# $U_p(4) \times U_q(4)$. Intensity lines.

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$$\left|\varphi^{\omega_1,J_1}_{n_1,L_1};\ \Lambda_1\right\rangle\ \left\langle\varphi^{\omega_2,J_2}_{n_2,L_2};\ \Lambda_2\right|\ \left\{\begin{matrix}\hat\omega_1,\hat J_1\\ \hat n_1,\hat L_1\end{matrix}\right\}_{\Lambda_1}\left|\hat\omega_1\hat J_1,\hat n_1\hat L_1;\Lambda_1\right\rangle\left\langle\hat\omega_2\hat J_2,\hat n_2\hat L_2;\Lambda_2\right|\ [\ \underline{\underline{C}}\ ] \tag{1}$$

## 0.1 Eigensystem

Hamiltonian:

$$\hat H\ =\ \hat H_{\rm mol}\ +\ \hat H_{\rm cage}\ +\ \hat H_{\rm int} \tag{2}$$

Eigenvalues problem:

$$\begin{aligned}\hat H\left|\varphi\right\rangle &= E\left|\varphi\right\rangle\\ \hat H\left|\varphi^{\omega,J}_{n,L};\ \Lambda\right\rangle &= \mathrm{E}^{\omega,J}_{n,L}\left|\varphi^{\omega,J}_{n,L};\ \Lambda\right\rangle\\ \left|\varphi^{\omega,J}_{n,L};\ \Lambda\right\rangle &= \sum_{\left\{\begin{smallmatrix}\hat\omega,\ \hat J\\ \hat n,\ \hat L\end{smallmatrix}\right\}_\Lambda}\mathcal{C}^{\Lambda}_{\hat\omega,\hat J;\hat n,\hat L}\left|\hat\omega\hat J,\hat n\hat L;\Lambda\right\rangle\end{aligned} \tag{3}$$

The quantum numbers of the eigenstates are assigned according to the maximum coefficient over the basis. The summation is over all the states that belong to the para/ortho $\Lambda$-block.

## 0.2 $\hat d^{(1)}$ dipolar operator

Let $\hat d^{(1)}$ be a dipolar operator which doesn't mix para and ortho states.

$$\left\langle\varphi^{\omega_1,J_1}_{n_1,L_1};\ \Lambda_1\right|\left|\hat d^{(1)}\right|\left|\varphi^{\omega_2,J_2}_{n_2,L_2};\ \Lambda_2\right\rangle = \tag{4}$$

$$= \left[\sum_{\left\{\begin{smallmatrix}\hat\omega_1,\ \hat J_1\\ \hat n_1,\ \hat L_1\end{smallmatrix}\right\}_{\Lambda_1}}\mathcal{C}^{\Lambda_1}_{\hat\omega_1,\hat J_1;\hat n_1,\hat L_1}\left\langle\hat\omega_1\hat J_1,\hat n_1\hat L_1;\Lambda_1\right|\right]\left|\hat d^{(1)}\right|\left[\sum_{\left\{\begin{smallmatrix}\hat\omega_2,\ \hat J_2\\ \hat n_2,\ \hat L_2\end{smallmatrix}\right\}_{\Lambda_2}}\mathcal{C}^{\Lambda_2}_{\hat\omega_2,\hat J_2;\hat n_2,\hat L_2}\left|\hat\omega_2\hat J_2,\hat n_2\hat L_2;\Lambda_2\right\rangle\right]$$

$$= \sum_{\left\{\begin{smallmatrix}\hat\omega_1,\ \hat J_1\\ \hat n_1,\ \hat L_1\end{smallmatrix}\right\}_{\Lambda_1}}\ \sum_{\left\{\begin{smallmatrix}\hat\omega_2,\ \hat J_2\\ \hat n_2,\ \hat L_2\end{smallmatrix}\right\}_{\Lambda_2}}\mathcal{C}^{\Lambda_1}_{\hat\omega_1,\hat J_1;\hat n_1,\hat L_1}\,\mathcal{C}^{\Lambda_2}_{\hat\omega_2,\hat J_2;\hat n_2,\hat L_2}\left\langle\hat\omega_1\hat J_1,\hat n_1\hat L_1;\Lambda_1\right|\left|\hat d^{(1)}\right|\left|\hat\omega_2\hat J_2,\hat n_2\hat L_2;\Lambda_2\right\rangle$$

$$= \left[\underline{\underline{\mathcal{C}^{\Lambda_1}_{\varphi_1}}}\right]^T\left[\underline{\underline{d^{(1)}_{\Lambda_1,\Lambda_2}}}\right]\left[\underline{\underline{\mathcal{C}^{\Lambda_2}_{\varphi_2}}}\right] \tag{5}$$

where $\left[\underline{\underline{\mathcal{C}^{\Lambda}_{\varphi}}}\right]$ is a ($\dim\_\Lambda\times 1$) matrix. The dimension of $\left[\underline{\underline{\mathcal{C}^{\Lambda_1}_{\varphi_1}}}\right]^T$ is ($1\times\dim\_\Lambda_1$), of $\left[\underline{\underline{d^{(1)}_{\Lambda_1,\Lambda_2}}}\right]$ is ($\dim\_\Lambda_1\times\dim\_\Lambda_2$), and $\left[\underline{\underline{\mathcal{C}^{\Lambda_2}_{\varphi_2}}}\right]$, ($\dim\_\Lambda_2\times 1$).

Now we need to build all the $\left[ \underline{\underline{d^{(1)}_{\Lambda_1,\Lambda_2}}} \right]$ for para and ortho cases when it's needed.

Steps:

1. Read experimental data and allocate the needed matrices.
2. Solve the eigensystem and compute the eigenstates
3. ...