On the numerical solution of ESE in the eigen-energy representation

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We have a list of J-levels $\{L_i \equiv \alpha_i J_i\}_{i=1}^{N_L}$ with N_L the number of levels. Then we have a list of lines $\{\ell_j \equiv (\alpha_k J_k, \alpha_l J_l)\}_{j=1}^{N_\ell}$ with the multiindex $j \equiv (k,l)$ and N_ℓ the number of lines. It is desirable that $E(\alpha_k J_k) < E(\alpha_l J_l)$ in terms of the level energies.

Every J-level consists of $2J+1$ Zeeman sublevels αJM and the corresponding density matrix of the J level has therefore $(2J+1)^2$ elements of the form $\rho_{MM'}(\alpha J)$. Firstly make an ordered list of the levels $\alpha_i J_j$. For each of them, make an ordered list of the MM' combinations. For practical implementation in Python, I would make a list like

$$[[L_1, M, M'], [L_1, M'', M'''], \cdots, [L_2, M, M'], [L_2, M'', M'''], \cdots]].$$

Then numerical representation of the atomic density matrix is then vector of density matrices ρ_p defined by the above list. For lines, similarly, we have a list $[[L_i, L_k], [L_l, L_m], \cdots]$.

An equation for the cohence is of the form

$$\frac{d\rho_{MM'}(\alpha J)}{dt} = \frac{d\rho_p}{dt} = -2\pi i \nu_L g_{\alpha J}(M - M')\rho_p + \sum_q \Pi_{pq}\rho_q \tag{1}$$

where the summation goes over all the q coherences of all the levels and the Π_{pq} elements are complex-valued.

A relatively simple algorithmn how to generate the ESE matrix elements could be as follows: Run a loop over these elements (rows of the ESE matrix) and for every $\rho_{MM'}(\alpha J)$ do the following

1. Initialize the ESE row corresponding to $\rho_{p=MM'}(\alpha J)$ to zero.
2. Run over the list of lines, $\{\ell_j \equiv (\alpha_k J_k, \alpha_l J_l)\}_{j=1}^{N_\ell}$. If αJ is not involved in ℓ_j, ignore the line, othewise continue with the following steps.
3. Make a loop over the columns. Every column corresponds to some ρ_q position where $q = NN'$ of some $\alpha' J'$ level. If ρ_q is not involved in ℓ_j, ignore it. Otherwise:
   (a) If ρ_q is above ρ_p then calculate $T_E(p \to q)$ and add it to the p position.
   (b) If ρ_q is below ρ_p then calculate $T_A(p \to q)$ and add it to the p position. The $\bar{J}$ tensor is known for the current line ℓ_i.
   (c) If ρ_q belongs to the same level αJ as ρ_p, then we may need to include relaxation rates. This is in the case that either $M = N$ or $M' = N'$. If any of these casses happens than run another loop over the lines and add the relaxation terms for to the ESE_{pq} position.
4. Add the term Hanle $-2\pi i \nu_L g_{\alpha J}(M - M')$ at the p column.

After the ESE matrix is filled, replace any row in ESE with a row that is zero except for the q positions corresponding to populations ($N = N'$) where we put 1. The right-hand-site of this row will also be 1. This will guarantee us that the sum of level populations is normalized to 1. Solve ESE (ideally using singular value decomposition but other LA methods would often work as well).