$U_p(4) \times U_q(4)$

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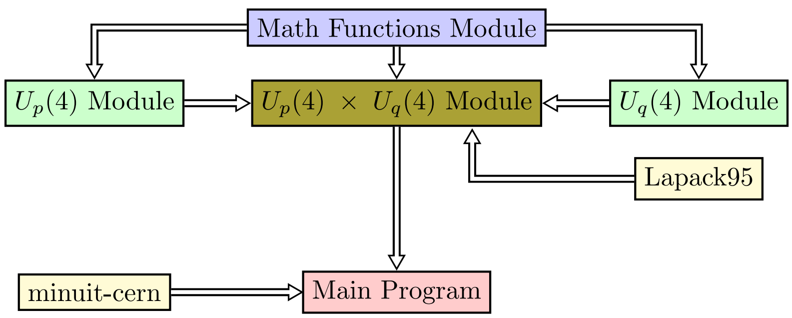
Chapter 1

Modules



1.1 Math Functions Module → `MOD_matfun.f90`

- Functions:

  - `p_symbol`(a,b) $=\ (a)_s\ =\ a(a+1)...(a+s-1)$
  - `factorial`(n) $=\ n!$
  - `delta_function`(a,b,c) $=\ \Delta$(abc)
  - `wigner_6j`$(j_1,j_2,j_3,l_1,l_2,l_3)\ =\ \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}$ [1]
  - `wigner_9j`$(j_1,j_2,j_3,l_1,l_2,l_3,k_1,k_2,k_3)\ =\ \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \\ k_1 & k_2 & k_3 \end{Bmatrix}\ =\ \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & J \end{Bmatrix}$ [2]

[1]Definition of the book *Nuclear Shell Theory* of Amos de-Shalit and Igal Talmi
[2]Integers only

1.2 $U_p(4)$ Module $\rightarrow$ `MOD_Up4.f90`

Hamiltonian:

$$\hat{H}_{U_p(4)} = \beta\,\hat{\mathcal{C}}_2\left[so_p(4)\right]+\gamma\,\hat{\mathcal{C}}_2\left[so_p(3)\right]+\gamma_2\,\left[\hat{\mathcal{C}}_2\left[so_p(3)\right]\right]^2+\kappa\,\hat{\mathcal{C}}_2\left[so_p(4)\right]\hat{\mathcal{C}}_2\left[so_p(3)\right] \tag{1.1}$$

- Global definitions:
  - Npval: $U(4)$ Totally symmetric representation.
- Functions:
  - Function: `RME_Casimir_SOp4`
  - Function: `RME_Casimir_SOp3`
  - Function: `RME_Qp2`
  - Function: `RME_np`

1.3 $U_q(4)$ Module $\rightarrow$ `MOD_Uq4.f90`

Hamiltonian:

$$\hat{H}_{U_q(4)} = a\,\hat{\mathcal{C}}_1\left[u_q(3)\right]+b\,\hat{\mathcal{C}}_2\left[u_q(3)\right]+c\,\hat{\mathcal{C}}_2\left[so_q(3)\right]+d\,\hat{\mathcal{C}}_2\left[so_q(4)\right] \tag{1.2}$$

- Global definitions:
  - Nqval: $U(4)$ Totally symmetric representation.
- Functions:
  - Function: `RME_Casimir_Uq3`
  - Function: `RME_Casimir_SOq3`
  - Function: `RME_Casimir_SOq4`
  - Function: `RME_Qq2`
  - Function: `RME_Dq_prima`

1.4 $U_p(4) \times U_q(4)$ Module $\rightarrow$ `MOD_Up_x_Uq.f90`

- Global definitions:
  - `basis_para(1:5, no of para-states)`: Integers. Para-states
  - `basis_ortho(1:5, no of ortho-states)`: Integers. Ortho-states
  - `dim_para(1:`$\Lambda_{\texttt{max}}$`)`: Integers. Para-dim blocks

- `dim_ortho(1:`$\Lambda_{\texttt{max}}$`)`: Integers. Ortho-dim blocks
- `ijk_para(1:`$\Lambda_{\texttt{max}}$`)`: Integers. Pseudo-pointer
- `ijk_ortho(1:`$\Lambda_{\texttt{max}}$`)`: Integers. Pseudo-pointer
- `lambda_max`: Integer. Maximum value of Λ
- Type `exp_point`: `exp_point%ist`, `exp_point%i_pos`,`exp_point%fst`,`exp_point%f_pos`, `exp_point%energy` and `exp_point%intensity`
- `total_exp`: Integer. Number of experimental data.
- `exp_data`: Type(`exp_point`)
- Type `matrix`: `matrix(`Λ`)%[SYM]`
- `Ham(1:`$\Lambda_{\texttt{max}}$`)`: Type(`matrix`). Hamiltonian para/ortho matrices
- `SOq4(1:`$\Lambda_{\texttt{max}}$`)`: Type(`matrix`). $\hat{\mathcal{C}}_2\left[SO_q(4)\right]$ para/ortho matrices
- `QpQq(1:`$\Lambda_{\texttt{max}}$`)`: Type(`matrix`). $\left[\hat{Q}_p^{(2)} \times \hat{Q}_q^{(2)}\right]^{(0)}$ para/ortho matrices
- `QpQqW(1:`$\Lambda_{\texttt{max}}$`)`: Type(`matrix`). $\left[\hat{Q}_p^{(2)} \times \hat{Q}_q^{(2)}\right]^{(0)} \hat{\mathcal{C}}_2\left[SO_p(4)\right] + c.c.$ para/ortho matrices
- `EnergiesPara(Prtho)(1:sum(dims))`. Where energies will be stored.
- `intop(no Exp data, 1:3)`: To save the expected values of the transitions operators in the EigenBasis.
- `Temp` : Reduced temperature

• Functions:

- Subroutine: `dimension_po`
- Subroutine: `build_basis_po`
- Subroutine: `initialize_position_index`
- Function: `RME_Qp_x_Qq_0`
- Function: `RME_Ip_x_SOq4`
- Function: `RME_QpQqSOp4`
- Subroutine: `build_Up_x_Uq_matrix`
- Function: `pretty_braket`
- Subroutine: `read_expdat`
- Function: `exp_lines`
- Subroutine: `build_ham`
- Function: `find_pos`
- Subroutine: `eigensystem`
- Function: `assig_state`
- Function: `chi2`

- Function: `FCN`
- Function: `RME_np_x_Dq_1` (Dipolar operator)
- Function: `RME_Qp2_x_Dq_1` (Dipolar operator)
- Function: `RMS_Qp2_x_nq_2` (Quadrupolar operator)
- Subroutine: `StoreEigenMatel`
- Subroutine: `EigenExpected` ($< \psi_1|\hat{T}|\psi_2 >$)
- Function: `chi2_int` (Chi2 to fit intensities)
- Function: `compute_ProbTrans`
- Function: `compute_transition`
- Subroutine: `FCN_int`
- Subroutine: `Save_energies`

1.4.1 Building the basis

We have a block-diagonalizable system dividing the problem in para ($\mathrm{mod}(J,2) = 0$) and ortho ($\mathrm{mod}(J,2) = 1$) cases, and separating by different Λ. The states will be stored in the same array sorted by Λ. The dimension of each block will be saved in `dim_[SYM]`$(\Lambda = 0)$, ... , `dim_[SYM]`$(\Lambda = \Lambda_{\max})$.

$$\begin{array}{c} \left.\begin{bmatrix} \left|\psi_1^{\Lambda=0}\right\rangle \\ \vdots \\ \left|\psi_{\texttt{dim\_[SYM]}(\Lambda=0)}^{\Lambda=0}\right\rangle \end{bmatrix}\right\} \to 1\text{:}\texttt{dim\_[SYM]}(\Lambda = 0) \\ \vdots \\ \left.\begin{bmatrix} \left|\psi_1^{\Lambda=\Lambda_{\max}}\right\rangle \\ \vdots \\ \left|\psi_{\texttt{dim\_[SYM]}(\Lambda=\Lambda_{\max})}^{\Lambda=\Lambda_{\max}}\right\rangle \end{bmatrix}\right\} \to 1\text{:}\texttt{dim\_[SYM]}(\Lambda = \Lambda_{\max}) \end{array} \tag{1.3}$$

Therefore, the basis array is as follow:

$$\texttt{basis\_[SYM]} = \left[\left|\psi_1^{\Lambda=0}\right\rangle, ..., \psi_{\texttt{dim\_[SYM]}(\Lambda=0)}^{\Lambda=0}, ..., \left|\psi_1^{\Lambda=\Lambda_{\max}}\right\rangle, ..., \psi_{\texttt{dim\_[SYM]}(\Lambda=\Lambda_{\max})}^{\Lambda=\Lambda_{\max}}\right] \tag{1.4}$$

Each element of the the basis must cotain information about quantum numbers:

$$\left|\psi_i^{\Lambda}\right\rangle = (w\ J;\ n\ L;\ \Lambda \in [|J - L|, J + L]) \tag{1.5}$$

Dimension: `dimension_po`

Fortran90 subroutine.
Inputs:

- Npval. Integer
- Nqval. Integer
- $\Lambda_{\max}$. Integer

Outputs:

- dim_para. Integer, dimension(0:$\Lambda_{\max}$)
- dim_ortho. Integer, dimension(0:$\Lambda_{\max}$)

Basis: `build_basis_po`

Inputs:

- Npval. Integer
- Nqval. Integer
- $\Lambda_{\max}$. Integer
- total_para. Integer, total dimension of para basis
- total_ortho. Integer, total dimension of ortho basis
- dim_para. Integer, dimension(0:$\Lambda_{\max}$)
- dim_ortho. Integer, dimension(0:$\Lambda_{\max}$)

Outputs:

- basis_para. Integer, dimension$\left(1:5,\ 1:\sum_{\Lambda=0}^{\Lambda_{\max}} \texttt{dim_para}(\Lambda)\right)$
- basis_ortho. Integer, dimension$\left(1:5,\ 1:\sum_{\Lambda=0}^{\Lambda_{\max}} \texttt{dim_ortho}(\Lambda)\right)$
  - basis_[SYM](1,:) $\longrightarrow$ w
  - basis_[SYM](2,:) $\longrightarrow$ J
  - basis_[SYM](3,:) $\longrightarrow$ n
  - basis_[SYM](4,:) $\longrightarrow$ L
  - basis_[SYM](5,:) $\longrightarrow$ Λ

Para-states

$$
\begin{array}{l}
\text{LOOP: } J = 0, 2, ..., N_p - \mathrm{mod}(N_p, 2) \\
\quad \text{LOOP: } L = 0, 1, ..., N_q \\
\quad\quad \text{CONDITIONAL: } |J - L| \leq \Lambda_{max} \text{ to continue, else go to next } L \\
\quad\quad\quad \text{LOOP: } \Lambda = |J - L|, |J - L| + 1, ..., \min(\Lambda_{max}, J + L) \\
\quad\quad\quad\quad \text{LOOP: } w = N_p - \mathrm{mod}(N_p, 2), N_p - \mathrm{mod}(N_p, 2) - 2, ..., J \\
\quad\quad\quad\quad\quad \text{LOOP: } n = L, L + 2, ..., Nq \\
\quad\quad\quad\quad\quad\quad \texttt{basis\_para}\,(1, \texttt{dim\_para}\,(\Lambda)) = w \\
\quad\quad\quad\quad\quad\quad \texttt{basis\_para}\,(2, \texttt{dim\_para}\,(\Lambda)) = J \\
\quad\quad\quad\quad\quad\quad \texttt{basis\_para}\,(3, \texttt{dim\_para}\,(\Lambda)) = n \\
\quad\quad\quad\quad\quad\quad \texttt{basis\_para}\,(4, \texttt{dim\_para}\,(\Lambda)) = L \\
\quad\quad\quad\quad\quad\quad \texttt{basis\_para}\,(5, \texttt{dim\_para}\,(\Lambda)) = \Lambda
\end{array}
\tag{1.6}
$$

Ortho-states

$$
\begin{array}{l}
\text{LOOP: } J = 1, 3, ..., N_p - (1 - \mathrm{mod}(N_p, 2)) \\
\quad \text{LOOP: } L = 0, 1, ..., N_q \\
\quad\quad \text{CONDITIONAL: } |J - L| \leq \Lambda_{max} \text{ to continue, else go to next } L \\
\quad\quad\quad \text{LOOP: } \Lambda = |J - L|, |J - L| + 1, ..., \min(\Lambda_{max}, J + L) \\
\quad\quad\quad\quad \text{LOOP: } w = N_p - (1 - \mathrm{mod}(N_p, 2)), N_p - (1 - \mathrm{mod}(N_p, 2)) - 2, ..., J \\
\quad\quad\quad\quad\quad \text{LOOP: } n = L, L + 2, ..., Nq \\
\quad\quad\quad\quad\quad\quad \texttt{basis\_ortho}\,(1, \texttt{dim\_ortho}\,(\Lambda)) = w \\
\quad\quad\quad\quad\quad\quad \texttt{basis\_ortho}\,(2, \texttt{dim\_ortho}\,(\Lambda)) = J \\
\quad\quad\quad\quad\quad\quad \texttt{basis\_ortho}\,(3, \texttt{dim\_ortho}\,(\Lambda)) = n \\
\quad\quad\quad\quad\quad\quad \texttt{basis\_ortho}\,(4, \texttt{dim\_ortho}\,(\Lambda)) = L \\
\quad\quad\quad\quad\quad\quad \texttt{basis\_ortho}\,(5, \texttt{dim\_ortho}\,(\Lambda)) = \Lambda
\end{array}
\tag{1.7}
$$

Pseudo-pointer: `initialize_position_index`

```
subroutine initialize_position_index(ijk,partial_dim,lambda_max)
!
! Inputs:
! o) partial_dim: Integer array dimension 0:lambda_max
! o) lambda_max
!
! Output:
! o) ijk: Integer array dimension 0:lambda_max
!
! This functions initializes the initial integer "pointer" ijk(0:lambda_max),
! so that
! ijk(0) = 1
! ijk(1) = position where lambda=1 block starts
! ...
! ijk(lambda_max) = position where lambda=lambda_max block stats
!
! This function is going to be of vital importance during the program's develop-
ment
!
```

Building all matrices: `build_Up_x_Uq_matrix`

This subroutine builds the matrices for the operators of $U_p(4) \times U_q(4)$ using para/ortho basis without mixing different Λ.

```
subroutine build_Up_x_Uq_matrix(basis,matrix,RME_fun,iprint)
!
! This function build the para / ortho matrices using the given basis.
! This procedure can be used to build Up4 x Uq4 operators' matrices.
!
! INPUTs:
! o) basis: para/ortho basis
! o) matrix: square matriz len(basis) x len(basis)
! o) RME_fun: function with w1,j1,n1,l1,lam1,w2,j2,n2,l2,lam2 dependences.
! o) iprint: printing control
!
! OUTPUT:
! o) matrix
!
! All position corresponding to lam1 /= lam2 will be ZERO!
!
```

The function `RME_fun` must deppend on $(\omega_1, J_1, n_1, L_1, \Lambda_1, \omega_2, J_2, n_2, L_2, \Lambda_2)$.

Braket notation output: `pretty_braket`

Useless gadget ... but very nice.

```
function pretty_braket(w,j,n,l,lam,bk,Np,Nq)
!
! INPUTs:
! o) Np(opt), Nq(opt), w, j, n, l, lam: Quantum numbers
! o) bk: one character = b (bra) or k (ket)
!
! OUTPUT:
! o) pretty_braket: character type
!
```

Chapter 2

Programs

2.1 BuckProgram_fit

See *BuckProgram_fit.f90* file and *BPfit.inp* input in scr/ folder.

2.2 IntProgram_fit

2.2.1 Input File

2.2.2 Definitions

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