Unitary group approach for effective potentials in 2D systems: application to carbon suboxide C_3O_2

Marisol Rodríguez Arcos

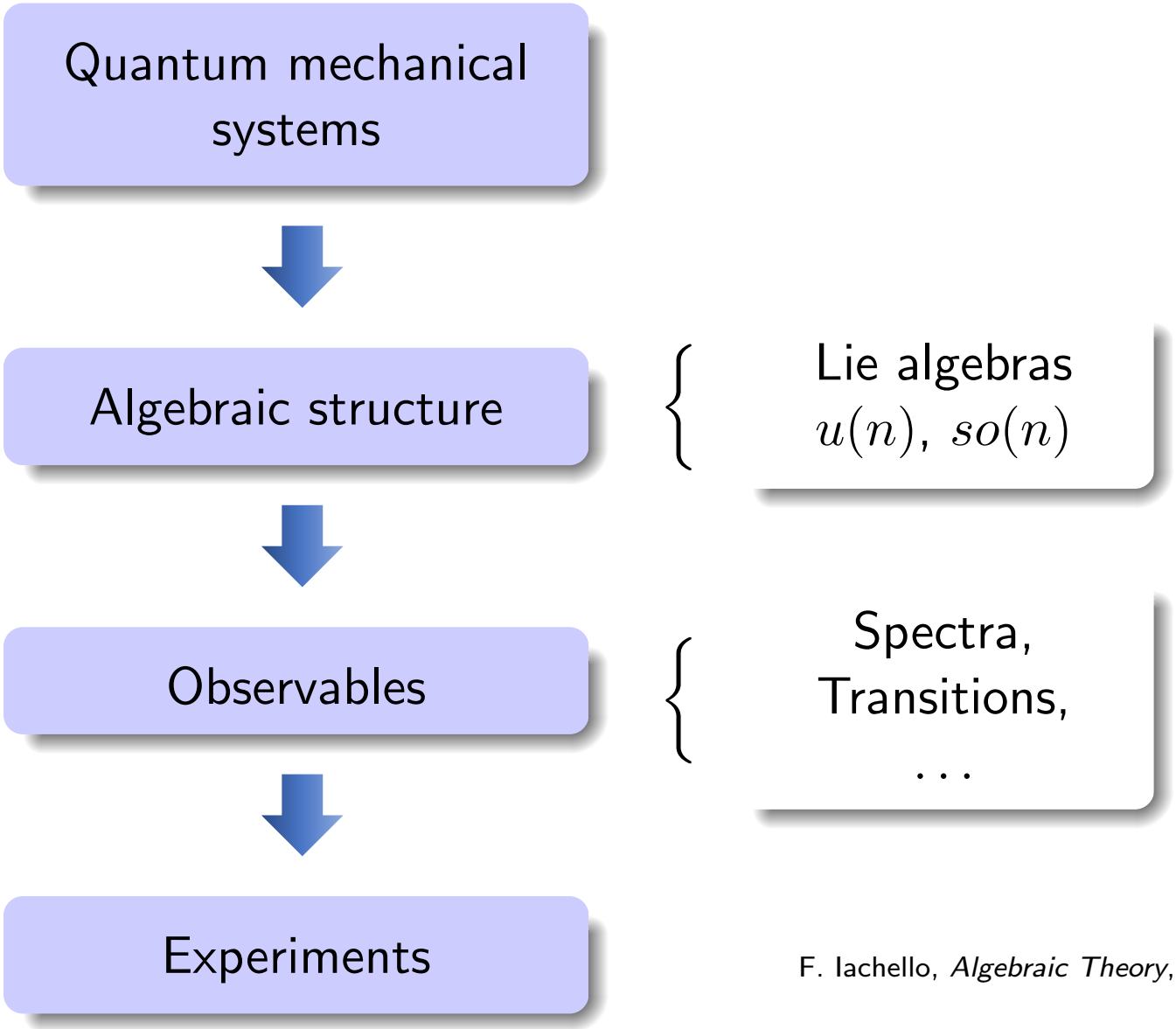
Nuclear Sciences Institute,
National Autonomous University of Mexico

in collaboration with Renato Lemus (ICN-UNAM)

Content

1. Algebraic methods
2. Connection between algebraic and configuration space
   - The $U(3)$ unitary group approach
   - Energy, coordinate and momentum representation
3. Algebraic representation of 2D Hamiltonian
   - Quartic potential
   - Energy spectra and wave functions
4. Application to carbon suboxide (C_3O_2)

Algebraic methods



F. Iachello, *Algebraic Theory*, **160**, 151 (1994).

Connection between the algebraic and configuration space

What is the translation of the coordinate q and momentum p from configuration into the algebraic space?

Connection between the algebraic and configuration space

What is the translation of the coordinate q and momentum p from configuration into the algebraic space?

Configuration space

$$\hat{H}_{cs}(\mathbf{q}, \mathbf{p})\psi_{\mathbf{n}}(\mathbf{q}) = E_{\mathbf{n}}\psi_{\mathbf{n}}(\mathbf{q})$$

Connection between the algebraic and configuration space

What is the translation of the coordinate q and momentum p from configuration into the algebraic space?

Configuration space

$$\hat{H}_{cs}(\mathbf{q},\mathbf{p})\psi_{\mathbf{n}}(\mathbf{q}) = E_{\mathbf{n}}\psi_{\mathbf{n}}(\mathbf{q})$$

Fock space

$$\hat{H}_{Fock}|\mathbf{n}\rangle = E_{\mathbf{n}}|\mathbf{n}\rangle$$

second quantization

Connection between the algebraic and configuration space

What is the translation of the coordinate q and momentum p from configuration into the algebraic space?

Configuration space

$$\hat{H}_{cs}(\mathbf{q},\mathbf{p})\psi_{\mathbf{n}}(\mathbf{q}) = E_{\mathbf{n}}\psi_{\mathbf{n}}(\mathbf{q})$$

Fock space

$$\hat{H}_{Fock}|\mathbf{n}\rangle = E_{\mathbf{n}}|\mathbf{n}\rangle$$

Algebraic space

$$\hat{H}^{U(\nu+1)}_{alg}|[N]\mathbf{n}\rangle = E_{\mathbf{n}}|[N]\mathbf{n}\rangle$$

?

Example. 1D harmonic oscillator

Configuration space

$$\hat{H}_{cs} = \frac{1}{2\mu}\hat{p}^2 + \frac{\omega^2\mu}{2}\hat{q}^2,$$

$$\psi_n(q) = N_n e^{(-q^2/2\lambda_0^2)} H_n(q/\lambda_0)$$

$$N_n = (n!2^n\lambda_0\sqrt{\pi})^{-1/2}$$

Example. 1D harmonic oscillator

Configuration space

$$\hat{H}_{cs} = \frac{1}{2\mu}\hat{p}^2 + \frac{\omega^2\mu}{2}\hat{q}^2,$$

$$\psi_n(q) = N_n e^{(-q^2/2\lambda_0^2)} H_n(q/\lambda_0)$$

$$N_n = (n!2^n\lambda_0\sqrt{\pi})^{-1/2}$$

Fock space

$$\hat{H}^{o.a}_{Fock} = \hbar\omega(\hat{n} + 1/2),$$
$$\hat{n} = \hat{a}^\dagger\hat{a}$$

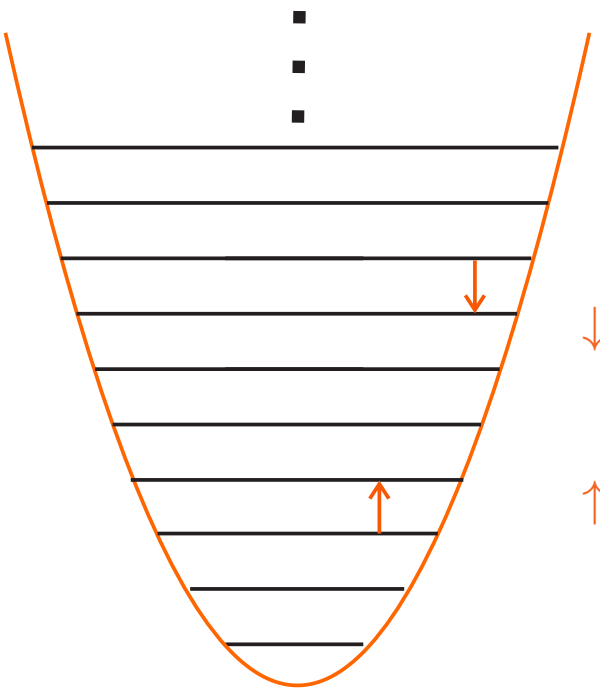
$$|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n|0\rangle.$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{\mu\omega}{\hbar}}\hat{q} - i\frac{\hat{p}}{\sqrt{\hbar\omega\mu}}\right),$$
$$\hat{a} = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{\mu\omega}{\hbar}}\hat{q} + i\frac{\hat{p}}{\sqrt{\hbar\omega\mu}}\right).$$

Fock space

1D harmonic oscillator

$$\hat{n} = \hat{a}^\dagger \hat{a}$$



$\hat{a}|n\rangle$

$\downarrow |n-1\rangle$

$\uparrow |n+1\rangle$

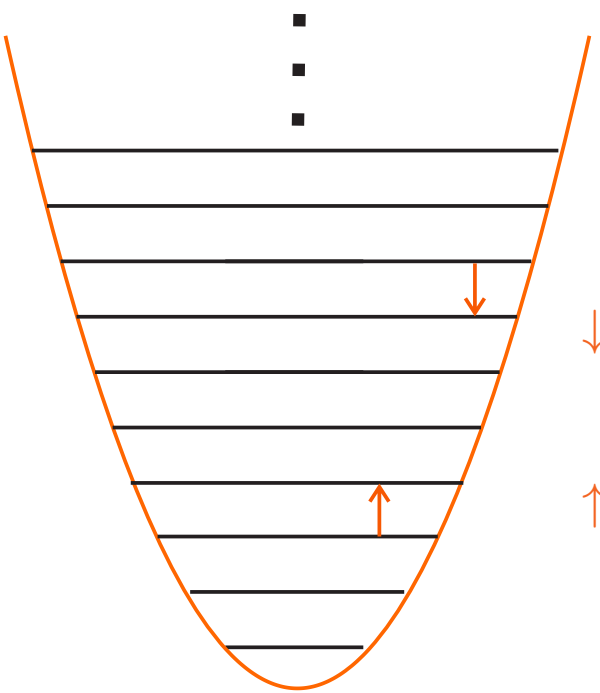
$\hat{a}^\dagger |n\rangle$

$$\sum_n^\infty |n\rangle\langle n| = 1$$

Fock space

1D harmonic oscillator

$$\hat{n} = \hat{a}^\dagger \hat{a}$$



$\hat{a}|n\rangle$

$\downarrow |n-1\rangle$

$\uparrow |n+1\rangle$

$\hat{a}^\dagger |n\rangle$

$$\sum_n^\infty |n\rangle\langle n| = 1$$

In practice, when the basis is cut off:

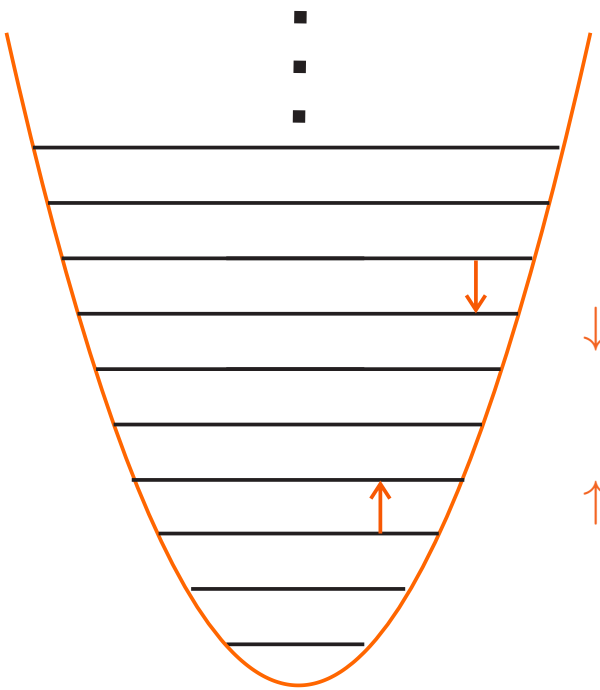
$$\sum_n^\infty |n\rangle\langle n| = 1$$

It is possible to use a harmonic oscillator basis and recover the closure condition?

Fock space

1D harmonic oscillator

$$\hat{n} = \hat{a}^\dagger \hat{a}$$



$\hat{a}|n\rangle$

$\downarrow |n-1\rangle$

$\uparrow |n+1\rangle$

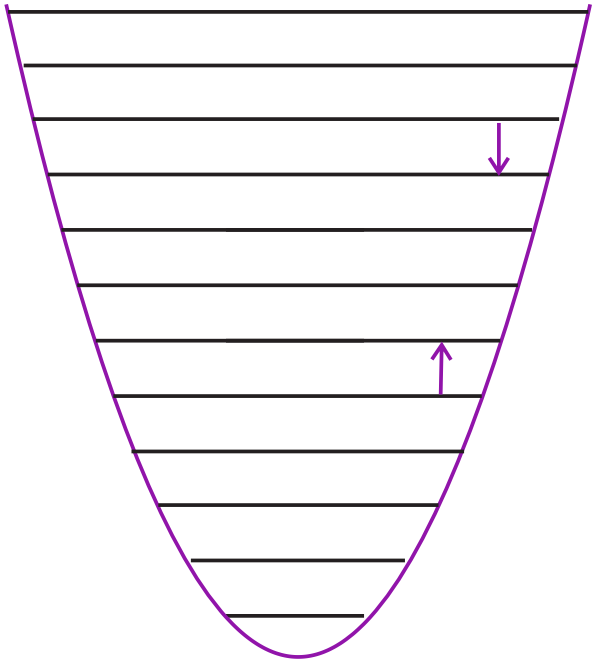
$\hat{a}^\dagger |n\rangle$

$$\sum_{n}^{\infty} |n\rangle\langle n| = 1$$

Algebraic space

Adding a scalar boson $s^\dagger(s)$

$$\hat{N} = \hat{a}^\dagger(\hat{a}) + s^\dagger(s)$$



$s^\dagger \hat{a}|[N]n\rangle$

$\downarrow |[N]n-1\rangle$

$\uparrow |[N]n+1\rangle$

$\hat{a}^\dagger s|[N]n\rangle$

$$\sum_{n}^{N} |[N]n\rangle\langle[N]n| = 1$$

1D Algebraic realization

Adding a scalar boson $s(s^\dagger)$ to the 1D oscillator:

1D Algebraic realization

Adding a scalar boson $s(s^\dagger)$ to the 1D oscillator:

$$G_{U(2)} = \{\hat{N}, \hat{n}, \hat{a}^\dagger s, s^\dagger \hat{a}\},$$

$$\hat{N} = \hat{a}^\dagger \hat{a} + s^\dagger s; \quad \hat{n} = \hat{a}^\dagger \hat{a}.$$

1D Algebraic realization

Adding a scalar boson $s(s^\dagger)$ to the 1D oscillator:

$$G_{U(2)} = \{\hat{N}, \hat{n}, \hat{a}^\dagger s, s^\dagger \hat{a}\},$$

$$\hat{N} = \hat{a}^\dagger \hat{a} + s^\dagger s; \quad \hat{n} = \hat{a}^\dagger \hat{a}.$$

The $U(2)$ group becomes a dynamical group.

1D Algebraic realization

Adding a scalar boson $s(s^\dagger)$ to the 1D oscillator:

$$G_{U(2)} = \{\hat{N}, \hat{n}, \hat{a}^\dagger s, s^\dagger \hat{a}\},$$

$$\hat{N} = \hat{a}^\dagger \hat{a} + s^\dagger s; \quad \hat{n} = \hat{a}^\dagger \hat{a}.$$

The $U(2)$ group becomes a dynamical group.

Coordinates and momenta take the form [5, 6]:

$$\hat{\mathcal{Q}} = \sqrt{\frac{\hbar}{2\mu\omega}} \frac{1}{\sqrt{N}} \left[\hat{a}^\dagger s + s^\dagger \hat{a}\right],$$

$$\hat{\mathcal{P}} = \frac{i}{\sqrt{2}} \sqrt{\hbar\mu\omega} \frac{1}{\sqrt{N}} \left[\hat{a}^\dagger s - s^\dagger \hat{a}\right].$$

[5]R. Lemus, *Mol. Phys.*, (2018).
[6] R.D. Santiago, *et al. Mol. Phys.*, **24**, 206 (2017).

1D Algebraic realization

Adding a scalar boson $s(s^\dagger)$ to the 1D oscillator:

$$G_{U(2)} = \{\hat{N}, \hat{n}, \hat{a}^\dagger s, s^\dagger \hat{a}\},$$

$$\hat{N} = \hat{a}^\dagger \hat{a} + s^\dagger s; \quad \hat{n} = \hat{a}^\dagger \hat{a}.$$

The $U(2)$ group becomes a dynamical group.

Coordinates and momenta take the form [5, 6]:

$$\hat{\mathcal{Q}} = \sqrt{\frac{\hbar}{2\mu\omega}} \frac{1}{\sqrt{N}} \left[\hat{a}^\dagger s + s^\dagger \hat{a}\right],$$

$$\hat{\mathcal{P}} = \frac{i}{\sqrt{2}} \sqrt{\hbar\mu\omega} \frac{1}{\sqrt{N}} \left[\hat{a}^\dagger s - s^\dagger \hat{a}\right].$$

$$\hat{q} \,|_{\hat{a}^\dagger(\hat{a}) \to \hat{b}^\dagger(\hat{b})} \to \hat{\mathcal{Q}}; \qquad \hat{p} \,|_{\hat{a}^\dagger(\hat{a}) \to \hat{b}^\dagger(\hat{b})} \to \hat{\mathcal{P}}.$$

$$\hat{b}^\dagger \equiv \frac{\hat{a}^\dagger s}{\sqrt{N}}; \qquad \hat{b} \equiv \frac{s^\dagger \hat{a}}{\sqrt{N}}$$

[5]R. Lemus, *Mol. Phys.*, (2018).
[6] R.D. Santiago, *et al. Mol. Phys.*, **24**, 206 (2017).

2D Systems. The $U(3)$ unitary group approach

Harmonic oscillator in 2D:

$$\text{O.A}\hat{H}_{Fock} = \frac{\hbar\omega}{2}\sum_{\sigma}(\hat{\tau}_{\sigma}^{\dagger}\hat{\tau}_{\sigma} + \hat{\tau}_{\sigma}\hat{\tau}_{\sigma}^{\dagger}), \qquad \sigma = \pm$$

$$\hat{\tau}_{\pm}^{\dagger} = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{\omega\mu}{\hbar}}\hat{Q}_{\pm} + i\frac{\hat{P}_{\mp}}{\sqrt{\hbar\omega\mu}}\right],$$

2D Systems. The $U(3)$ unitary group approach

Harmonic oscillator in 2D:

$$\text{O.A}\hat{H}_{Fock} = \frac{\hbar\omega}{2}\sum_{\sigma}(\hat{\tau}^{\dagger}_{\sigma}\hat{\tau}_{\sigma} + \hat{\tau}_{\sigma}\hat{\tau}^{\dagger}_{\sigma}), \qquad \sigma = \pm$$

$$\hat{\tau}^{\dagger}_{\pm} = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{\omega\mu}{\hbar}}\hat{Q}_{\pm} + i\frac{\hat{P}_{\mp}}{\sqrt{\hbar\omega\mu}}\right],$$

The $U(3)$ space is generated by adding a scalar boson $\sigma^{\dagger}(\sigma)$ to the 2D oscillator space:

$$\begin{aligned}
\hat{D}_{\pm} &= \sqrt{2}(\pm\tau^{\dagger}_{\pm}\sigma \mp \sigma^{\dagger}\tau_{\mp}), & \hat{R}_{\pm} &= \sqrt{2}(\tau^{\dagger}_{\pm}\sigma + \sigma^{\dagger}\tau_{\mp}),\\
\hat{Q}_{\pm} &= \sqrt{2}\tau^{\dagger}_{\pm}\tau_{\mp}, & \hat{n}_{\sigma} &= \sigma^{\dagger}\sigma,\\
\hat{n} &= \tau^{\dagger}_{+}\tau_{+} + \tau^{\dagger}_{-}\tau_{-}, & \hat{l} &= \tau^{\dagger}_{+}\tau_{+} - \tau^{\dagger}_{-}\tau_{-}.
\end{aligned}$$

Subalgebra chains of algebra $U(3)$

The algebra $U(3)$ provides the following three chains:

Chain	Casimir operator
$U(3) \supset U(2) \supset SO(2)$	$\hat{C}_{U(2)} = \hat{n}$
$U(3) \supset SO(3) \supset SO(2)$	$\hat{C}_{SO(3)} = \hat{W}^2 = D^2 + l^2$
$U(3) \supset S\bar{O}(3) \supset SO(2)$	$\hat{C}_{S\bar{O}(3)} = \hat{\bar{W}}^2 = R^2 + l^2$

Subalgebra chains of algebra $U(3)$

The algebra $U(3)$ provides the following three chains:

Chain	Casimir operator
$U(3) \supset U(2) \supset SO(2)$	$\hat{C}_{U(2)} = \hat{n}$
$U(3) \supset SO(3) \supset SO(2)$	$\hat{C}_{SO(3)} = \hat{W}^2 = D^2 + l^2$
$U(3) \supset S\bar{O}(3) \supset SO(2)$	$\hat{C}_{S\bar{O}(3)} = \hat{\bar{W}}^2 = R^2 + l^2$

The bases associated with the Casimir Operators:

$$\hat{n}|[N]; nl\rangle = n|[N]; nl\rangle,$$

$$\hat{W}^2|[N]; \zeta l\rangle = \zeta(\zeta+1)|[N]; \zeta l\rangle,$$

$$\hat{\bar{W}}^2|[N]; \bar{\zeta} l\rangle = \bar{\zeta}(\bar{\zeta}+1)|[N]; \bar{\zeta} l\rangle,$$

Subalgebra chains of algebra $U(3)$

The algebra $U(3)$ provides the following three chains:

Chain	Casimir operator
$U(3) \supset U(2) \supset SO(2)$	$\hat{C}_{U(2)} = \hat{n}$
$U(3) \supset SO(3) \supset SO(2)$	$\hat{C}_{SO(3)} = \hat{W}^2 = D^2 + l^2$
$U(3) \supset S\bar{O}(3) \supset SO(2)$	$\hat{C}_{S\bar{O}(3)} = \hat{\bar{W}}^2 = R^2 + l^2$

The bases associated with the Casimir Operators:

$$\hat{n}|[N]; nl\rangle = n|[N]; nl\rangle,$$

$$\hat{W}^2|[N]; \zeta l\rangle = \zeta(\zeta+1)|[N]; \zeta l\rangle,$$

$$\hat{\bar{W}}^2|[N]; \bar{\zeta} l\rangle = \bar{\zeta}(\bar{\zeta}+1)|[N]; \bar{\zeta} l\rangle,$$

the bases satisfy:

$$\sum_{n,l}^{N} |[N]nl\rangle\langle[N]nl| = \sum_{\zeta,l}^{N} |[N]\zeta l\rangle\langle[N]\zeta l| = \sum_{\bar{\zeta},l}^{N} |[N]\bar{\zeta} l\rangle\langle[N]\bar{\zeta} l| = 1.$$

Algebraic representation of the coordinate and momentum

Using a mapping to the 2D h. o. basis, the coordinates and momenta take the form [7]:

$$\hat{Q}_\pm \to \hat{\mathcal{Q}}_\pm \qquad \hat{P}_\pm \to \hat{\mathcal{P}}_\pm$$

$$\hat{\mathcal{Q}}_\pm = \pm\frac{1}{2}\sqrt{\frac{\hbar}{\mu\omega}}\frac{1}{\sqrt{N}}\hat{D}_\pm, \qquad \hat{\mathcal{P}}_\pm = -\frac{i}{2}\sqrt{\hbar\mu\omega}\frac{1}{\sqrt{N}}\hat{R}_\mp.$$

Algebraic representation of the coordinate and momentum

Using a mapping to the 2D h. o. basis, the coordinates and momenta take the form [7]:

$$\hat{Q}_\pm \to \hat{\mathcal{Q}}_\pm \qquad \hat{P}_\pm \to \hat{\mathcal{P}}_\pm$$

$$\hat{\mathcal{Q}}_\pm = \pm\frac{1}{2}\sqrt{\frac{\hbar}{\mu\omega}}\frac{1}{\sqrt{N}}\hat{D}_\pm, \qquad \hat{\mathcal{P}}_\pm = -\frac{i}{2}\sqrt{\hbar\mu\omega}\frac{1}{\sqrt{N}}\hat{R}_\mp.$$

The operators $\hat{W}^2$ and $\hat{\bar{W}}^2$ associated with the $SO(3)$ and $S\bar{O}(3)$ subalgebras:

$$\hat{W}^2 = D^2 + l^2 \qquad \hat{\bar{W}}^2 = R^2 + l^2.$$

Algebraic representation of the coordinate and momentum

Using a mapping to the 2D h. o. basis, the coordinates and momenta take the form [7]:

$$\hat{Q}_\pm \to \hat{\mathcal{Q}}_\pm \qquad \hat{P}_\pm \to \hat{\mathcal{P}}_\pm$$

$$\hat{\mathcal{Q}}_\pm = \pm\frac{1}{2}\sqrt{\frac{\hbar}{\mu\omega}}\frac{1}{\sqrt{N}}\hat{D}_\pm, \qquad \hat{\mathcal{P}}_\pm = -\frac{i}{2}\sqrt{\hbar\mu\omega}\frac{1}{\sqrt{N}}\hat{R}_\mp.$$

The operators $\hat{W}^2$ and $\hat{\bar{W}}^2$ associated with the $SO(3)$ and $S\bar{O}(3)$ subalgebras:

$$\hat{W}^2 = N\frac{2\mu\omega}{\hbar}\hat{\mathcal{Q}}^2 + \hat{l}^2, \qquad \hat{\bar{W}}^2 = N\frac{2}{\hbar\mu\omega}\hat{\mathcal{P}}^2 + \hat{l}^2.$$

Algebraic representation of the coordinate and momentum

Using a mapping to the 2D h. o. basis, the coordinates and momenta take the form [7]:

$$\hat{Q}_\pm \to \hat{\mathcal{Q}}_\pm \qquad \hat{P}_\pm \to \hat{\mathcal{P}}_\pm$$

$$\hat{\mathcal{Q}}_\pm = \pm\frac{1}{2}\sqrt{\frac{\hbar}{\mu\omega}}\frac{1}{\sqrt{N}}\hat{D}_\pm, \qquad \hat{\mathcal{P}}_\pm = -\frac{i}{2}\sqrt{\hbar\mu\omega}\frac{1}{\sqrt{N}}\hat{R}_\mp.$$

The operators $\hat{W}^2$ and $\hat{\bar{W}}^2$ associated with the $SO(3)$ and $S\bar{O}(3)$ subalgebras:

$$\hat{W}^2 = N\frac{2\mu\omega}{\hbar}\hat{\mathcal{Q}}^2 + \hat{l}^2, \qquad \hat{\bar{W}}^2 = N\frac{2}{\hbar\mu\omega}\hat{\mathcal{P}}^2 + \hat{l}^2.$$

This result leads to the identification:

$$U(3) \supset SO(3) \supset SO(2) \to \text{coordinate}$$
$$U(3) \supset S\bar{O}(3) \supset SO(2) \to \text{momentum}$$

[7] M. M. Estévez-Fregoso and R. Lemus, *Mol. Phys.*, (2018).

Algebraic representation of energy

The harmonic oscillator hamiltonian can be written in the algebraic space:

$$_{\text{O.A}}\hat{H}^{\text{U(3)}}_{alg} = -\frac{1}{2}g_{+-}\ (\hat{\mathcal{P}}_{+}\hat{\mathcal{P}}_{-} + \hat{\mathcal{P}}_{-}\hat{\mathcal{P}}_{+}) - \frac{1}{2}f_{+-}\ (\hat{\mathcal{Q}}_{+}\hat{\mathcal{Q}}_{-} + \hat{\mathcal{Q}}_{-}\hat{\mathcal{Q}}_{+}),$$

Algebraic representation of energy

The harmonic oscillator hamiltonian can be written in the algebraic space:

$$\text{O.A}\hat{H}^{\text{U(3)}}_{alg} = -\frac{1}{2}g_{+-}\ (\hat{\mathcal{P}}_+\hat{\mathcal{P}}_- + \hat{\mathcal{P}}_-\hat{\mathcal{P}}_+) - \frac{1}{2}f_{+-}\ (\hat{\mathcal{Q}}_+\hat{\mathcal{Q}}_- + \hat{\mathcal{Q}}_-\hat{\mathcal{Q}}_+),$$

and in terms of the $\hat{C}_{U(2)} = \hat{n}$ operator:

$$\text{O.A}\hat{H}^{\text{U(3)}}_{alg} = \hbar\omega\left\{\left(1 - \frac{1}{2N}\right)\hat{n} + 1 - \frac{\hat{n}^2}{N}\right\}.$$

Algebraic representation of energy

The harmonic oscillator hamiltonian can be written in the algebraic space:

$$\text{O.A}\hat{H}^{\text{U(3)}}_{alg} = -\frac{1}{2}g_{+-}\ (\hat{\mathcal{P}}_+\hat{\mathcal{P}}_- + \hat{\mathcal{P}}_-\hat{\mathcal{P}}_+) - \frac{1}{2}f_{+-}\ (\hat{\mathcal{Q}}_+\hat{\mathcal{Q}}_- + \hat{\mathcal{Q}}_-\hat{\mathcal{Q}}_+),$$

and in terms of the $\hat{C}_{U(2)} = \hat{n}$ operator:

$$\text{O.A}\hat{H}^{\text{U(3)}}_{alg} = \hbar\omega\left\{\left(1 - \frac{1}{2N}\right)\hat{n} + 1 - \frac{\hat{n}^2}{N}\right\}.$$

We can thus identify the chain as the energy representation:

$$U(3) \supset U(2) \supset SO(2) \rightarrow \text{energy}$$

Algebraic representation of energy

The harmonic oscillator hamiltonian can be written in the algebraic space:

$$\text{O.A}\hat{H}^{\text{U(3)}}_{alg} = -\frac{1}{2}g_{+-}\ (\hat{\mathcal{P}}_+\hat{\mathcal{P}}_- + \hat{\mathcal{P}}_-\hat{\mathcal{P}}_+) - \frac{1}{2}f_{+-}\ (\hat{\mathcal{Q}}_+\hat{\mathcal{Q}}_- + \hat{\mathcal{Q}}_-\hat{\mathcal{Q}}_+),$$

and in terms of the $\hat{C}_{U(2)} = \hat{n}$ operator:

$$\text{O.A}\hat{H}^{\text{U(3)}}_{alg} = \hbar\omega\left\{\left(1 - \frac{1}{2N}\right)\hat{n} + 1 - \frac{\hat{n}^2}{N}\right\}.$$

We can thus identify the chain as the energy representation:

$$U(3) \supset U(2) \supset SO(2) \rightarrow \text{energy}$$

The results are summarized in:

Chain	Basis	Representation
$U(3) \supset U(2) \supset SO(2)$	$\lvert[N]; nl\rangle$	Energy
$U(3) \supset SO(3) \supset SO(2)$	$\lvert[N]; \zeta l\rangle$	Coordinate
$U(3) \supset S\bar{O}(3) \supset SO(2)$	$\lvert[N]; \bar{\zeta} l\rangle$	Momentum

A hamiltonian in the algebraic space :

$$\hat{H}_{cs} = \frac{\mathbf{P}^2}{2\mu} + V(\sqrt{\mathbf{Q}^2}) \quad \rightarrow \quad \hat{H}^{\mathsf{U(3)}}_{alg} = \frac{\hat{\mathcal{P}}^2}{2\mu} + V(\sqrt{\hat{\mathcal{Q}}^2}).$$

A hamiltonian in the algebraic space :

$$\hat{H}_{cs} = \frac{\mathbf{P}^2}{2\mu} + V(\sqrt{\mathbf{Q}^2}) \quad \rightarrow \quad \hat{H}^{\mathsf{U(3)}}_{alg} = \frac{\hat{\mathcal{P}}^2}{2\mu} + V(\sqrt{\hat{\mathcal{Q}}^2}).$$

Adding and subtracting the term $-\frac{\mu\omega}{2}\hat{\mathcal{Q}}^2$:

A hamiltonian in the algebraic space :

$$\hat{H}_{cs} = \frac{\mathbf{P}^2}{2\mu} + V(\sqrt{\mathbf{Q}^2}) \quad \rightarrow \quad \hat{H}^{\mathsf{U(3)}}_{alg} = \frac{\hat{\mathcal{P}}^2}{2\mu} + V(\sqrt{\hat{\mathcal{Q}}^2}).$$

Adding and subtracting the term $-\frac{\mu\omega}{2}\hat{\mathcal{Q}}^2$:

$$\hat{H}^{\mathsf{U(3)}}_{alg} = \frac{\hat{\mathcal{P}}^2}{2\mu} + \frac{\mu\omega}{2}\hat{\mathcal{Q}}^2 - \frac{\mu\omega}{2}\hat{\mathcal{Q}}^2 + V(\sqrt{\hat{\mathcal{Q}}^2}),$$

A hamiltonian in the algebraic space :

$$\hat{H}_{cs} = \frac{\mathbf{P}^2}{2\mu} + V(\sqrt{\mathbf{Q}^2}) \quad \rightarrow \quad \hat{H}^{\mathsf{U(3)}}_{alg} = \frac{\hat{\mathcal{P}}^2}{2\mu} + V(\sqrt{\hat{\mathcal{Q}}^2}).$$

Adding and subtracting the term $-\frac{\mu\omega}{2}\hat{\mathcal{Q}}^2$:

$$\hat{H}^{U(3)}_{alg} = \hbar\omega \left[\left(1 - \frac{1}{2N}\right)\hat{n} + 1 - \frac{\hat{n}^2}{N} \right] + \kappa V'(\sqrt{\hat{\mathcal{Q}}^2}),$$

where:

$$V'(\hat{\mathcal{Q}}^2) = -\frac{m\omega^2}{2}\hat{\mathcal{Q}}^2 + V(\sqrt{\hat{\mathcal{Q}}^2}), \;\; \kappa \in [0,1].$$

A hamiltonian in the algebraic space :

$$\hat{H}_{cs} = \frac{\mathbf{P}^2}{2\mu} + V(\sqrt{\mathbf{Q}^2}) \quad \rightarrow \quad \hat{H}^{\mathsf{U(3)}}_{alg} = \frac{\hat{\mathcal{P}}^2}{2\mu} + V(\sqrt{\hat{\mathcal{Q}}^2}).$$

Adding and subtracting the term $-\frac{\mu\omega}{2}\hat{\mathcal{Q}}^2$:

$$\hat{H}^{U(3)}_{alg} = \hbar\omega \left[\left(1 - \frac{1}{2N}\right)\hat{n} + 1 - \frac{\hat{n}^2}{N}\right] + \kappa V'(\sqrt{\hat{\mathcal{Q}}^2}),$$

where:

$$V'(\hat{\mathcal{Q}}^2) = -\frac{m\omega^2}{2}\hat{\mathcal{Q}}^2 + V(\sqrt{\hat{\mathcal{Q}}^2}), \;\; \kappa \in [0,1].$$

We have the following matrix elements in the coordinate representation:

$$\langle [N]\zeta' l|\hat{\mathcal{Q}}^2|[N]\zeta l\rangle = \frac{d^2}{2}\frac{[\zeta(\zeta+1) - l^2]}{N}\,\delta_{\zeta',\zeta}, \quad d = \sqrt{\hbar/\mu\omega}$$

Algebraic representation of 2D Hamiltonian

Hence the matrix elements of the Hamiltonian (for a given l) in the energy representation take the general form:

$$\boxed{\mathbf{H}^{(E)} = \mathbf{\Lambda}^{(E)} + \kappa \mathbf{T}^{\dagger} \mathbf{\Lambda}^{(Q)} \mathbf{T},}$$

Algebraic representation of 2D Hamiltonian

Hence the matrix elements of the Hamiltonian (for a given l) in the energy representation take the general form:

$$\mathbf{H}^{(E)} = \mathbf{\Lambda}^{(E)}$$

where:

$$||\mathbf{\Lambda}^{(E)}|| = \hbar\omega \left[\left(1 - \frac{1}{2N}\right)\hat{n} + 1 - \frac{\hat{n}^2}{N}\right]\delta_{n',n},$$

Algebraic representation of 2D Hamiltonian

Hence the matrix elements of the Hamiltonian (for a given l) in the energy representation take the general form:

$$\mathbf{H}^{(E)} = \mathbf{\Lambda}^{(E)} + \mathbf{\Lambda}^{(Q)}$$

where:

$$||\mathbf{\Lambda}^{(E)}|| = \hbar\omega \left[\left(1 - \frac{1}{2N}\right)\hat{n} + 1 - \frac{\hat{n}^2}{N}\right]\delta_{n',n},$$

$$||\mathbf{\Lambda}^{(Q)}|| = \hbar\omega\left[-\frac{1}{2}\frac{\xi(\zeta,l)^2}{2N} + \frac{1}{\hbar\omega}V\left(d\frac{\xi(\zeta,l)}{\sqrt{2N}}\right)\right]\delta_{\zeta,\zeta'},$$

with $\xi(\zeta,l) = \sqrt{\zeta(\zeta+1) - l^2}$ and $\kappa \in [0,1]$.

Algebraic representation of 2D Hamiltonian

Hence the matrix elements of the Hamiltonian (for a given l) in the energy representation take the general form:

$$\mathbf{H}^{(E)} = \mathbf{\Lambda}^{(E)} + \kappa \mathbf{T}^{\dagger} \mathbf{\Lambda}^{(Q)} \mathbf{T},$$

where:

$$||\mathbf{\Lambda}^{(E)}|| = \hbar\omega \left[\left(1 - \frac{1}{2N} \right) \hat{n} + 1 - \frac{\hat{n}^2}{N} \right] \delta_{n',n},$$

$$||\mathbf{\Lambda}^{(Q)}|| = \hbar\omega \left[-\frac{1}{2} \frac{\xi(\zeta,l)^2}{2N} + \frac{1}{\hbar\omega} V\left(d \frac{\xi(\zeta,l)}{\sqrt{2N}} \right) \right] \delta_{\zeta,\zeta'},$$

with $\xi(\zeta,l) = \sqrt{\zeta(\zeta+1) - l^2}$ and $\kappa \in [0,1]$.

$\mathbf{T}$ stands for the transformation brackets:

$$\mathbf{T} = ||\langle [N]\zeta l | [N] n l \rangle||,$$

which connect energy and coordinate representations.

Quartic potential in algebraic space

The Hamiltonian to be considered is given by:

$$\hat{H} = \frac{\mathbf{P}^2}{2\mu} - \alpha\mathbf{Q}^2 + \beta\mathbf{Q}^4$$

Quartic potential in algebraic space

The Hamiltonian to be considered is given by:

$$\hat{H} = \frac{\mathbf{P}^2}{2\mu} - \alpha\mathbf{Q}^2 + \beta\mathbf{Q}^4$$

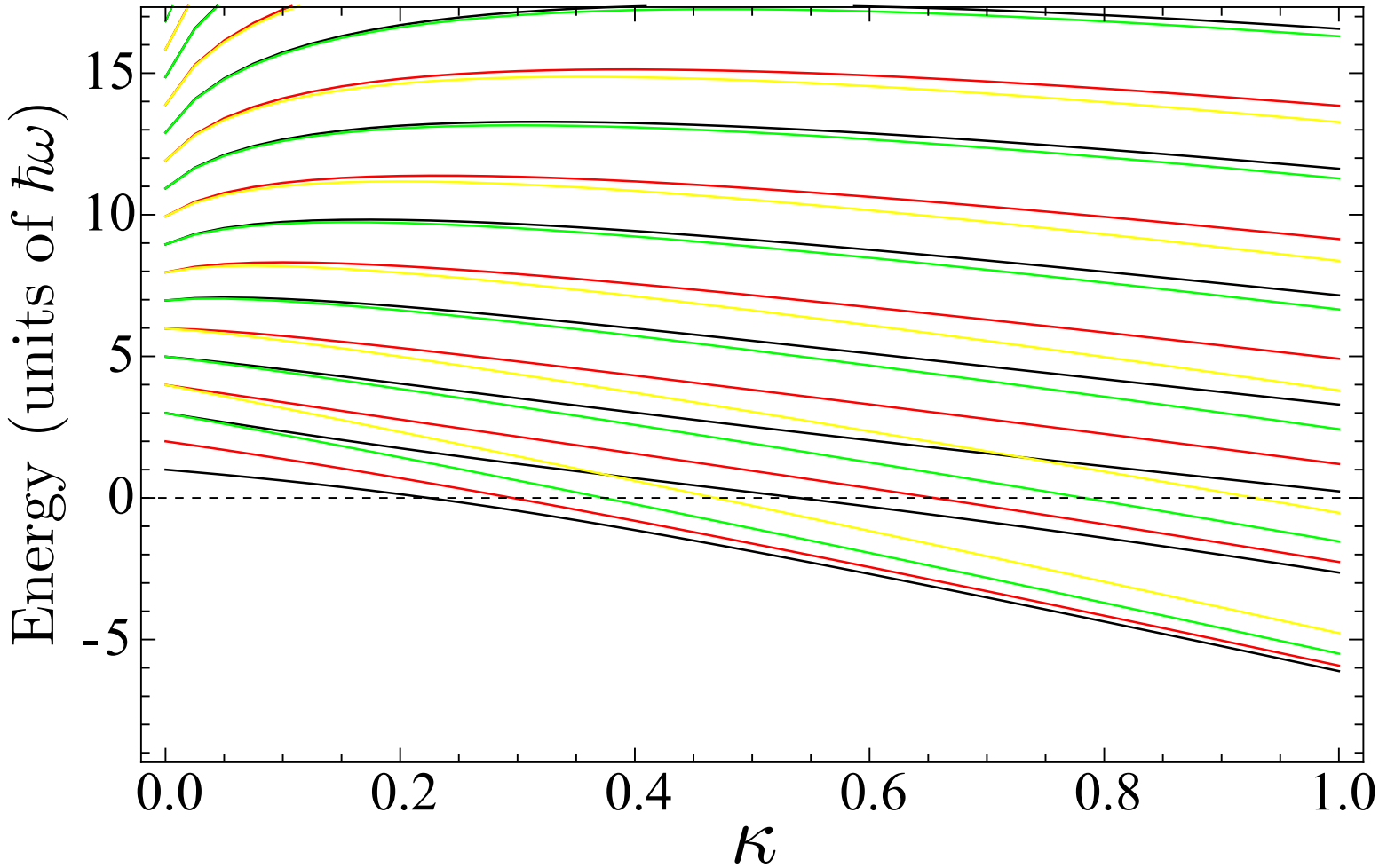
can be expressed in matrix form:

$$\boxed{\mathbf{H}^{(E)} = \mathbf{\Lambda}^{(E)} + \kappa\mathbf{T}^{\dagger}\mathbf{\Lambda}^{(Q)}\mathbf{T},}$$

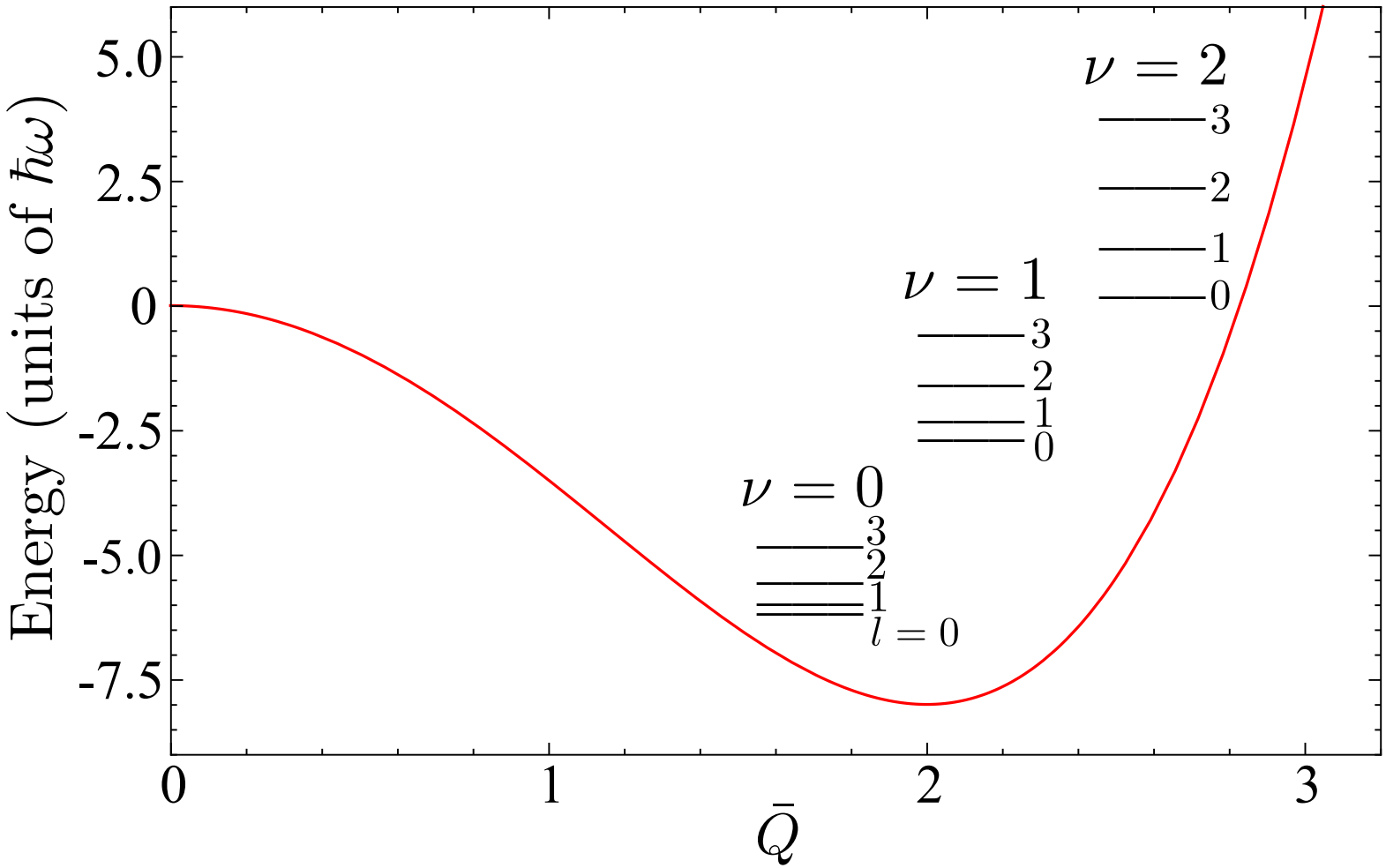
where:

$$||\mathbf{\Lambda}^{(Q)}|| = \hbar\omega\left[-\left(\frac{1}{2}+\bar{\alpha}\right)\frac{\xi(\zeta,l)^2}{2N} + \bar{\beta}\left(\frac{\xi(\zeta,l)^2}{\sqrt{2N}}\right)\right]\delta_{\zeta,\zeta'},$$

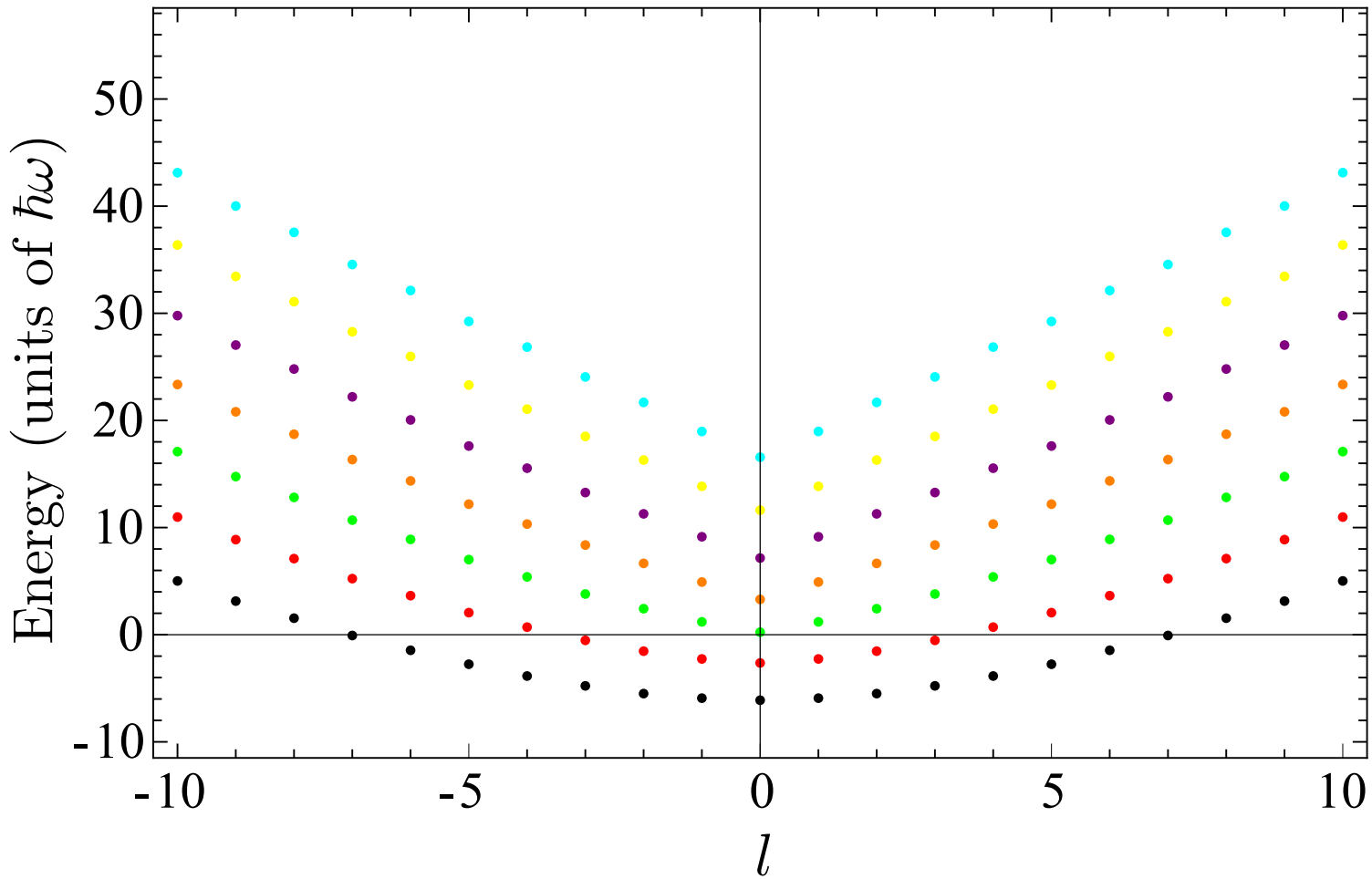
$$\bar{\alpha} = \frac{\alpha}{\mu\omega^2}; \quad \bar{\beta} = \frac{\beta\hbar}{\mu^2\omega^3}.$$



Correlation diagram from harmonic oscillator ($\kappa = 0$) to quartic potential ($\kappa = 1$). The parameters used N=1500, $\bar{\alpha}$= 4.0, $\bar{\beta}$= 0.5. The levels with angular momentum l=0,1,2,3. The lowest level in black of each group corresponds to l=0. The correlation between the linear and the displaced oscillator provides the labeling ν for the vibrational states for the bending modes through $\nu = (n - |l|)/2$.



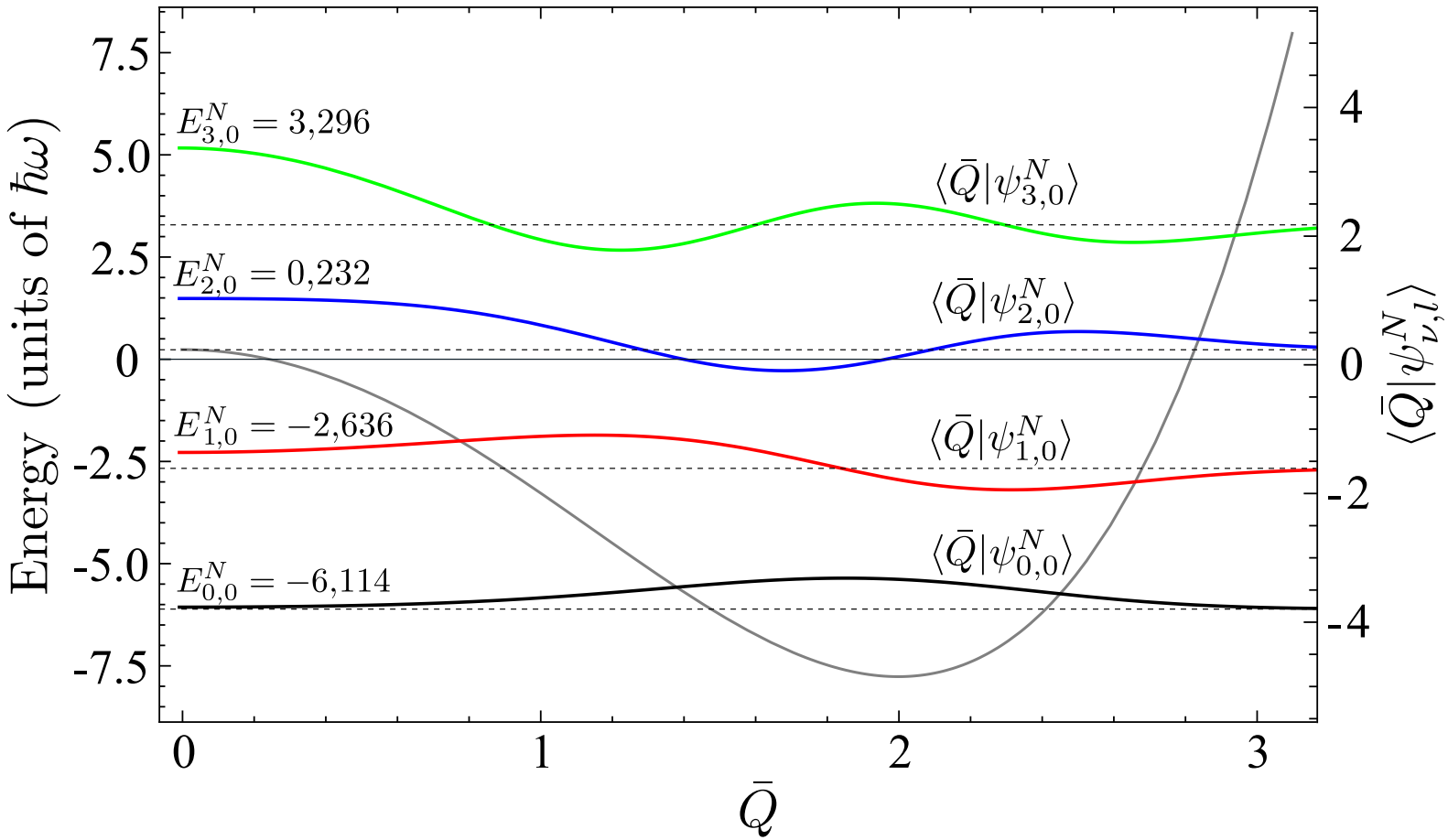
Quartic potential with parameters N=1500, $\bar{\alpha}$= 4.0, $\bar{\beta}$= 0.5, choosing $\bar{Q}_0 = 2$. The energy levels for ν=0, 1, 2 and l=0, 1, 2, 3 are displayed.



Energy levels as a function of angular momentum (l) with the parameters N=1500, $\bar{\alpha}$= 4.0, $\bar{\beta}$= 0.5 and κ=1.0.

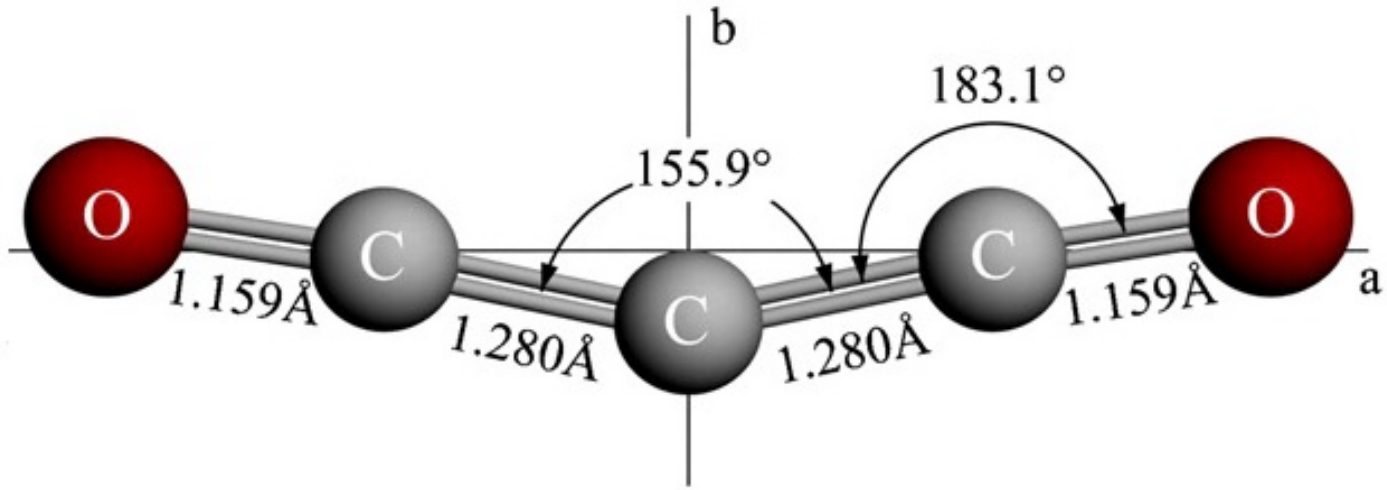
The eigenstates are given as an expansion in terms of the eigenkets $|[N]nl\rangle$ in the following form

$$|\psi^N_{\nu,l}\rangle = \sum_{n=0}^{N} \langle [N]nl|\psi^N_{\nu,l}\rangle |[N]nl\rangle$$



Energy levels and calculated radial wave functions with angular momentum l=0 and ν=0, 1, 2, 3 with the parameters N=1500, $\bar{\alpha}$= 4.0, $\bar{\beta}$= 0.5 and κ=1.0.

Application to carbon suboxide C_3O_2



The structure of C_3O_2 with *ab initio* parameters in the principal axis system [8].

[8] M. Winnewisser *et al.*, *J. Mol. Struct.* **798**, 1 (2006).

The Hamiltonian in algebraic space used for describe the CCC bending modes is given by:

$$\hat{H} = \hbar\omega\left\{\left(1 - \frac{1}{2N}\right)\hat{n} + 1 - \frac{\hat{n}^2}{N}\right\} - \left(\frac{\mu\omega^2}{2} + \alpha\right)\mathcal{Q}^2 + \beta\mathcal{Q}^4$$

The best spectroscopic description was obtained with the parameters:

$$\omega = 5{,}09607 \times 10^{12}\ \text{Hz}, \quad \alpha = 27{,}25889\ cm^{-1}/\text{Å}^2, \quad \beta = 17{,}72693\ cm^{-1}/\text{Å}^4.$$

Bending mode	Observed [9]	Residual	Residual Ref. [10]
0^0	0.00	0.00	0.0
1^1	18.33	-3.55	-2.37
2^2	46.26	-4.26	-3.74
2^0	60.70	-0.29	-0.7
3^3	80.85	-2.74	-4.85
3^1	97.30	-1.03	-2.70
4^4	120.68	-1.14	-5.82
4^2	137.41	-2.01	-4.49
4^0	144.30	-1.44	-3.3
5^5	164.88	3.51	-6.82
5^3	181.25	0.23	-6.15
5^1	191.14	-0.29	-4.96
6^6	212.87	6.34	-7.73
6^4	228.55	0.67	-7.75
6^2	239.70	-1.70	-6.9
6^0	244.70	-1.36	-5.5
values in cm^{-1}	$rms =$	2.56	5.14

[9]L. Fusina, I.M. Mills, *J. Mol. Spectrosc.*, **79** (1980) 123.
[10]J. Koput, *Chem. Phys. Lett.*. **320** (2000) 237.

The Hamiltonian in algebraic space used for describe the CCC bending modes is given by:

$$\hat{H} = \hbar\omega\left\{\left(1-\frac{1}{2N}\right)\hat{n}+1-\frac{\hat{n}^2}{N}\right\}-\left(\frac{\mu\omega^2}{2}+\alpha\right)\mathcal{Q}^2+\beta\mathcal{Q}^4$$

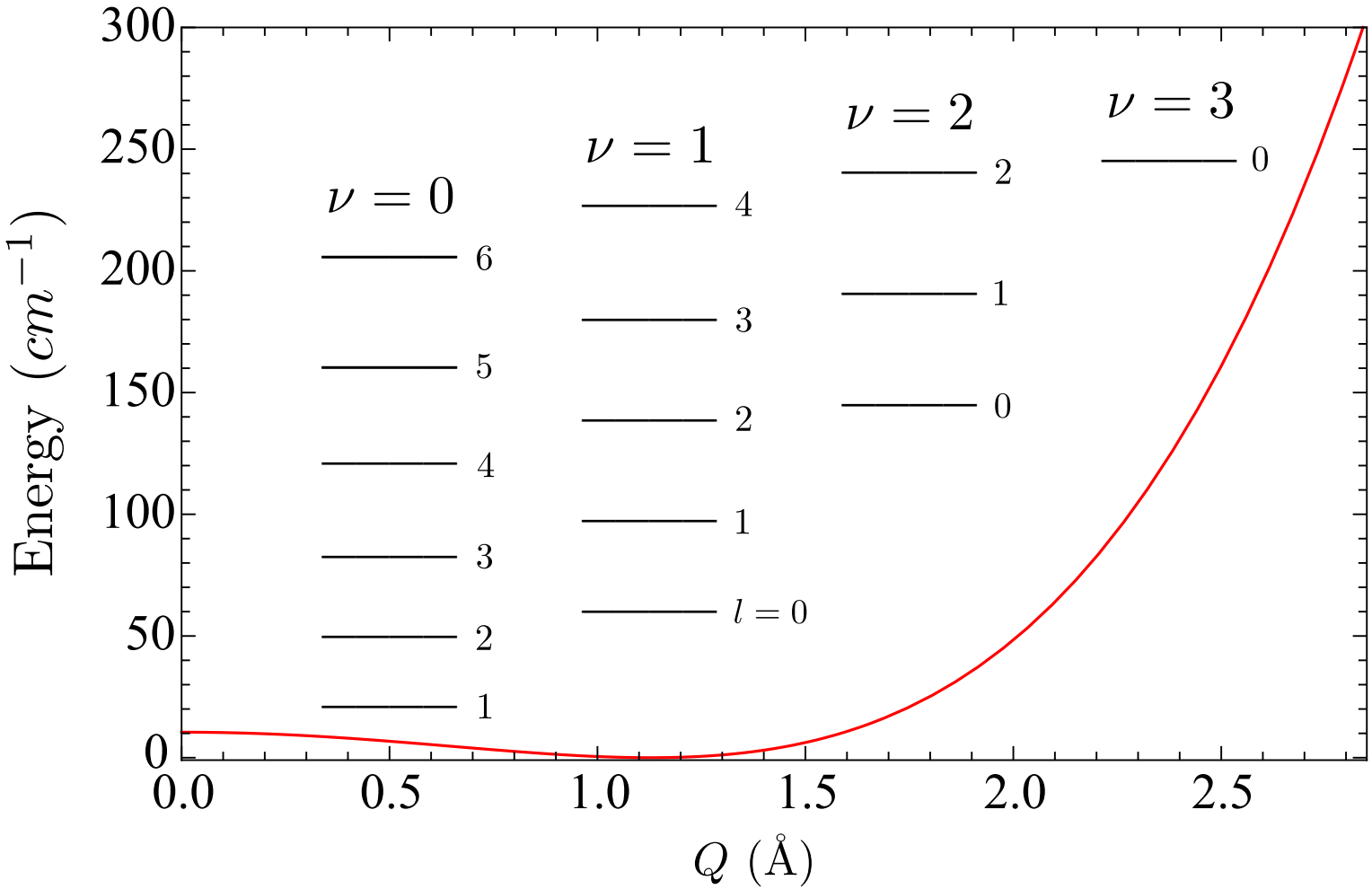
The best spectroscopic description was obtained with the parameters:

$$\omega = 5{,}09607\times10^{12}\ \text{Hz}, \quad \alpha = 27{,}25889\ cm^{-1}/\text{Å}^2, \quad \beta = 17{,}72693\ cm^{-1}/\text{Å}^4.$$

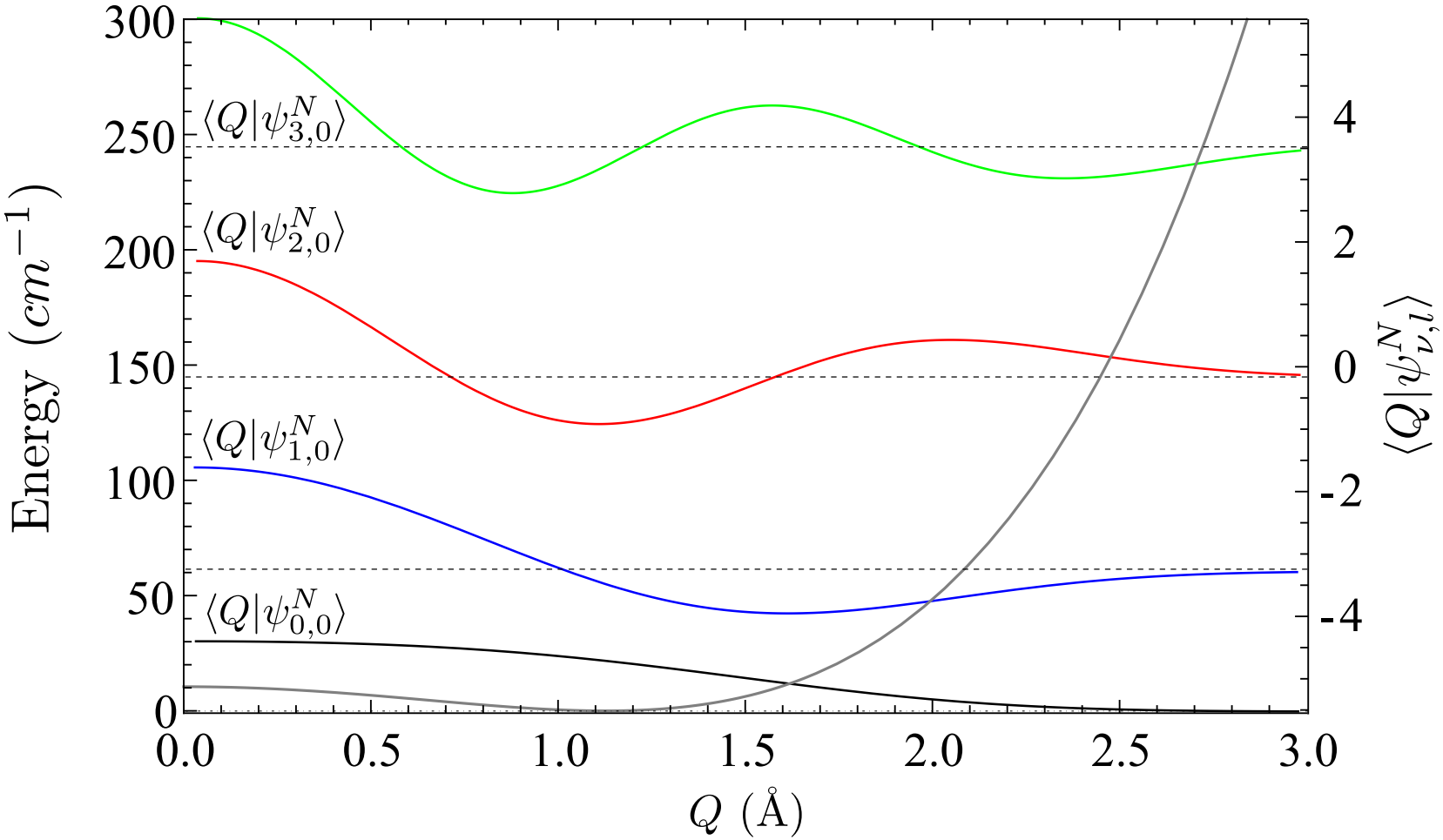
Bending mode	Observed [9]	Residual	Residual Ref. [10]
0^0	0.00	0.00	0.0
1^1	18.33	-3.55	-2.37
2^2	46.26	-4.26	-3.74
2^0	60.70	-0.29	-0.7
3^3	80.85	-2.74	-4.85
3^1	97.30	-1.03	-2.70
4^4	120.68	-1.14	-5.82
4^2	137.41	-2.01	-4.49
4^0	144.30	-1.44	-3.3
5^5	164.88	3.51	-6.82
5^3	181.25	0.23	-6.15
5^1	191.14	-0.29	-4.96
6^6	212.87	6.34	-7.73
6^4	228.55	0.67	-7.75
6^2	239.70	-1.70	-6.9
6^0	244.70	-1.36	-5.5
values in cm^{-1}	$rms =$	2.56	5.14

[9]L. Fusina, I.M. Mills, *J. Mol. Spectrosc.*, **79** (1980) 123.
[10]J. Koput, *Chem. Phys. Lett.*. **320** (2000) 237.

M.Rodríguez-Arcos and R. Lemus,
Chem. Phys. Lett., **713** (2018) 266.



Energy levels of the molecule C_3O_2 calculated with the quartic potential taking the parameters $N = 1500$, $\alpha = 27.26 \pm 0.45\ cm^{-1}/\text{Å}^2$ and $\beta = 17.73 \pm 0.74\ cm^{-1}/\text{Å}^4$, with minimum located in Q_0=1.127 Å.



Calculated radial wave functions with angular momentum l=0 and ν=0, 1, 2, 3. The parameters used for the quartic potential was N=1500, $\alpha = 27.26 \pm 0.45\ cm^{-1}/\text{Å}^2$ and $\beta = 17.73 \pm 0.74\ cm^{-1}/\text{Å}^4$.

Summary

- As a crucial ingredient of our approach an algebraic realization of the coordinates and momenta is obtained.

Summary

- As a crucial ingredient of our approach an algebraic realization of the coordinates and momenta is obtained.
- This feature provides the tools to obtain the algebraic representation of a 2D Hamiltonian in terms of similitude transformation of a diagonal matrix.

Summary

- As a crucial ingredient of our approach an algebraic realization of the coordinates and momenta is obtained.
- This feature provides the tools to obtain the algebraic representation of a 2D Hamiltonian in terms of similitude transformation of a diagonal matrix.
- The $U(3)$ algebraic approach may be applied to: linear-bend transitions of non rigid molecules, for example C_3O_2.

Thank you very much for your attention!