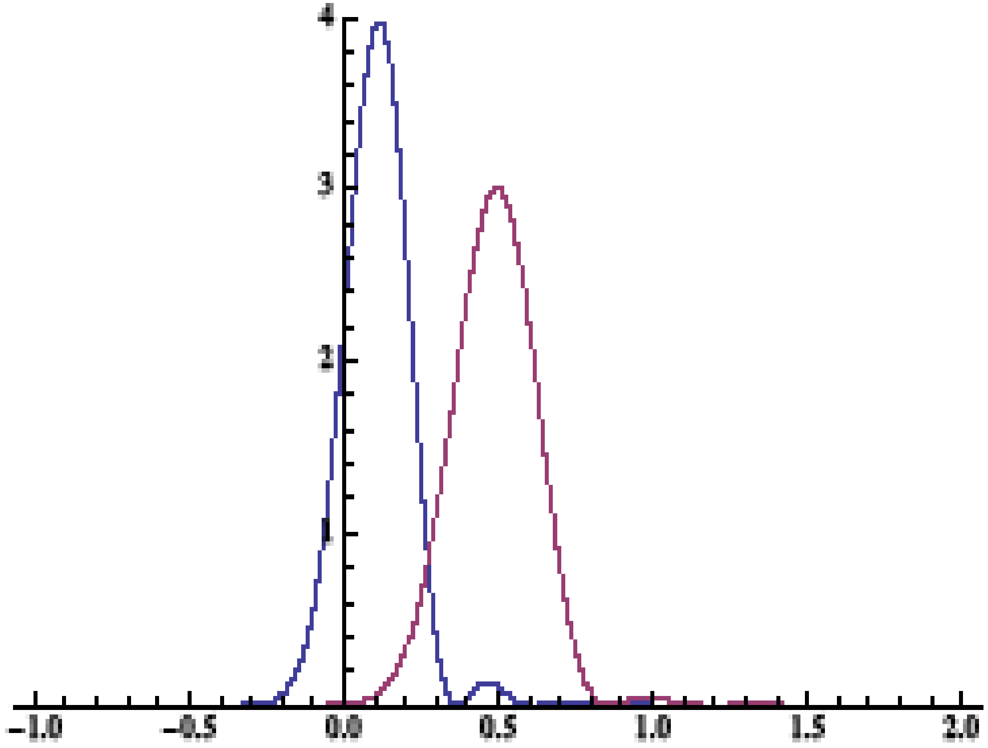
Fig: Time evolution of *e*-type

(a) coherent states and (b) squeezed coherent states for HCl

Probability distributions :

$$P_o(z,\gamma,n) = \frac{1}{N_o^{\upsilon}(z,\gamma)} \frac{|Z_o(z,\gamma,n)|^2}{n!}$$

$$P_e(z,\gamma,n) == \frac{1}{N_e^{\upsilon}(z,\gamma)} \frac{\Gamma(2p-n)}{\Gamma(2p)} \frac{|Z_e(z,\gamma,n)|^2}{n!}$$



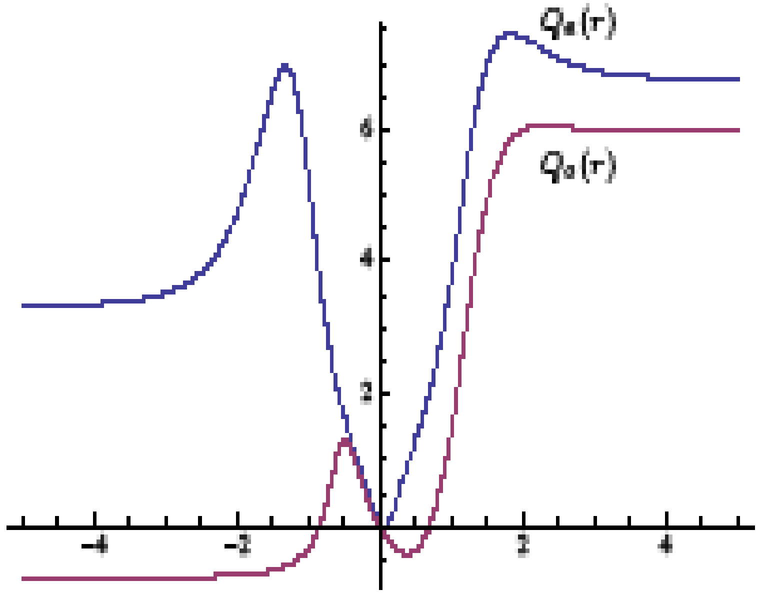
Density probabilities of squeezed coherent states, $z=2$, $\gamma=0.6$
e-type (blue), *o*-type (red), for HCl

Mandel parameter Q

is used to study the statistical properties of CS and SQS,

$$Q(z,\gamma)=\frac{(\Delta N)^2-\langle N\rangle^2}{\langle N\rangle}$$

$$\langle N\rangle=\sum_{n=0} nP(z,\gamma,n), \qquad (\Delta N)^2=\sum_{n=0} n^2P(z,\gamma,n)-\left(\sum_{n=0} nP(z,\gamma,n)\right)^2$$



SCS

Poissonian stats

photon bunching

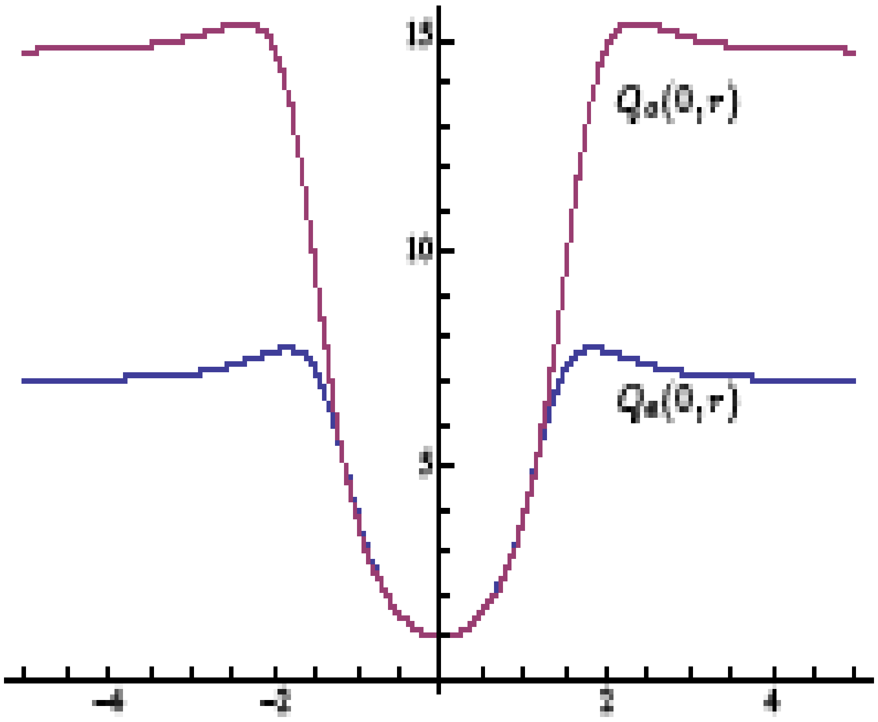
$Q(z,\gamma)>0$

$Q(z,\gamma)<0$

super Poissonian stats

antibunching

Fig: Mandel parameter for *e*-type (blue) and *o*-type (red) states for $z=2$ for HCl



Comparison of Mandel Parameter in the vacuum *z=0* for *o*-type (red) and *e*-type (blue) squeezes states

5. Conclusions

• *q*-deformations of general Hamiltonian, which in different approximations lead to Morse potential or Dunham expansion;

• New physical interpretations of quantum deformation parameters, related to finite number of states;

• Parameters calculated in terms of experimental constants;

• Generalised and Gaussian coherent states of Morse potential;

• Oscillator-like and energy-like coherent and squeezed coherent states defined by ladder operators;

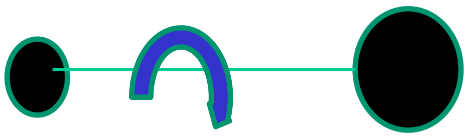
Questions:

Why do energy-like coherent states behave better?

Why there is a squeezing effect in the coherent states?

FutureWork

• bending modes [Iachello&Oss]
modified Pöschl-Teller potential

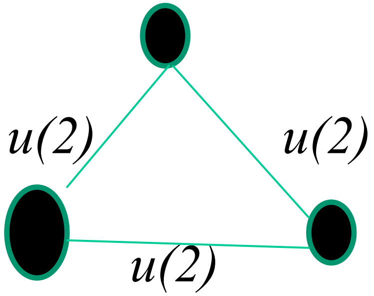


• Generalize the model

-Include other bonds

-Include interactions between bonds

$u(2)\times u(2)\times u(2)\ldots$



• Extend the model to 2 and 3 dimensions

Franco Iachello, thank you for showing us that beauty in physics is in its simplicity