Three-particle corrections to the Effective Hamiltonian for Thallium

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This is a summary of the calculations in October 2011 of the 3e-corrections in Thallium

PACS numbers:

A. Background

We calculate Tl in V^{N-3} approximation within CI+MBPT approach using second order MBPT. The complete set of second order diagrams include one-, two-, and three-electron contributions. Three-electron contribution to the energies in thallium was first estimated in Ref. [1] and found to be very small (V^{N-1} approximation was used). Since then three-electron contribution was usually neglected (see, for example, Refs. [2–5]). Very recently Berengut calculated five-electron ion Cr II and showed that there three-electron contribution is as important as two others [6].

Here we want to calculate three-electron corrections not only to the energies, but to other observables as well. That requires more accurate calculation of the many-electron wave functions. Technically three-electron Hamiltonian is very difficult to use because it has much more non-zero matrix elements and its matrix is not sparse. Consequently, Davidson-like methods of diagonalization become inefficient. Because of that we made a compromise and calculated three-electron diagrams only for the relatively small block of the Hamiltonian of a size $N_1 \times N_2$, where $N_1 N_2 \sim 10^6$. Effective Hamiltonian in our approach is symmetrical, so there is no need to calculate and store transposed block $N_2 \times N_1$. We increased the size of the block and saw that three-electron corrections are sufficiently close to saturation (say, within 10%). After three-electron corrections are included in the Hamiltonian matrix, we use exactly the same machinery, as we do for the two-electron case. Effective operators for all observables were calculated within RPA approximation. No structural radiation, two-particle, and normalization corrections were included.

B. Technical issues

Calculations are done in four steps:

1. Two-particle part is calculated as usual. The files `SGC.CON` and `SCRC.CON` store second order one- and two-electron MBPT amplitudes. The code `conf` is used to calculate the matrix of the effective Hamiltonian (`CONF.HIJ`) and it's eigenvectors (`CONF.XIJ`).

2. Three-electron contribution is calculated by the code `conf_3d`. It uses <u>all</u> CONF.* files from the previous step and forms the file `CONF_3D.HIJ` with three-electron block of the Hamiltonian.

   - The size of the block is given from console as the numbers of configurations `Nc1` and `Nc2` (`Nc1` $\leq$ `Nc2`).

   - Parameter `Nc1` can be increased in the consecutive calculations appending existing file `CONF_3D.HIJ`. This way one can study saturation without recalculating previous step.

   - After forming the block the code calculates corrections to the energies by diagonalization of the three-electron part *in the subspace of the eigenvectors* stored in the file CONF.XIJ. This method is good enough for the energies, but generally is not applicable to other observables, as it <u>does not reproduce</u> all configurational mixings.

   The size of the three-particle block is limited by the parameter `IP1` in the following way. The numbers of determinants `Nd1` and `Nd2` which correspond to `Nc1` and `Nc2` should be `Nd1` $\cdot$ `[Nd2` $-$ `(Nd1` $-$ `1)/2]` $\leq$ `IP1`^{2}.

3. The files `CONF.HIJ` and `CONF_3D.HIJ` are merged together in the file `3e.HIJ` by the code `form_3e`. The file `3e.HIJ` has the same structure and format, as `CONF.HIJ`.

4. The file `3e.HIJ` is renamed to `CONF.HIJ`. After that the code `conf` is executed with the key `Kl=1`. In this case the code diagonalizes matrix from `CONF.HIJ` and finds new eigenvectors. These eigenvectors can be used to calculate different amplitudes in a standard way.

C. Results

Table I gives corrections to the valence energies and to the transition frequencies from the ground state. Table II gives corrections to the magnetic hyperfine constants A. E1 amplitudes are listed in Table III.

We use `ine` code to calculate polarizabilities, EDM enhancement factor, and PNC transition amplitude. Results are in Table IV.

TABLE I: Valence energies (a.u.) and transition frequencies (cm^{-1}) in two-electron and three-electron variants of CI+MBPT. Relative differences are given in percent.

J^p	CI+MBPT(2e)		CI+MBPT(3e)		
$\frac{1}{2}^-$	2.103344	0.0	2.103093	−0.012%	0.0	0.00%
$\frac{3}{2}^-$	2.067301	7910.4	2.067030	−0.013%	7914.9	0.06%
$\frac{1}{2}^-$	1.949108	33850.8	1.949093	−0.001%	33799.1	−0.15%
$\frac{3}{2}^-$	1.944492	34863.9	1.944466	−0.001%	34814.6	−0.14%
$\frac{1}{2}^+$	1.984266	26134.6	1.984255	−0.001%	26082.1	−0.20%
$\frac{3}{2}^+$	1.940815	35670.9	1.940758	−0.003%	35628.4	−0.12%
$\frac{5}{2}^+$	1.940420	35757.6	1.940357	−0.003%	35716.5	−0.11%
$\frac{1}{2}^+$	1.928521	38369.0	1.928519	0.000%	38314.7	−0.14%

TABLE II: Magnetic hyperfine constants A (MHz).

State	(2e)	(3e)	Diff.
$6p_{1/2}$	22423.7	22440.7	0.08%
$6p_{3/2}$	91.6	71.7	−21.72%
$7p_{1/2}$	2268.5	2273.8	0.23%
$7p_{3/2}$	304.4	302.2	−0.72%
$7s_{1/2}$	12793.7	12791.1	−0.02%
$6d_{3/2}$	−47.9	−44.8	−6.44%
$6d_{5/2}$	168.9	163.7	−3.04%
$8s_{1/2}$	4039.1	4040.8	0.04%

D. Conclusions

As expected, the three-electron corrections to the valence energies and to other observables are small. On the other hand, they are not negligible and should be in-cluded in the calculations claiming sub-percent accuracy. Relative corrections to some hfs constants are rather large, because these constants are anomalously small and

TABLE III: Reduced matrix elements for E1 amplitudes (a.u.).

Transition	(2e)	(3e)	Diff.
$6p_{1/2} - 7s_{1/2}$	1.792	1.794	0.10%
$6p_{1/2} - 6d_{3/2}$	2.419	2.421	0.09%
$6p_{1/2} - 8s_{1/2}$	0.533	0.533	−0.03%
$6p_{3/2} - 7s_{1/2}$	3.414	3.420	0.17%
$6p_{3/2} - 6d_{3/2}$	1.464	1.465	0.09%
$6p_{3/2} - 6d_{5/2}$	4.295	4.299	0.11%
$6p_{3/2} - 8s_{1/2}$	0.783	0.782	−0.04%

TABLE IV: Polarizabilities of the states $6p_{1/2}$ and $6p_{3/2}$ (in a.u.), EDM enhancement factor $K_{\mathrm{at}}(6p_{1/2})$, and PNC transition amplitude (in $10^{-9}Q_w/(-N)$ a.u.).

	(2e)	(3e)	Diff.
$\alpha_0(6p_{1/2})$	46.135	46.323	0.41%
$\alpha_0(6p_{3/2})$	78.665	79.067	0.51%
$\alpha_2(6p_{3/2})$	−26.502	−26.662	0.60%
$K_{\mathrm{at}}(6p_{1/2})$	−585.10	−587.01	0.33%
$E1_{\mathrm{PNC}}(6p_{1/2}, 6p_{3/2})$	0.7268	0.7289	0.29%

the role of <u>all</u> corrections is enhanced. Three-electron corrections for these constants are still smaller than other second order corrections. **Three-particle corrections calculated here can be added to the more accurate calculations.**

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