Manual for MQDT solver

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1 Theory background

The energy eigen wave function for a atomic excited complex should be a superposition of the eigenchannel wavefunctions,

$$\Psi^{J^{\pi}} = \sum_{\alpha}^{N_p} A_{\alpha} \psi_{\alpha}^{J\pi}(E), \tag{1}$$

where N_p is the number of physical channels.

The asymptotic boundary condition (for bound and continuum) leads to a set of secular equations,

$$\begin{cases}
\sum_{\alpha} U_{i\alpha} \sin \pi (\nu_i + \mu_\alpha) A_\alpha^\rho = 0 & \text{for } i \in \text{closed channels,} \\
\sum_{\alpha} U_{i\alpha} \sin \pi (-\tau^\rho + \mu_\alpha) A_\alpha^\rho = 0 & \text{for } i \in \text{open channels.}
\end{cases} \tag{2}$$

The existence of non-trivial solution A^{ρ}_{α} in eqns. (2) requires the determinant of coefficients matrix to vanish, which gives rise to the multichannel quantum defect theory (MQDT) eqns. (3a):

$$F(x_i, U_{i\alpha}, \mu_{\alpha}) = \det[U_{i\alpha} \sin \pi (x_i + \mu_{\alpha})] = 0,$$
 (3a)

where,

$$x_i = \begin{cases} v_i & \text{for } i \in \text{closed channels,} \\ -\tau & \text{for } i \in \text{open channels,} \end{cases}$$

and the effective principle quantum number are defined by,

$$E = I_i - q^2 / v_i^2. \tag{3b}$$

We can employ the graphic solution method to solve the MQDT equation in autoionization region naturally. However, it's beneficial to also treat the bound energy region in the similar fashion(i.e., Lu-Fano plot) by the fact that the phase shift can be smoothly connected with the quantum defect number by the analytical continuation property of S matrix.

There are situations where we need to treat several channels, that corresponds to more than one thresholds, as openned ones (denote as $\{I_o\}$). However, due to the limitation of 2D illustration of the Lu-Fano type plot, only one energy relation condition line can be presented to find the physical discrete levels. In such situations, we need to project these channels onto one of these thresholds (e.g. an arbitrary one $I_y \in \{I_o\}$), via the following additional constrains,

$$-\tau_i = \begin{cases} -\tau_i & i = y, \\ -\tau_y + \Delta_{i,y} & i \neq y, \end{cases}$$
 (4a)

where,

$$\Delta_{i,y} = \nu_i - \nu_y = \left[\frac{1}{\nu_x^2} - \frac{I_i - I_x}{q^2} \right]^{-1/2} - \left[\frac{1}{\nu_x^2} - \frac{I_y - I_x}{q^2} \right]^{-1/2}.$$
 (4b)

As we can see constrains (4) varies smoothly and fulfills the Rydberg energy relation at the physical discrete levels.

The mixing coefficients can be easily shown to be proportional to the cofactor $C_{i\alpha}$ of $F(x_i, U_{i\alpha}, \mu_{\alpha})$ by the analogy of the secular eqns (2) and the definition of determinant.

$$A_{\alpha} = C_{i\alpha} / (\sum_{\alpha} C_{i\alpha}^2)^{1/2}, \quad \forall i \le N_p$$
 (5)

2 Program structure

```
# global constants and parameters
 constants
                # user defined complex data structure for easier data communication
2 type_def
            # frequently used numerical algorithms
3 numerical
              # dynamical array for easier data storage
4 darray
file_cmdl_io # file i/o and commandline parser
              # frequently used string operations and block output.
6 stdio
                # seting up machine-dependent systematic parameters (EPS, PI, Nan ...)
7 envset
  gengrid
                # generating X and Y grids.
9 SOLVMQDT
              # solving the MQDT equations
```

3 Numerical algorithms

- (i) X-grid
 - uniform
 - divide X-axis into several segments based on the eigenchannel quantum defect $\mu_{\alpha} \pm \delta_{\alpha}/2$.
 - δ_{α} is the resonance width estimated by the imaginary part of projected K_{cc} matrix. (J. M. Lecomte, J. Phys. B: At. Mol. Phys. 20 (1987) 3645-3662.)
 - (Optional) manually set x-segments and increase grid density.
 - (Not useful) alternatively, divide X-axis into several segments based on effective eigenchannel quantum defect $\tilde{\mu}_{\alpha} \pm \delta_{\alpha}/2$. Where the effective eigenchannel quantum defect $\tilde{\mu}_{\alpha}$ is obtained by diagonalizing the real part of projected K_{cc} matrix.(J. M. Lecomte, J. Phys. B: At. Mol. Phys. 20 (1987) 3645-3662.). But it seems working poorly in the test.

(ii) Y-grid

- For the first x step $v_x^{(0)}$, initiate the Y-grid segments with $\mu_{\alpha}(\alpha \in \text{open channels})$. Use rather dense y grid to search.
- Second x step $v_x^{(1)}$: update Y-grid segments with the results first step. Only a few grid per segment is needed from now on.
- n > 2 x step: update Y-grid segments with the extrapolation of the result of n 1'th and n 2'th x step.
- Be careful with sudden jump due to modulo 1.
- (Optional)manually set y-segments and increase grid density.

(iii) equation solver

- Newton-Ralphson.
- Bisect search.
- Hybrid of Newton and bisect updating formula.
- A relaxation coefficient can be used to slow down the oscillation.
- For autoionization(continuum) region, Greene's generalized eigenvalue technique is now implemented too improve efficiency. Caveate could be that now I am using Lapack routine, so only double precision is possible, which only allows for not so high dimension problems (where the efficiency of the original root finding version is tolerable).

4 Program input

Required input files:

```
miuang.out  # S matrix prepared by smooth-toolkits
mqdt.in  # MQDT solver control file
dalfa.in  # dipole matrix elements (optional)
```

The major control file *mqdt.in*. The input file is case-insensitive. You can add blank lines and # to comment. You can also use {} to wrap the data block, you can put them in one line or break the wrapper into multiple lines.

Below is a sample input file.

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