2D Vibron Model Program Suite

U(3) Dynamical Algebra

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Contents

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1 Abstract

This is the documentation of the `2DVM_U3` program suite that is composed of mainly `Fortran 90` but also `Perl` and `Python` scripts to perform calculations using the 2D limit of the Vibron model (2DVM).

2 Theory Outline

The original paper where the 2DVM was presented is Ref.~[1]. We also make extensive use of the detailed description of the model provided in Ref.~[2]. Other references deal mainly with the application of the 2DVM to molecular bending vibrations [3, 4, 5], quantum phase transitions [6, 7, 8, 9, 10, 11, 12, 13], or both [14, 15]. New developments also consider the coupling of several $U(3)$ dynamical algebras for the modeling of systems with several degrees of freedom [16, 17, 18, 19, 20].

We proceed to review the main theory results used in this program suite.

The 2DVM has an $U(3)$ dynamical algebra whose nine generators are built as bilinear products of one scalar $\sigma^\dagger$ and two circular $\tau^\dagger_\pm$ bosonic creation operators with the corresponding annihilation operators, $\sigma, \tau_\pm$ [2]. The nine generators are recasted to provide a deeper physical insight as [1]

$$\begin{array}{lcl} \hat{n} = \tau^\dagger_+\tau_+ + \tau^\dagger_-\tau_- & , & \hat{n}_s = \sigma^\dagger\sigma \\ \hat{\ell} = \tau^\dagger_+\tau_+ - \tau^\dagger_-\tau_- & , & \hat{Q}_\pm = \sqrt{2}\,\tau^\dagger_\pm\tau_\mp \\ \hat{D}_\pm = \sqrt{2}(\pm\tau^\dagger_\pm\sigma \mp \sigma^\dagger\tau_\mp) & , & \hat{R}_\pm = \sqrt{2}(\tau^\dagger_\pm\sigma + \sigma^\dagger\tau_\mp)\ . \end{array} \tag{1}$$

There are two possible subalgebra chains starting from the dynamical algebra $U(3)$ and ending in the symmetry algebra $SO(2)$. The symmetry algebra has the 2D angular momentum $\hat{\ell}$ as generator, which imply that this is a conserved quantity:

$$\begin{array}{ccccc} & & U(2) & & Chain(I) \\ & \nearrow & & \searrow & \\ U(3) & & & & SO(2) \\ & \searrow & & \nearrow & \\ & & SO(3) & & Chain(II) \end{array} \tag{2}$$

The corresponding subalgebras are composed by the following elements

$$\begin{array}{cc} U(2) & \{\hat{n}, \hat{\ell}, \hat{Q}_+, \hat{Q}_-\} \\ SO(3) & \{\hat{l}, \hat{D}_+, \hat{D}_-\} \\ SO(2) & \{\hat{l}\} \end{array} \tag{3}$$

where the $SO(3)$ elements satisfy the usual angular momentum commutation relations. Because of an automorphism of the Lie algebra $U(3)$ constructed with $\tau_\pm$, σ there is an alternative $SO(3)$ subalgebra of $U(3)$, called $\overline{SO(3)}$, with elements

$$\overline{SO(3)} \quad \{\hat{l}, \hat{R}_+, \hat{R}_-\}\ . \tag{4}$$

Another ingredient of the algebraic approach are the Casimir (or invariant) operators associated to each subalgebra chain [21, 22]. The first and second order Casimir operators for the subalgebras in Eqs.\ (3) and (4) are

$$\begin{array}{lcl} \hat{C}_1[U(2)] = \hat{n} & , & \hat{C}_2[U(2)] = \hat{n}(\hat{n}+1) \\ \hat{C}_2[SO(3)] = \hat{W}^2 = (\hat{D}_+\hat{D}_- + \hat{D}_-\hat{D}_+)/2 + \hat{l}^2 & & \\ \hat{C}_1[SO(2)] = \hat{l} & , & \hat{C}_2[SO(2)] = \hat{l}^2 \end{array} \tag{5}$$

and

$$\hat{C}_2[\overline{SO(3)}] = \hat{\bar{W}}^2 = (\hat{R}_+\hat{R}_- + \hat{R}_-\hat{R}_+)/2 + \hat{\ell}^2 \ . \tag{6}$$

We proceed to state the basis quantum numbers and branching rules for each dynamical symmetry.

2.1 $U(2)$ or Cylindrical Oscillator Dynamical Symmetry

In this chain states are labeled by the quantum numbers n and ℓ

$$\left| \begin{array}{ccccc} U(3) & \supset & U(2) & \supset & SO(2) \\ [N] & & n & & \ell \end{array} \right\rangle \ , \tag{7}$$

and the basis is $|[N];n,\ell\rangle$. An alternative notation, often used in molecular physics, is $|[N];n^\ell\rangle$. The quantum number N labels the totally symmetric representation of $U(3)$, $[N]$, and it is related to the total number of bound states of the system, n is the vibrational quantum number, and ℓ is the vibrational angular momentum. The branching rules are

$$\begin{aligned} &n = N, N-1, N-2, \ldots, 0 \\ &l = \pm n, \pm(n-2), \ldots, \pm 1 \text{ or } 0 \ , \ \ (n = \text{odd or even}) \ . \end{aligned} \tag{8}$$

This is the natural basis to fit experimental bending vibration data in the case of linear and quasilinear molecules.

2.2 $SO(3)$ or Displaced Oscillator Dynamical Symmetry

States in this chain are characterized by the quantum numbers

$$\left| \begin{array}{ccccc} U(3) & \supset & SO(3) & \supset & SO(2) \\ [N] & & \omega & & \ell \end{array} \right\rangle \ . \tag{9}$$

and will be labelled as $|[N];\omega,\ell\rangle$. The branching rules are

$$\begin{aligned} &\omega = N, N-2, N-4, \ldots, 1 \text{ or } 0 \ , \ \ (N = \text{odd or even}), \\ &l = \pm\omega, \pm(\omega-1), \ldots, 0 \ . \end{aligned} \tag{10}$$

In this case, it is convenient to introduce a vibrational quantum number v, which can be identified with the number of quanta of excitation in the displaced oscillator:

$$v = \frac{N-\omega}{2} \ . \tag{11}$$

The branching rules in this case are

$$\begin{aligned} v &= 0, 1, \ldots, \frac{N-1}{2} \text{ or } \frac{N}{2} \ , \ \ (N = \text{odd or even}), \\ l &= 0, \pm 1, \pm 2, \ldots, \pm(N-2v) \ . \end{aligned} \tag{12}$$

This is the natural basis to fit experimental bending vibration data in the case of quasi-rigid and rigidly-bent molecules.

2.3 2DVM Hamiltonians included in the program suite

We present the three different Hamiltonians that are considered in the present programs. The simplest Hamiltonian, used mainly in the study of QPTs and ESQPTs, is the so called model Hamiltonian, that includes the $\hat{n} = \tau_+^\dagger \tau_+ + \tau_-^\dagger \tau_-$ operator from the dynamical symmetry (I) (DS-I) and the) and the Pairing operator $\hat{P}$ which is built adding a diagonal contribution to the $SO(3)$ second order Casimir operator $\hat{W}^2 = (\hat{D}_+\hat{D}_- + \hat{D}_-\hat{D}_+)/2 + \hat{\ell}^2$. The Pairing operator is $\hat{P} = N(N+1) - \hat{W}^2$. the $SO(3)$ algebra).

The model Hamiltonian $\hat{\mathscr{H}}$ is then

$$\hat{\mathscr{H}} = \varepsilon \left[(1-\xi)\hat{n} + \frac{\xi}{N-1}\hat{P} \right] \ . \tag{13}$$

The Hamiltonian has two parameters: a global energy scale ε and a control parameter ξ such that for $\xi = 0.0$ the system is in the DS-I and for $\xi = 1.0$ the system is in the DS-I. This is specially adequate to characterize the ground state and excited state QPTs as there is a second order ground state QPT for the critical value $\xi_c = 0.2$ [2].

A second Hamiltonian is $\hat{H}_{2b}$, the most general one- and two-body Hamiltonian of the 2DVM defined in [1].

$$\hat{H}_{2b} = E_0 + \varepsilon\hat{n} + \alpha\hat{n}(\hat{n}+1) + \beta\hat{\ell}^2 + A\hat{P} \ , \tag{14}$$

where the operators $\hat{n}$ and $\hat{n}(\hat{n}+1)$ belong to the DS-I and the pairing operator $\hat{P}$ to the DS-II while the vibrational angular momentum, $\hat{\ell}$, is common to both dynamical chains. In fact in all the cases considered the angular momentum is a constant of the motion, ℓ is a good quantum number, and the Hamiltonian are block diagonal in ℓ, a fact that simplifies the numerical calculations reducing the dimension of the considered matrices. In addition to this, as in the absence of external fields, the first order angular momentum operator $\hat{\ell}$ is not included there is a degeneracy between positive and negative ℓ values for $\ell \neq 0$ and only $\ell \geq 0$ are considered. The formula for the dimension of a subspace of the totally symmetric representation N with angular momentum ℓ is $(N - | \ll |)/2 + 1$, if N and ℓ have the same parity, and $(N - |\ell| + 1)/2$ if they have different parity. Both cases are considered simultaneously in the programs as

$$dim(N,\ell) = \frac{N - |\ell| + mod(N - |\ell|, 2) + 1}{2} \ . \tag{15}$$

The third and last Hamiltonian considered is $\hat{H}_{4b}$, the most general 1-, 2-, 3-, and 4-body Hamiltonian, that can be expressed in terms of the Casimir operators $\hat{n}$, $\hat{n}^2$, $\hat{\ell}^2$, $\hat{W}^2$, and $\hat{\overline{W}}^2$ can be expressed as follows

$$\begin{aligned}
\hat{H}_{4b} =& P_{11}\hat{n} \\
&+ P_{21}\hat{n}^2 + P_{22}\hat{\ell}^2 + P_{23}\hat{W}^2 \\
&+ P_{31}\hat{n}^3 + P_{32}\hat{n}\hat{\ell}^2 + P_{33}(\hat{n}\hat{W}^2 + \hat{W}^2\hat{n}) \\
&+ P_{41}\hat{n}^4 + P_{42}\hat{n}^2\hat{\ell}^2 + P_{43}\hat{\ell}^4 + P_{44}\hat{\ell}^2\hat{W}^2 \\
&+ P_{45}(\hat{n}^2\hat{W}^2 + \hat{W}^2\hat{n}^2) + P_{46}\hat{W}^4 + P_{47}(\hat{W}^2\hat{\overline{W}}^2 + \hat{\overline{W}}^2\hat{W}^2)/2 \ .
\end{aligned} \tag{16}$$

The Hamiltonian has fourteen spectroscopic constants P_{ij}, where the subindeces indicate that this parameter corresponds to the j-th operator of the i-body operators.

From the matrix elements of the creation and annihilation sigma and tau bosons in the two dynamical symmetries published in [2], the ensuing operator matrix elements can be derived.

2.3.1 Operator Matrix Elements in the Dynamical Symmetry (I)

The diagonal operators in this dynamical symmetry are

Operator $\hat{n}^p$ $\langle [N];n^\ell|\hat{n}^p|[N];n^\ell\rangle = n^p$ for $p = 1,2,3,4$.

Operator $\hat{\ell}^{2q}$ $\langle [N];n^\ell|\hat{\ell}^{2q}|[N];n^\ell\rangle = \ell^{2q}$ for $q = 1,2$.

Operator $\hat{n}^p\hat{\ell}^{2q}$ $\langle [N];n^\ell|\hat{n}^p\ell^{2q}|[N];n^\ell\rangle = n^p\ell^{2q}$ for $p = 1,2$ and $q = 1$.

The non-diagonal matrix elements in this basis are

$SO(3)$ **Casimir Operator** $\hat{W}^2$

$$\begin{aligned}\langle [N];n_2^l|\hat{W}^2|[N];n_1^l\rangle = &\left[(N-n_1)(n_1+2)+(N-n_1+1)n_1+l^2\right]\delta_{n_2,n_1}\\ &-\sqrt{(N-n_1+2)(N-n_1+1)(n_1+l)(n_1-l)}\,\delta_{n_2,n_1-2}\\ &-\sqrt{(N-n_1)(N-n_1-1)(n_1+l+2)(n_1-l+2)}\,\delta_{n_2,n_1+2}\ .\end{aligned} \tag{17}$$

Note that this is the main nondiagonal operator in this case and it is a band matrix as the non-zero matrix elements are located in the main and first diagonals only.

Operator $\hat{n}\hat{W}^2+\hat{W}^2\hat{n}$ As the operator $\hat{n}$ is diagonal the matrix is also band diagonal with matrix elements

$$\begin{aligned}\langle [N];n_2^l|\hat{n}\hat{W}^2+\hat{W}^2\hat{n}|[N];n_1^l\rangle =&2n_1\left[(N-n_1)(n_1+2)+(N-n_1+1)n_1+l^2\right]\delta_{n_2,n_1}\\ &-(2n_1-2)\sqrt{(N-n_1+2)(N-n_1+1)(n_1+l)(n_1-l)}\,\delta_{n_2,n_1-2}\\ &-(2n_1+2)\sqrt{(N-n_1)(N-n_1-1)(n_1+l+2)(n_1-l+2)}\,\delta_{n_2,n_1+2}\ .\end{aligned} \tag{18}$$

Operator $\hat{\ell}^2\hat{W}^2$ This operator is computed for $\ell \neq 0$ multiplying the $\hat{W}^2$ operator matrix times ℓ^2.

Operator $\hat{n}^2\hat{W}^2+\hat{W}^2\hat{n}^2$ This is computed as the $\hat{n}\hat{W}^2+\hat{W}^2\hat{n}$ operator.

$$\begin{aligned}\langle [N];n_2^l|\hat{n}^2\hat{W}^2+\hat{W}^2\hat{n}^2|[N];n_1^l\rangle =&2n_1^2\left[(N-n_1)(n_1+2)+(N-n_1+1)n_1+l^2\right]\delta_{n_2,n_1}\\ &-[n_1^2+(n_1-2)^2]\sqrt{(N-n_1+2)(N-n_1+1)(n_1+l)(n_1-l)}\,\delta_{n_2,n_1-2}\\ &-[n_1^2+(n_1+2)^2]\sqrt{(N-n_1)(N-n_1-1)(n_1+l+2)(n_1-l+2)}\,\delta_{n_2,n_1+2}\ .\end{aligned} \tag{19}$$

Operator $\hat{W}^4$ This operator is computed as the matrix product of the $\hat{W}^2$ operator matrix times itself.

Operator $\hat{W}^2\hat{\overline{W}}^2+\hat{\overline{W}}^2\hat{W}^2$ In this basis the only difference between the matrix elements of the $\hat{W}^2$ and $\hat{\overline{W}}^2$ operators is the sign of the non-diagonal contribution, which is positive in this case. The full operator is computed via matrix multiplication.

2.3.2 Operator Matrix Elements in the Dynamical Symmetry (II)

The diagonal operators in this dynamical symmetry are

$SO(3)$ **Casimir Operator** $\hat{W}^2$ $\langle [N];\omega\ell|\hat{W}^2|[N];\omega\ell\rangle = \omega(\omega+1)$.

Operator $\hat{\ell}^{2q}$ $\langle [N];\omega\ell|\hat{\ell}^{2q}|[N];\omega\ell\rangle = \ell^{2q}$ for $q = 1,2$.

Operator $\hat{\ell}^2\hat{W}^2$ $\langle [N];\omega\ell|\hat{\ell}^2\hat{W}^2|[N];\omega\ell\rangle = \ell^2\omega(\omega+1$.

Operator $\hat{W}^4$ $\langle [N];\omega\ell|\hat{W}^2|[N];\omega\ell\rangle = \omega^2(\omega+1)^2$.

The non-diagonal matrix elements in this basis are

Operator $\hat{n}$

$$\langle [N];w_2^l|\hat{n}|[N];w_1^l\rangle = \left\{ \frac{(N-w_1)\left[(w_1-l+2)(w_1-l+1)+(w_1+l+2)(w_1+l+1)\right]}{2(2w_1+1)(2w_1+3)} \right. \\ \left. + \frac{(N+w_1+1)\left[(w_1+l)(w_1+l-1)+(w_1-l)(w_1-l-1)\right]}{2(2w_1+1)(2w_1-1)} \right\} \delta_{w_2,w_1} \tag{20}$$

$$+\sqrt{\frac{(N-w_1)(N+w_1+3)(w_1-l+2)(w_1-l+1)(w_1+l+2)(w_1+l+1)}{(2w_1+1)(2w_1+3)^2(2w_1+5)}}\,\delta_{w_2,w_1+2}$$

$$+\sqrt{\frac{(N-w_1+2)(N+w_1+1)(w_1-l)(w_1-l-1)(w_1+l)(w_1+l-1)}{(2w_1-3)(2w_1-1)^2(2w_1+1)}}\,\delta_{w_2,w_1-2} \tag{21}$$

Note that this is the main nondiagonal operator in this case and it is again a band matrix with non-zero matrix elements are located in the main and first diagonals only. The $\hat{n}$ matrix element in this basis are taken from [2] with a typo that has been corrected.

Operators $\hat{n}^2$**,** $\hat{n}^3$**, and** $\hat{n}^4$ These three operators are computed by matrix multiplication of the basic operator (20)

Operator $\hat{n}\hat{\ell}^2$ This operator is computed for $\ell \neq 0$ multiplying the $\hat{n}$ operator matrix times ℓ^2.

Operator $\hat{n}\hat{W}^2 + \hat{W}^2\hat{n}$ As the operator $\hat{n}$ is band diagonal $\hat{W}^2$ is diagonal this operator matrix is also band diagonal with matrix elements

$$\langle[N];w_2\ell|\hat{n}\hat{W}^2+\hat{W}^2\hat{n}|[N];w_1\ell\rangle = 2\omega_1(\omega_1+1)\left\{\frac{(N-w_1)\left[(w_1-l+2)(w_1-l+1)+(w_1+l+2)(w_1+l+1)\right]}{2(2w_1+1)(2w_1+3)}\right.$$
$$\left.+\frac{(N+w_1+1)\left[(w_1+l)(w_1+l-1)+(w_1-l)(w_1-l-1)\right]}{2(2w_1+1)(2w_1-1)}\right\}\delta_{w_2,w_1} \tag{22}$$
$$+\left[\omega_1(\omega_1+1)+(\omega_1+2)(\omega_1+3)\right]$$
$$\times\sqrt{\frac{(N-w_1)(N+w_1+3)(w_1-l+2)(w_1-l+1)(w_1+l+2)(w_1+l+1)}{(2w_1+1)(2w_1+3)^2(2w_1+5)}}\delta_{w_2,w_1+}$$
$$+\left[(\omega_1-2)(\omega_1-1)+\omega_1(\omega_1+1)\right]$$
$$\times\sqrt{\frac{(N-w_1+2)(N+w_1+1)(w_1-l)(w_1-l-1)(w_1+l)(w_1+l-1)}{(2w_1-3)(2w_1-1)^2(2w_1+1)}}\delta_{w_2,w_1-2}$$

Operator $\hat{n}^2\hat{W}^2+\hat{W}^2\hat{n}^2$ This is computed in the same way that the $\hat{n}\hat{W}^2+\hat{W}^2\hat{n}$ operator but taking into account that the $\hat{n}^2$ operator is double banded. Therefore the operator matrix elements can be expressed as follow

$$\begin{aligned}\langle[N];w_2\ell|\hat{n}^2\hat{W}^2+\hat{W}^2\hat{n}^2|[N];w_1\ell\rangle = {}& 2\omega_1(\omega_1+1)[\hat{n}^2]_{w_1,w_1}\,\delta_{w_2,w_1}\\ &+\left[\omega_1(\omega_1+1)+(\omega_1+2)(\omega_1+3)\right][\hat{n}^2]_{w_1,w_1+2}\delta_{w_2,w_1+2}\\ &+\left[(\omega_1-2)(\omega_1-1)+\omega_1(\omega_1+1)\right][\hat{n}^2]_{w_1,w_1-2}\delta_{w_2,w_1-2}\\ &+\left[\omega_1(\omega_1+1)+(\omega_1+4)(\omega_1+5)\right][\hat{n}^2]_{w_1,w_1+4}\delta_{w_2,w_1+4}\\ &+\left[(\omega_1-4)(\omega_1-3)+\omega_1(\omega_1+1)\right][\hat{n}^2]_{w_1,w_1-4}\delta_{w_2,w_1-4}\,,\end{aligned} \tag{23}$$

where $[\hat{n}^2]_{w_i,w_j}$ are the $\hat{n}^2$ operator matrix elements.

Operator $\hat{W}^2\hat{\overline{W}}^2+\hat{\overline{W}}^2\hat{W}^2$ In this basis we need first to compute the matrix elements of the $\hat{\overline{W}}^2$ making use of Eqs.\ (37) and (38) of Ref.\ [2].

$$\langle[N];w_2\ell_2|\hat{R}_-|[N];w_1\ell_1\rangle = A_{w_1,\ell_1}\delta_{w_2,w_1}\delta_{\ell_2,\ell_1-1}+B_{w_1,\ell_1}\delta_{w_2,w_1-2}\delta_{\ell_2,\ell_1-1}+C_{w_1,\ell_1}\delta_{w_2,w_1+2}\delta_{\ell_2,\ell_1-1}\,, \tag{24}$$

where

$$\begin{aligned}A_{w,\ell} =& \frac{(2N+3)(2\ell+1)}{(2w-1)(2w+3)}\sqrt{(w+\ell)(w-\ell+1)/2}\\ B_{w,\ell} =& -\sqrt{\frac{2(N+w+1)(N-w+2)(w+\ell)(w-\ell)(w+\ell-1)(w+\ell-2)}{(2w+1)(2w-1)^2(2w-3)}}\\ C_{w,\ell} =& \sqrt{\frac{2(N+w+3)(N-w)(w+\ell+1)(w-\ell+1)(w-\ell+2)(w-\ell+3)}{(2w+1)(2w+3)^2(2w+5)}}\,.\end{aligned}$$

The previous result can be used for the obtention of an expression for the $\hat{R}_+$ operator matrix elements

$$\begin{aligned}\langle[N];w_2\ell_2|\hat{R}_-|[N];w_1\ell_1\rangle^\dagger =& \langle[N];w_1\ell_1|\hat{R}_+|[N];w_2\ell_2\rangle \\ =& A_{w_2,\ell_2+1}\delta_{w_1,w_2}\delta_{\ell_1,\ell_2+1}+B_{w_2+2,\ell_2+1}\delta_{w_1,w_2-2}\delta_{\ell_1,\ell_2+1}+C_{w_2-2,\ell_2+1}\delta_{w_1,w_2+2}\delta_{\ell_1,\ell_2+1}\,.\end{aligned} \tag{25}$$

The upper diagonal matrix elements of the Casimir operator $\hat{\overline{W}}^2 = \hat{R}_+\hat{R}_- + \hat{\ell}^2$ can then be expressed as

$$\begin{aligned}\langle [N]; w_2\ell|\hat{\overline{W}}^2|[N]; w_1\ell\rangle = & A^2_{w_1,\ell_1} + B^2_{w_1,\ell_1} + C^2_{w_1,\ell_1}\,\delta_{w_2,w_1} \\ & +(A_{w_1,\ell}B_{w_1+2,\ell} + C_{w_1,\ell}A_{w_1+2,\ell})\delta_{w_2,w_1+2} \\ & +C_{w_1,\ell}B_{w_1+4,\ell})\delta_{w_2,w_1+4}\ ,\end{aligned} \tag{26}$$

and the lower diagonal matrix elements can be computed from this equation.

The $\hat{W}^2\hat{\overline{W}}^2 + \hat{\overline{W}}^2\hat{W}^2$ operator is then computed as in Eq. (23)

$$\begin{aligned}\langle [N]; w_2\ell|\hat{W}^2\hat{\overline{W}}^2 + \hat{\overline{W}}^2\hat{W}^2|[N]; w_1\ell\rangle = & \ 2\omega_1(\omega_1+1)[\hat{\overline{W}}^2]_{w_1,w_1}\,\delta_{w_2,w_1} \\ & +[\omega_1(\omega_1+1)+(\omega_1+2)(\omega_1+3)]\,[\hat{\overline{W}}^2]_{w_1,w_1+2}\delta_{w_2,w_1+2} \\ & +[(\omega_1-2)(\omega_1-1)+\omega_1(\omega_1+1)]\,[\hat{\overline{W}}^2]_{w_1,w_1-2}\delta_{w_2,w_1-2} \\ & +[\omega_1(\omega_1+1)+(\omega_1+4)(\omega_1+5)]\,[\hat{\overline{W}}^2]_{w_1,w_1+4}\delta_{w_2,w_1+4} \\ & +[(\omega_1-4)(\omega_1-3)+\omega_1(\omega_1+1)]\,[\hat{\overline{W}}^2]_{w_1,w_1-4}\delta_{w_2,w_1-4}\ ,\end{aligned} \tag{27}$$

where $[\hat{n}^2]_{w_i,w_j}$ are the $\hat{n}^2$ operator matrix elements.

3 Programs included in the package

We proceed to describe the different programs provided. Compiled `Fortran` programs have names with the suffix `_gfortran` or `_ifort` depending on the compiler used.

The subroutine used for matrix diagonalization is `LA_SYEVR` from the `Lapack95` [23], the `Fortran 95` interface to `Lapack` [24].

3.1 `Fortran` programs to compute eigenvectors, eigenvalues, and other quantities

3.1.1 Programs `avec_U3_U2_mh` and `avec_U3_SO3_mh`

The programs `avec_U3_XX_mh` compute, and eventually save, eigenvalues and eigenvectors of the model Hamiltonian (13) using the `XX = U2` -Eq. (7)- or `SO3` -Eq. (9)- basis. The input file for this program is of `namelist` type with the following syntax

```
#
#       INPUT FILE FOR 2DVM U(3) Calculations
#       Model Hamiltonian
&par_aux Iprint = 1, Eigenvec_Log = .T., Excitation_Log = .F., Save_avec_Log = .T.  /
&par_0   N_val = 20, L_val = 0 /
&par_1   epsilon = 1.0,   xi = 0.4 /
```

And the different variables are:

- `Iprint` *Integer variable*. Control program verbosity.
- `Eigenvec_Log` *Logical variable* If the variable is `.True.` eigenvalues and eigenvectors are computed.
- `Excitation_Log` *Logical variable* If the variable is `.True.` excitation energies wrt the ground state energy are reported.
- `Save_avec_Log` *Logical variable* If the variable is `.True.` eigenstates are saved in a file with the name `eigvec_XX_NYY_LZZ.dat` where `XX = u2/so3`, `YY = N_val`, and `ZZ = L_val`.
- `N_val` *Integer variable* Totally symmetric irrep of $U(3)$. Determines the Hilbert space size.
- `L_val` *Integer variable* Vibrational (2D) angular momentum ℓ value.
- `epsilon` *Real (DP) variable* Model Hamiltonian global energy scale ε in Eq.(13).
- `xi` *Real (DP) variable* Model Hamiltonian control parameter, $0 \leq \xi \leq 1$ defined in Eq. (13).

The result of running the program using the `U2` basis with the previous input file is

```
$ ../bin/avec_U3_U2_mh_gfortran < u3_modham.inp
 L_val =            0
           0   4.7178381890544925
  -6.6913473582377064E-002 |           0 >
   0.26757490446002280     |           2 >
  -0.50918508872650692     |           4 >
   0.59782591356876802     |           6 >
  -0.47489555175329112     |           8 >
   0.26470245150057914     |          10 >
  -0.10411984650838124     |          12 >
    2.8307962444698111E-002 |          14 >
   -5.0262214812812631E-003 |          16 >
    5.1057145041144211E-004 |          18 >
   -1.9360623933001603E-005 |          20 >
.
.
.
          20   20.560646361706880
    4.8846592744607648E-008 |           0 >
    7.4751184587909931E-007 |           2 >
    6.4855302773322584E-006 |           4 >
    4.1763856737063440E-005 |           6 >
    2.2180851797258004E-004 |           8 >
    1.0276743631749022E-003 |          10 >
    4.3044673503380383E-003 |          12 >
    1.6740682624946063E-002 |          14 >
    6.2024723264416194E-002 |          16 >
   0.22776900283209650      |          18 >
   0.97158341333025411      |          20 >
```

A file named `eigvec_u2_N20_L0.dat` is created. This file includes the energies, the Hamiltonian matrix diagonal[1] and the eigenstates in column-major order and it has the following structure, where `XX = u2` or `so3`, depending on the basis selected.

```
# N =           N_val ; L =            L_val  ; XX basis
# Eigenvalues
  E_1       E_2    ....... E_dim
# Hamiltonian Diagonal
  H_11      H_22    ...... H_dimdim
  Psi_1_1   Psi_2_1 ...... Psi_dim_1
  ................................
  Psi_dim_1 Psi_dim_2 .... Psi_dim_dim
```

3.1.2 Programs `avec_U3_U2` and `avec_U3_SO3`

3.1.3 Programs `ipr_U3_U2_mh` and `ipr_U3_SO3_mh`

3.1.4 Program `ipr_Husimi_U3_U2_mh`

3.1.5 Programs `ipr_U3_U2` and `ipr_U3_SO3`

3.1.6 Program `ipr_4b_U3_U2` and `ipr_4b_U3_SO3`

3.2 Programs to fit experimental vibrational bending spectra

3.2.1 Program `chi2_U3`

3.3 `Perl` scripts

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[1] In case `Excitation_Log = .True.` the ground state energy is also substracted from the Hamiltonian matrix diagonal.

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