Rigorous \textit{ab initio} study of Allowed and Forbidden transition amplitudes of Tl\textsuperscript{2+}

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Abstract. We report here ‘allowed’ and ‘forbidden’ electromagnetic transition amplitudes among various low lying states of doubly ionized Thallium (Tl\textsuperscript{2+}) using relativistic coupled cluster method based on Dirac-Fock hybrid basis functions. These transitions are of importance in astrophysics and plasma research. The effect of core correlation, pair correlation and core polarization on these transitions are estimated.

1. Introduction
Atomic experiments and the inputs they provide toward understanding of fundamental physics are amongst the fore-front research area that has come in limelight in recent years due to advancements in technology. Transitions among mixed parity states in different atoms/ions have been used to estimate weak interaction parameter as accurately as possible to quantify physics beyond the ‘Standard Model’ of particle physics. One of the important goals of these studies is to select an atomic or ionic candidate for large parity non-conservation (PNC) effect. Precise understanding of atomic structure is one of the basic requirement of this processes. In the present work, we assess the potential of doubly ionized thallium for such experiments.

Elements heavier than iron show over-abundance in the peculiar star, HgMn \chi Lupi \cite{2}. The observed abundance of ionized Thallium in the evolved stars are important inputs for the characterization of different astronomical bodies \cite{1}. We estimate in the present work the competence of doubly ionized thallium for the precise estimation of these abundances. The reliability of these estimates depends on the accuracy of transition probabilities that are determined using an approximate quantum mechanical model. This is especially important for forbidden transition where experimental measurements are difficult. Some of these forbidden transitions between states of same principle quantum numbers correspond to longer wavelengths compared to normal allowed transitions. This long wavelength transitions can provide information about the thermal Doppler effect in many physical systems \cite{3}. There are also other important astronomical features for transition in infrared and radio regions \cite{4}. The lack of accurate knowledge of energy levels of Tl\textsuperscript{+2} seems to be an important reason why many wavelengths that are observed in an astronomical spectrum are hitherto un-identified.

Our goal in the present work to calculate all the bound energy levels of the Tl\textsuperscript{2+} system. The calculated energy wavefunctions are then used to estimate the electromagnetic transition amplitudes among the atomic/ionic energy levels. We have employed n the present work the
highly correlated relativistic coupled cluster method (RCC), with single and double excitations [5].

2. Theory

The reference state used to obtain the correlated state for Tl$^{2+}$ is the Dirac-Fock closed-shell state for Tl$^{3+}$, which is an eigen state of the Dirac Fock Hamiltonian:

$$H_{DF}|\Phi_{DF}\rangle = E_0|\Phi_{DF}\rangle,$$

with the Dirac Fock Hamiltonian $H_{DF}$ given by

$$H_{DF} = \sum_i c\tilde{\alpha}_i\tilde{\beta}_i + (\beta_i - 1)c^2 + V_N(r_i) + U_{DF}(r_i),$$

where $\tilde{\alpha}_i$ and $\beta_i$ are Dirac matrices, and $V_N(r_i)$ and $U_{DF}(r_i)$ are respectively the nuclear potential and Dirac-Fock potential for the $i$'th electron. The correlated wave function for Tl$^{3+}$ can be obtained from the Dirac-Fock(DF) wavefunction $|\Phi_{DF}\rangle$ as

$$|\Psi\rangle = \Omega|\Phi_{DF}\rangle,$$

where the wave operator, $\Omega$ is expressed in powers of interaction potential [6] $V_{es} = \sum_{i<j} \frac{1}{r_{ij}} - \sum_i U_{DF}(r_i)$ which corresponds to the ‘correlation’ left out of the Dirac-Fock formalism. Very often this residual correlation is addressed using the Brillouin-Wigner perturbation technique [6].

The coupled cluster theory is based on following ansatz for the wave operator [6]

$$\Omega = e^T,$$

Where the cluster operator $T$ is expressed in terms of certain connected diagrams of the wave operator [6]. It is well known that the operator $T$ can be expressed in terms of cluster operator $\{T_n\}$, where $n$ stands for simultaneous excitations of the core and valence electrons from the DF state, $|\Phi_{DF}\rangle$.

Any state of Tl$^{2+}$ with one valence electron in the $v$'th orbital is described using open shell coupled cluster approach as

$$|\Psi_v\rangle = e^T\{e^{S_v}\}|\Phi_v\rangle = e^T\{1 + S_v\}a_v^\dagger|\Phi_{DF}\rangle.$$

The operators $T$ and $S_v$ are the single and double excitation cluster operators associated with closed- and open shell hole-particle excitations, respectively [6, 7]. In our calculation, only four power of single ($T_1$) and two power of double ($T_2$) normal ordered core excitation operators are considered to contribute in the Dirac-Coulomb matrix. Likewise, at the most one power of normal ordered single valence $S_{1v}$ and core-valence $S_{2v}$ excitation operators are considered to contribute to the RCC equations, as seen from eq. (2.5). Partial triple excitations [8, 9] are obtained in combination with the above mentioned $T$ and $S_v$ operators. For computational simplicity, the $T$ amplitudes are solved first for the closed-shell system, Tl$^{3+}$. The wavefunction for Tl$^{2+}$ is then enhanced to include an additional electron in the $v$'th orbital to obtain the open-shell wavefunctions [10]. The normal ordering Hamiltonian, $H_N$, can be written as $H_N = f_N + V_N$, i.e., sum over one-body
and two-body terms. The dressed operator of the normal order Hamiltonian is $H_N = e^{-T}H_N e^T$. $\Delta E_{corr}$ is the correlation energy of the initial reference state $Tl^{3+}$ is given by:

$$\langle \Phi_{DF}|H_N|\Phi_{DF} \rangle = \Delta E_{corr}.$$  \hspace{1cm} (6)

Besides, we have:

$$\langle \Phi_{DF}^*|H_N|\Phi_{DF} \rangle = 0,$$ \hspace{1cm} (7)

where $|\Phi_{DF}\rangle$ and $|\Phi_{DF}^*\rangle$ are two different Dirac-Fock states of $Tl^{3+}$ corresponding to configurations in the orthogonal space of the state function of $Tl^{3+}$.

For the open-shell RCC calculation, the $S_v$ operators are solved by the following equations

$$\langle \Phi_v|H_N\{1 + S_v\}|\Phi_v \rangle = -\Delta E_v,$$ \hspace{1cm} (8)

$$\langle \Phi_v^*|H_N\{1 + S_v\}|\Phi_v \rangle = -\Delta E_v\langle \Phi_v^*|\{S_v\}|\Phi_v \rangle,$$ \hspace{1cm} (9)

where $\Delta E_v$ is the ionization potential (IP) of the corresponding valence electron $v$. Here, $|\Phi_v^*\rangle$ are the states excited from $|\Phi_v\rangle$.

The matrix element of an arbitrary operator can be expressed as

$$O_{fi} = \frac{\langle \Psi_f|O|\Psi_i \rangle}{\sqrt{\langle \Psi_f|\Psi_f \rangle \langle \Psi_i|\Psi_i \rangle}}$$

$$= \frac{\langle \Phi_i|\{1 + S_f\} e^{T} O e^{T}\{1 + S_i\}|\Phi_i \rangle}{\sqrt{\langle \Phi_i|\{1 + S_f\} e^{T} e^{T}\{1 + S_f\}|\Phi_f \rangle \langle \Phi_i|\{1 + S_i\} e^{T} e^{T}\{1 + S_i\}|\Phi_i \rangle}}$$ \hspace{1cm} (10)

The normalization factors are obtained using the following relation:

$$Norm = \langle \Psi_f|O|\Psi_i \rangle \left( \frac{1}{\sqrt{(1 + N_f)(1 + N_i)}} - 1 \right)$$ \hspace{1cm} (11)

with $N_v = \{S_v^\dagger e^T e^T S_v\}$ for an electron $v$, where $v = i$ for the initial state and $f$ for the final state.

The one-electron reduced matrix elements of the E1, M1 and E2 operators are given by [11, 12].

$$\langle k_f||q_{m}^{(E1)}||k_i \rangle = \langle k_f||C_m^{(1)}||k_i \rangle$$

$$\times \int dr \left[ r(P_f(r)P_i(r) + Q_f(r)Q_i(r)) + \frac{\alpha}{10}(k_f - k_i)(\epsilon_i - \epsilon_f)r^2[P_f(r)Q_i(r) + Q_f(r)P_i(r)] + \frac{\alpha}{5}(\epsilon_i - \epsilon_f)r^2[P_f(r)Q_i(r) - Q_f(r)P_i(r)] \right]$$ \hspace{1cm} (12)

$$\langle k_f||q_{m}^{(M1)}||k_i \rangle = \langle k_f||C_m^{(1)}||k_i \rangle \frac{6\kappa_i + \kappa_f}{\alpha k} \left[ \int dr j_1(kr)(P_f(r)Q_i(r) + Q_f(r)P_i(r)) \right]$$ \hspace{1cm} (13)

and

$$\langle k_f||q_{m}^{(E2)}||k_i \rangle = \langle k_f||C_m^{(2)}||k_i \rangle \frac{15}{k^2}$$

$$\times \left[ \int dr j_2(kr)(P_f(r)P_i(r) + Q_f(r)Q_i(r)) + j_3(kr)\frac{k_f - k_i}{3}(P_f(r)Q_i(r) + Q_f(r)P_i(r)) + (P_f(r)Q_i(r) - Q_f(r)P_i(r)) \right]$$ \hspace{1cm} (14)
respectively. Here, $j_i$ and $\kappa_i \left( = \pm (j_i + \frac{1}{2}) \right)$ for $j_i = l_i \pm \frac{1}{2}$ are the total angular momentum and relativistic angular momentum quantum numbers, respectively, of the $i$th electron orbital. The quantity $C_{l_m}^{(l)}$ is the Racah tensor and $j_l(kr)$ is the spherical Bessel function of order $l$. $P_l(r)$ and $Q_l(r)$ are the large and small radial components of the Dirac wavefunctions.

3. Result & discussion

The DF orbitals of $Tl^{3+}$ are generated from the universal Gaussian type orbital (GTO) basis functions [13] using $\alpha_0 = 0.00825$ and $\beta = 2.91$ and considering Fermi nuclear distribution. The choice of the parameters are based on the agreement of DF energies and wavefunctions for the bound GTO orbitals with the numerical DF orbitals obtained using the GRASP program [14]. Once the exponent parameters are fixed, the number of single particle orbital base function that are chosen with different symmetries depend on the convergence criteria of the DF energies of the system and individual bound orbitals. There are 32s, 32p, 30d, 25f, 20g symmetry bases used for the GTO calculations. The number of DF orbitals for different symmetries used in the RCC calculations are based on the convergence criteria for core correlation energy. We consider all core orbitals to be active except the 1s orbitals. Since the wave operator (eq. 2.4) has an exponential form with reference to the cluster operator $T$ and $S$, most of the many-body correlation is comprehensively addressed through the single and double excitations. In fact, from the combination single and double excitation operators, some triples excitations are also considered.

The ‘allowed’ electric dipole transition amplitudes among various low-lying states with different correlation contributions are presented in table I. The table shows that the Dirac-Fock (DF) transition amplitude for $6s_{1/2} \rightarrow 7p_{1/2}$ transition is unusually low compared to that for $6s_{1/2} \rightarrow 7p_{3/2}$. However, all order strong core-polarizations contributions (i.e. $\bar{O}S_{2v}$ +c.c.) to these transition amplitudes enhance the transition amplitude of the former significantly, and hence reverse the order of the total amplitudes compared to DF results. We have confirmed these result by checking them using GRASP [14], the Multiconfiguration Dirac-fock (MCDF) method. Similar correlation effects are seen in the transitions in $6s \rightarrow 8p$ region presented in table I. This may be due to the fact that core polarization contributions are more strong compared to the DF contributions in transitions involving $6s$ state due to its large overlap with core orbitals. Similar core-polarization contribution features are seen in other systems like Ca$^+$, Sr$^+$ and Ba$^+$ [15]. One needs to carry out further studies to understand such anomalous behaviour by using different many-body approaches.

Comparison of generalized oscillator strength (gf) between the RRC and the MCDF [1] for low lying states is presented in table II. The MCDF is a variational approach involving coupled differential equations. The dominant contributions to the precision in this formalism comes from the increment of number of configurations considered in the calculations. The RCC is a diagrammatic approach where unlike the MCDF method the effect of positive energy orbitals are taken into account. Table II shows that the results from both approaches are in good agreement.

The ‘forbidden’ magnetic dipole and electric quadrupole transition amplitudes among few low lying states along with their different correlation contributions are presented in tables III and IV respectively. Table III shows that for the few cases where the DF contributions to M1 amplitudes are relatively weak, dominant contributions come from the pair correlation. Exceptions are from $P_{3/2}$ to $P_{3/2}$ transitions, where major contributors are the core correlations. Table IV shows that the core correlation contributions is larger than the DF part for E2 transitions between fine structure states of $6p$, $7p$, but not in the case of $8p$. From table I, we see that
| Transition | λ(A)   | Dirac Fock | Core correlation | Pair correlation | Core polarization | Norm   | Transition Amplitude |
|------------|--------|------------|------------------|------------------|------------------|--------|---------------------|
| 6s\(1/2\) → 6p\(1/2\) | 1566.79 | 2.0245     | -0.0055          | -0.0509          | -0.4551          | -0.0318 | 1.5128              |
| 6s\(1/2\) → 6p\(3/2\) | 1270.67 | -2.8304    | 0.0066           | 0.0732           | 0.5900           | 0.0449  | -2.1608             |
| 7p\(1/2\) → 7p\(1/2\) | 638.39  | -0.0038    | 0.0010           | -0.0212          | -0.1794          | 0.0027  | -0.1854             |
| 7p\(3/2\) → 7p\(3/2\) | 621.21  | -0.2454    | 0.0015           | 0.0417           | 0.2738           | -0.0006 | 0.0405              |
| 8p\(1/2\) → 8p\(1/2\) | 525.95  | -0.0250    | 0.0003           | 0.0044           | -0.1266          | 0.0018  | -0.1381             |
| 8p\(3/2\) → 8p\(3/2\) | 520.66  | -0.0987    | 0.0012           | 0.0086           | 0.2006           | -0.0010 | 0.0930              |
| 7s\(1/2\) → 6p\(1/2\) | 1341.33 | -1.2603    | 0.0005           | 0.0842           | -0.0215          | 0.0168  | -1.1777             |
| 7s\(1/2\) → 6p\(3/2\) | 1675.63 | 2.3457     | -0.0015          | -0.1254          | -0.0236          | -0.0303 | 2.1653              |
| 7p\(1/2\) → 7p\(1/2\) | 5474.78 | 4.2560     | -0.0106          | -0.0483          | -0.1709          | -0.0330 | 4.0181              |
| 7p\(3/2\) → 7p\(3/2\) | 4425.44 | -5.8005    | 0.0063           | 0.0534           | 0.2063           | 0.0544  | -5.5114             |
| 8p\(1/2\) → 8p\(1/2\) | 1932.30 | 0.0320     | -0.0059          | -0.0213          | -0.0855          | 0.00037 | -0.0577             |
| 8p\(3/2\) → 8p\(3/2\) | 1862.71 | -0.4834    | 0.0028           | 0.0440           | 0.1137           | 0.0031  | -0.3533             |
| 8s\(1/2\) → 6p\(1/2\) | 845.76  | -0.3824    | 0.0045           | 0.0245           | -0.0089          | 0.0047  | -0.3637             |
| 8s\(1/2\) → 6p\(3/2\) | 967.46  | 0.6040     | -0.0008          | -0.0195          | -0.0168          | -0.0072 | 0.5716              |
| 7p\(1/2\) → 7p\(1/2\) | 3934.17 | -2.7423    | -0.0002          | 0.1356           | -0.0331          | 0.0181  | -2.6173             |
| 7p\(3/2\) → 7p\(3/2\) | 4742.21 | 4.8556     | -0.0037          | -0.1967          | 0.0185           | -0.0398 | 4.6349              |
| 8p\(1/2\) → 8p\(1/2\) | 12395.05| 7.1344     | -0.0223          | -0.0124          | -0.0761          | -0.0368 | 7.0168              |
| 8p\(3/2\) → 8p\(3/2\) | 9998.64 | -9.6134    | 0.0007           | 0.0894           | -0.0894          | 0.0733  | -9.4725             |
Table 2. Comparison of generalized oscillator strength (gf) of Tl\(^{2+}\) for electric dipole transition

| Transitions   | gf (RCC) | gf (MCDF)[1] |
|---------------|----------|--------------|
| 6s\(_{1/2}\) → 6p\(_{1/2}\) | 0.4437   | 0.402        |
| 6s\(_{1/2}\) → 6p\(_{3/2}\) | 1.1161   | 1.015        |
Table 3. Transition amplitude of Tl$^{2+}$ for magnetic dipole transition

| Transitions | $\lambda$(Å) | Dirac correlation | Core-correlation | Pair-polarization | Core-correlation | Norm | Transition Amplitude |
|-------------|---------------|-------------------|-------------------|------------------|------------------|------|----------------------|
| $6s_{1/2}$  | 722.66        | -0.0001           | -0.0036           | 0.0726           | 0.0004           | -0.0011 | 0.0844              |
| $\rightarrow 7s_{1/2}$ | 549.26        | -0.0001           | -0.0023           | 0.0313           | 0.0002           | -0.0004 | 0.0350              |
| $7s_{1/2}$  | 2289.17       | -0.0001           | -0.0011           | 0.0843           | 0.0001           | -0.0005 | 0.0920              |
| $6p_{1/2}$  | 6723.29       | -1.1399           | 0.0018            | 0.0011           | -0.0001          | 0.0246  | -1.1383             |
| $\rightarrow 7p_{3/2}$ | 1029.34       | -0.0967           | 0.0008            | 0.0109           | -0.0001          | 0.0017  | -0.0973             |
| $\rightarrow 8p_{1/2}$ | 791.73        | -0.0001           | 0.0001            | 0.0149           | 0.0000           | -0.0003 | 0.0188              |
| $\rightarrow 8p_{3/2}$ | 779.80        | -0.0496           | 0.0002            | 0.0067           | 0.0000           | 0.0008  | -0.0509             |
| $6p_{3/2}$  | 1282.96       | -0.1150           | -0.0004           | -0.0098          | -0.0001          | 0.0017  | -0.1300             |
| $\rightarrow 7p_{1/2}$ | 1215.42       | -0.0002           | -0.0011           | 0.2151           | 0.0001           | -0.0046 | 0.2682              |
| $\rightarrow 7p_{3/2}$ | 897.42        | -0.0537           | 0.0005            | -0.0032          | -0.0001          | 0.00071 | -0.0510             |
| $\rightarrow 8p_{1/2}$ | 882.11        | -0.0001           | -0.0005           | 0.0964           | 0.0001           | -0.0021 | 0.1294              |
| $7p_{1/2}$  | 23089.08      | -1.1389           | 0.0024            | 0.0001           | -0.0000          | 0.0129  | -1.1375             |
| $\rightarrow 8p_{1/2}$ | 2986.32       | -0.0000           | -0.0006           | 0.0360           | -0.0000          | -0.0003 | 0.0405              |
| $\rightarrow 8p_{3/2}$ | 2823.29       | -0.0948           | 0.0014            | 0.0087           | 0.0000           | 0.0009  | -0.0937             |
| $7p_{3/2}$  | 3429.95       | -0.1141           | -0.0008           | -0.0065          | -0.0001          | 0.0011  | -0.1120             |
| $\rightarrow 8p_{3/2}$ | 3216.61       | -0.0001           | -0.0009           | 0.2293           | 0.0000           | -0.0033 | 0.2734              |
| $8p_{1/2}$  | 51716.46      | -1.1388           | 0.0041            | -0.0005          | 0.0000           | 0.0101  | -1.1367             |
| $\rightarrow 8p_{3/2}$ | 41712.46      | -1.1388           | 0.0041            | -0.0005          | 0.0000           | 0.0101  | -1.1367             |
Table 4. Transition amplitude of Ti$^{2+}$ for electric quadrupole transition

| Transitions | $\lambda$(Å) | Dirac core-Fock correlation | Core-correlation | Pair-correlation | Core-polarization | Norm | Transition Amplitude |
|-------------|--------------|-----------------------------|-----------------|-----------------|------------------|------|----------------------|
| $6p_{1/2}$  |              |                             |                 |                 |                  |      |                      |
| $\rightarrow 6p_{3/2}$ | 6723.29      | -8.4550                     | 43.7982         | 0.6335          | 0.2106           | 0.7695 | 35.5451             |
| $\rightarrow 7p_{3/2}$ | 1029.34      | 4.0864                      | 0.4803          | 3.1709          | 0.1580           | -0.1495 | 8.5520              |
| $\rightarrow 8p_{3/2}$ | 779.80       | 1.5425                      | 0.5322          | -0.4480         | 0.1438           | -0.0282 | 1.6973              |
| $7p_{1/2}$  |              |                             |                 |                 |                  |      |                      |
| $\rightarrow 6p_{3/2}$ | 1282.96      | 7.1895                      | 0.7556          | 3.0908          | 0.0051           | -0.1775 | 11.4093             |
| $\rightarrow 7p_{3/2}$ | 23089.08     | -37.1077                    | 140.2954        | 1.6740          | 0.0722           | -1.1880 | 14.0121             |
| $\rightarrow 8p_{3/2}$ | 2823.29      | 16.0059                     | 4.6142          | -1.4155         | 0.0806           | -0.1993 | 18.8730             |
| $8p_{1/2}$  |              |                             |                 |                 |                  |      |                      |
| $\rightarrow 6p_{3/2}$ | 897.42       | 1.9944                      | 0.2455          | 4.3223          | -0.0237          | -0.0872 | 6.2913              |
| $\rightarrow 7p_{3/2}$ | 3429.95      | 26.3867                     | 1.8948          | 4.7290          | 0.0275           | -0.3196 | 32.8751             |
| $\rightarrow 8p_{3/2}$ | 51716.46     | -104.6131                   | -1.2113         | 2.4885          | 0.0638           | 0.9126  | -102.9726           |
| $6p_{3/2}$  |              |                             |                 |                 |                  |      |                      |
| $\rightarrow 7p_{3/2}$ | 1215.42      | 6.0147                      | 0.06495         | 0.6142          | 0.0287           | -0.0843 | 4.8881              |
| $\rightarrow 8p_{3/2}$ | 779.80       | 1.9712                      | 0.5723          | -0.4726         | 0.0592           | -0.0338 | 2.0678              |
| $7p_{3/2}$  |              |                             |                 |                 |                  |      |                      |
| $\rightarrow 8p_{3/2}$ | 3216.61      | 22.1031                     | 5.2137          | -3.4181         | 0.0689           | -0.2872 | 23.4896             |
the core-polarization terms contribute significantly to the E1 transitions, whereas they are less
significant for the M1 and E2 transition amplitudes. The DF transition amplitudes of E2 tran-
sitions reported in table IV show the amplitudes between the same principle quantum number
are negative, whereas others are positive. This difference has to come from the radial integral
since the remaining terms involve identical angular factors. That is because of the nature of
radial parts.

4. conclusion
We have reported important E1, E2 and M1 transition amplitudes among few low-lying states of
doubly ionized thallium employing the highly correlated RCC theory at the level of single, dou-
ble and partial triple excitations. The power of the RCC theory has been exploited to obtain a
quantitative understanding of different correlation effects in transition amplitudes. We have ob-
served strong contributions from core-polarization to the E1 transitions. Also, core-correlations
contributes strongly to the E2 transitions. The results of the optical transitions between the
fine structure states of 6p may be useful for the study of fundamental atomic physics, and as
benchmarks for testing relativistic many-body theories.

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