Configuration-interaction many-body perturbation theory for La ii electric-dipole transition probabilities

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Accurate configuration-interaction many-body-perturbation theory La II electric-dipole transition probabilities

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Accurate transition probabilities of La II ion are calculated using configuration-interaction many-body perturbation theory with 10 adjustable parameters, seven of which are evaluated from energies of the La III single-valence electron ion. Comparison is given for transitions probabilities and lifetimes with experiments and theories. Close agreement with experiment is observed for most transitions. The theoretical approach can be extended to other divalent atoms and ions with strong valence-core interactions and to more complex atoms. The theory will be useful for opacity evaluation and astrophysical applications.

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I. INTRODUCTION

Calculations of heavy element abundances from observed spectra, including containing La II ions, have become more and more important in recent years [1]. Astrophysical applications are in need of accurate transition probabilities, which can be obtained from branching ratios and lifetimes. Multiple La II measurements of lifetimes and transition probabilities were carried out in the past [2–7, 9]. Few theoretical methods were applied to La II transitions: multi-configuration Dirac-Fock (MCDF) calculations [11] of 6s2 ^{1}S$_0$-6s6p ^{1}P$_1$, ^{3}P$_1$ transitions; the Hartree-Fock with relativistic corrections (HFR) method [10] modified by inclusion of core-valence corrections with semi-classical core-polarization potentials. This method used parametric fitting to obtain close agreement for energy levels, in most cases tens of inverse cm. In addition calculations based on Cowan's code [8] were also presented [9] and some criterion was applied to select the transitions that can be described by this approach.

Neutral or close to neutral lanthanides and actinides are challenging for atomic theory primary due to difficulties related to including very strong valence-valence interactions, especially in cases when the number of valence electrons exceeds 3, with strong valence-core correlations and relativistic corrections further complicating the matter. The approach of configuration-interaction many-body perturbation theory (CI-MBPT) has been very successful in light atoms, including Si I [13], Be I, Mg I, Ca I, Ne I , and some others. However, in actinides and lanthanides, because valence-core interaction is strong and CI-MBPT approach includes it only in the second order, which is insufficient, the accuracy is quite low. Previously, we attempted to improve accuracy by introducing adjustable parameters. Such parameters simulate the modification of second-order correction due to screening. While energies were definitely improved and level identification was possible, the transition probabilities did not agree accurately with experiment, although this can be partially attributed to limited accuracy of experimental measurements. Moreover, the adjustable parameters were optimized without considering physical constraints. In Th I, it was found [14] that different sets of quite different parameters can lead to similar wavefunctions and atomic properties. However, it was not clear how to find the best minimum because the number of adjustable parameters was as larger as 9 and finding absolute minimum in such a large dimension was technically very difficult or altogether impossible. The question remains whether the result would be quite accurate if we were able to find the absolute minimum. On the other hand, at least 7 out of 9 parameters can be found from energies of the corresponding one-valence ion; then only 2 or 3 parameters remain for optimization, and such an optimization problem is much easier to solve. Apart from the question of optimization, the optimal set of parameters depends on the basis, whether it is large enough to account for valence-valence interactions. In the systems with more than 3 valence electrons, this is difficult technically, because the optimization of parameters would take a very long time. Thus two-valence electron atoms can be a good testing ground for studying the optimization of parameters when the valence-valence interaction is saturated.

In this work we considered La II ion. It has two valence electron, so the question of saturation of valence-valence configuration space is not an issue, and the focus can be placed on valence-core interactions, which are significant and cannot be accounted sufficiently accurately with *ab initio* second-order MBPT. On the other hand, by introducing adjustable parameters in CI-MBPT, good accuracy is possible to achieve, as it will be illustrated in this paper. In contrast to our previous work, we found or constrained 7 parameters by adjusting them to obtain good agreement for energies of a single-valence ion (La III), and then only 3 parameters were completely fit to obtain agreement for 2-valence energies. Afterward, one or two of the initially estimated 7 parameters were minimally adjusted for the best energy fit, but this fit was much more constrained by physical meaning of parameters than in [14].

II. CI-MBPT APPROACH

To calculate La II energies a CI+MBPT method developed for open shell atoms with multiple valence electrons is used (see for example [15]). The theory can be summarized as follows. The effective CI+MBPT Hamiltonian for La II is split into two parts:

$$H^{eff} = \sum_{i=1}^{M} h_{1i} + \sum_{i\neq j}^{M} h_{2ij}. \quad (1)$$

The one-electron contribution

$$h_1 = c\alpha\cdot\mathbf{p} + (\beta-1)mc^2 - Ze^2/r + V^{N-3} + \Sigma_1 \quad (2)$$

in addition to the V^{N-3} Dirac-Hartree-Fock (DHF) potential contains the valence electron self-energy correction, Σ_1 [16]. In the current CI+MBPT program, the self-energy correction is calculated with the second-order MBPT. The term Σ_1 is regulated with seven scaling factors each for a specific one-electron relativistic angular momentum number: $s_{1/2}$, $p_{1/2}$, $p_{3/2}$, $d_{3/2}$, $d_{5/2}$,$f_{5/2}$, $f_{7/2}$. These factors not only take into account some omitted high-order MBPT corrections, but also relativistic effects such as single-particle Breit terms. The two-electron Hamiltonian is

$$h_2 = e^2/|\mathbf{r_1} - \mathbf{r_2}| + \Sigma_2 \quad (3)$$

where Σ_2 is the term accounting for Coulomb interaction screening arising from the presence of the core [17]. In the CI-MBPT program used, the screening is also calculated in the second order. For fitting the two additional scaling factors are introduced for zero and first-order multipolarity of the Coulomb interaction. Further details on the CI+MBPT approach can be found in Ref.[18]. In terms of specific numerical steps, first, the DHF V^{N-3} potential for the closed-shell La III ion is calculated. Second, the basis in the frozen V^{N-3} potential is calculated with the help of a B-spline subroutine for the ion in a cavity of radius $R = 30$ a.u. The basis is then used to evaluate the CI+MBPT terms in Eq. 1. Finally, the eigenvalue problem is solved for the effective Hamiltonian matrix. The program can generate a set of configurations by single-, double-, etc. excitations of the input configurations limited by a given maximum angular momentum l_{max} and N_{max}. In case of La II, we chose single and double excitations limited by: $n = 15$ for s and p states, $n = 14$ for d states, 13 for f states, and $n = 12$ for g states. The effective Hamiltonian matrix generation is repeated multiple times for different scaling factors (10 total) and optimization procedure described below is used until some optimum is reached. The electric dipole matrix elements are evaluated only. Random-phase approximation (RPA) corrections are added to take into account core-polarization corrections for the matrix elements.

III. OPTIMIZATION OF Σ_1 AND Σ_2 PARAMETERS

Seven Σ_1 parameters were estimated from La III energies, Table I. Each parameter affects only valence electrons of specific symmetry: $s_{1/2}$, $p_{1/2}$, $p_{3/2}$, etc, so the minimization is straightforward. While it is possible to find parameters that would minimize the deviation for the lowest states of given symmetry, the next excited states of the same symmetry will have substantial deviation. This is the limitation of the scaling theory. In two-valence La II, the expansion shows the dominant contribution from the lowest states, so it is reasonable to assume that the 7 parameters optimal for La III lowest energies are quite physical and are a good starting approximation. Indeed we find that slight adjustment are needed to improve the two-valence energies. It can be noted that f electrons have the largest deviations for the next in n level $5f$.

With Σ_1 parameters obtained from La III energies, three most important Σ_2 parameters were found from fitting La II energies, different for different J and parity. For optimization of Σ_2 parameters first and some re-optimization of some Σ_1 and Σ_2 parameters, we used the particle swarm method [19, 20]. This method has an advantage that it can accelerate the optimization by engaging multiple computer cores.

IV. LA II CI-MBPT ENERGIES AND G-FACTORS

The CI-MBPT energies with optimized 10 parameters using the procedure described above are shown in Tables II,III,IV for J=1-3 even states and in Tables V,VI,VII for J=1-3 odd states. It can be noted that the same Σ_1 parameters: 0.7600,0.8100,0.8100,0.8450,0.8550,0.8100,0.8150 give a good agreement for energies with experiment and also that they are quite close to the estimated Σ_1 parameters shown in Table I. However, the Σ_2 parameters differ: 0.9133,0.8900,0.890 for J=1, 0.8600,0.7163,0.750, for J=2, and 0.8610,0.7400,0.700, for J=3, although the change is not very large. The deviations of CI-MBPT energies from the experimental values for J=1, J=2, and J=3 even states are 118, 261, and 143, which are in the expected range. On the other hand, the odd states have the first parameter different from that of the even state 0.8159, instead of 0.7600, while the other Σ_1 are the same: 0.81,0.81,0.845,0.855,0.81,0.815. More substantial changes can be observed for Σ_2 parameters of odd states: 1.0525,0.8707,2.00 for J=1, 0.9923,0.7593,1.445 for J=2, 0.9564,0.7357,0.8000, for J=3. The CI-MBPT energy deviations from the experiment are 360, 38, and 326 cm^{-1} for J=1,2,3. It is especially small for J=2 and gives some assurance that the theory works particularly well for these states.

Apart from energies, g-factors are also calculated and

TABLE I: The estimates of Σ_1 parameters from energies of La III (NIST [21]). Energies (one-electron removal energies) are given in cm^{-1}. Because the lowest states of given symmetry dominate the expansion of the two-valence La II ion, the parameters were adjusted to fit well these levels. The comparison for second next levels for each symmetry is also given to illustrate the fact that it is impossible to have complete agreement for all levels. This can be the reason why in two-valence ions some adjustment of Σ_1 is needed to improve agreement for energies.

Par.	Par. Value	Levels	Expt. Energy	Th. Energy	Eth-Expt.
1	0.782	$6s_{1/2}$	141084	141072	-12
1	0.782	$7s_{1/2}$	72328	71924	-404
2	0.835	$6p_{1/2}$	112660	112651	-7
2	0.835	$7p_{1/2}$	61443	61114	-329
3	0.835	$6p_{3/2}$	109564	109539	-25
3	0.835	$7p_{3/2}$	60214	59912	-301
4	0.85	$5d_{3/2}$	154675	154658	-17
4	0.85	$6d_{3/2}$	72294	71599	-695
5	0.86	$5d_{5/2}$	153072	153066	-6
5	0.86	$6d_{5/2}$	71861	71188	-673
6	0.83	$4f_{5/2}$	147480	147562	82
6	0.83	$5f_{5/2}$	62221	61392	-829
7	0.83	$4f_{7/2}$	145980	145880	-100
7	0.83	$5f_{7/2}$	62141	61322	-819

compared with experiment. In most cases the agreement is better than 1%, but there are a few anomalies with substantial disagreement. This can be traced to strong mixing between adjacent states with small energy intervals. It can be expected that transition properties might exhibit similar anomalies due to strong mixing.

V. TRANSITION LA II CI-MBPT LINE STRENGTHS WITH NIST VALUES

In Tables VIII,IX,X La II CI-MBPT line strengths for J=2 even to J=1-3 odd transitions are compared with NIST values. This comparison shows that agreement with NIST values is quite accurate, with a few exception which can be due to strong sensitivity of involved transitions to mixing coefficients, since the NIST value accuracy is higher. The 2-2 transitions are expected to be most accuracy since the agreement for energies of J=2 odd states is much better than for energies of J=2 and J=3 odd states, but this is not actually observed. Thus the agreement for energies is not an obvious indication for high accuracy of transitions. More comparison for transition probabilities and lifetimes is given in following sections.

VI. ELECTRIC-DIPOLE TRANSITION PROBABILITY COMPARISON BETWEEN THEORIES AND EXPERIMENTS.

In order to carefully evaluate the current theory, we calculate multiple electric-dipole (E1) transition probabilities and compare them (Table XI) with other theories [9, 10] and accurate experimental measurements [7, 12]. The E1 transition probabilities A are calculated from line strengths S:

$$A = \frac{2.142 \times 10^{10} \omega^3 S}{2J+1} \tag{4}$$

where ω is the experimental transition energy in atomic units, J is the total angular momentum of the upper state. In most cases, our CI-MBPT results are in close agreement with the two experiments. When the values are relatively small, as expected, due to cancellation effects, the theoretical values have some disagreement with experiments, but for values greater than $2\times\ 10^7$ s^{-1}, the agreement is consistently on the order of 10% and in some cases the theory agrees with experiment within error bars. The agreement of the current theory is somewhat better than of previous ones. For example in the 5d6p $^3D_2$ - 5d6s $^3D_1$ transition, our value 2.71 is much closer to the experimental values of 3.10 and 2.72 than the two theories, 5.59 and 6.75 (in units of 10^7 s^{-1}). Nevertheless, the approach of HFR+FIT+CP, which in some sense is similar to CI-MBPT with adjustable parameters, is also successful. Thus the fit alone is not sufficient, even when the fitted energies are very close to experiment, as it is the case of HFR+FIT+CP theory.

Also we notice that in one case when the two experiments disagree, the 6s6p $^3P_2$ - 5d^2 $^3P_1$ transition, our value is closer to the experiment [12]. Surprisingly, the transition probabilities of some suppressed transitions still agree with the experiments.

TABLE II: The CI-MBPT energies and g-factors for J=1 even states of La II with comparison with NIST values [21]. Theoretical and experimental (NIST) energies are given in cm^{-1} and are aligned for the first level. The optimized CI-MBPT Σ_1 and Σ_2 parameters are the following: 0.7600,0.8100,0.8100,0.8450,0.8550,0.8100,0.8150;0.9133,0.8900,0.8900. Note that Σ_1 parameters were slightly changed from the ones giving the best La III single-valence energy for the lowest states. The standard deviation for energy is 118 cm^{-1}.

Level	Conf.	g-factor	E	Conf.	E	dE	g-factor	dg
#	NIST	NIST	NIST	CI-MBPT	CI-MBPT		CI-MBPT	
1	5d6s	0.498	1895	6s5d	1895	0	0.5	0.002
2	$5d^2$	1.497	5718	5d2	5562	-156	1.5	0.003
3	4f6p	0.497	38534	4f6p	38578	44	0.5	0.003
4	5d7s	0.5	49733	5d7s	49509	-224	0.5006	0.0006
5	5d6d	0.621	52169	5d6d	52036	-133	0.6244	0.0034
6	5d6d	1.335	53302	5d6d	53149	-153	1.3575	0.0225
7	5d6d	1.455	54365	5d6d	54217	-148	1.4205	-0.0345
8	5d6d	1.552	55230	5d6d	54889	-341	1.5978	0.0458
9	6s7s	1.955	60660	6s7s	60435	-225	1.939	-0.016
10	$6p^2$	1.528	61128	$6p^2$	60787	-341	1.5595	0.0315
11	$4f^2$	1.471	63703	$4f^2$	63563	-140	1.4968	0.0258
12	6s6d	0.506	64361	6s6d	64293	-68	0.5038	-0.0022

TABLE III: The CI-MBPT energies and g-factors for J=2 even states of La II with comparison with NIST values [21]. Theoretical and experimental (NIST) energies are given in cm^{-1} and are aligned for the first level. The optimized CI-MBPT Σ_1 and Σ_2 parameters are the following: 0.7600,0.8100,0.8100,0.8450,0.8550,0.8100,0.8150;0.8600,0.7163,0.7500. Note that Σ_1 parameters are the same as in case of J=1 even states, which are slightly different from the ones giving the best La III single-valence energy for the lowest states. The standard deviation for energy is 261 cm^{-1}. It is interesting to observe that the energy are well reproduced for highly excited states up to 59900 cm^{-1}.

Level	Conf.	g-factor	E	Conf.	E	dE	g-factor	dg
#	NIST	NIST	NIST	CI-MBPT	CI-MBPT		CI-MBPT	
1	$5d^2$	0.721	0	$5d^2$	0	0	0.707	-1.4%
2	$5d^2$	0.977	1394	5d6s	1531	137	0.997	2.0%
3	5d6s	1.133	2591	5d6s	2736	145	1.1355	0.2%
4	$5d^2$	1.481	6227	$5d^2$	6220	-7	1.4881	0.7%
5	5d6s	1.005	10095	5d6s	10915	820	1.0056	0.1%
6	4f6p	0.719	35787	4f6p	36112	325	0.7114	-0.8%
7	4f6p	1.071	38221	4f6p	38626	405	1.0864	1.5%
8	4f6p	1.036	40457	4f6p	40955	498	1.0356	0.0%
9	5d7s	1.117	49884	5d7s	49851	-33	1.1217	0.5%
10	5d7s	1.036	51523	5d7s	51488	-35	1.0446	0.9%
11	5d6d	1.154	52734	5d6d	52758	24	1.161	0.7%
12	5d6d	0.751	53885	5d6d	53801	-84	0.7512	0.0%
13	5d6d	1.183	55184	5d6d	55049	-135	1.2241	4.1%
14	5d6d	1.203	56036	5d6d	55895	-141	1.1961	-0.7%
15	$4f^2$	0.675	57399	$4f^2$	57583	184	0.674	-0.1%
16	$6p^2$	1.035	59900	$6p^2$	59951	51	1.0448	1.0%

VII. CI-MBPT LIFETIME CALCULATIONS

We have calculated lifetimes for several excited states, Table XII. Lifetimes are direct measurements, and they are used to derive transition probabilities from branching ratios. Thus lifetime errors can propagate to errors in transition probabilities. Several experimental lifetime measurements are available as well as calculations. One additional issue for getting transition probabilities from lifetimes is that not all possible transitions are accounted in the experiment, so this can be a source of additional error. Theory is better in this respect since

TABLE IV: The CI-MBPT energies and g-factors for J=3 even states of La II with comparison with NIST values [21]. Theoretical and experimental (NIST) energies are given in cm^{-1} and are aligned for the first level. The optimized CI-MBPT Σ_1 and Σ_2 parameters are the following: 0.7600,0.8100,0.8100,0.8450,0.8550,0.8100,0.8150;0.8610,0.7400,0.7000. Note that Σ_1 parameters are the same as in case of J=1 even states, which are slightly different from the ones giving the best La III single-valence energy for the lowest states. The standard deviation for energy is 143 cm^{-1}. It is interesting to observe that the energy are well reproduced for highly excited states up to 57919 cm^{-1}.

Level	Conf.	g-factor	E	Conf.	E	dE	g-factor	dg
#	NIST	NIST	NIST	CI-MBPT	CI-MBPT		CI-MBPT	
1	$5d^2$	1.083	1016	$5d^2$	1016	0	1.0834	0.0%
2	5d6s	1.334	3250	5d6s	3451	201	1.3333	-0.1%
3	4f6p	0.876	35453	4f6p	35813	360	0.8773	0.1%
4	4f6p	1.061	36955	4f6p	37271	316	1.0439	-1.7%
5	4f6p	0.944	37210	4f6p	37554	345	0.9601	1.6%
6	4f6p	1.274	39403	4f6p	39814	411	1.2854	1.1%
7	5d7s	1.315	51229	5d7s	51245	16	1.3293	1.4%
8	5d6d	0.987	52138	5d6d	52246	108	0.9996	1.3%
9	5d6d	0.861	52858	5d6d	53003	145	0.8644	0.3%
10	5d6d	1.218	53690	5d6d	53783	93	1.2245	0.6%
11	5d6d	1.088	54840	5d6d	54824	-16	1.0823	-0.6%
12	$4f^2$	1.085	57919	$4f^2$	58121	203	1.0833	-0.2%

TABLE V: The CI-MBPT energies and g-factors for J=1 odd states of La II with comparison with NIST energies [21]. Theoretical and experimental (NIST) energies are given in cm^{-1} and are aligned for the first level. The optimized CI-MBPT Σ_1 and Σ_2 parameters are the following: 0.8159,0.81,0.81,0.845,0.855,0.81,0.815;1.0525,0.8707,2.000. Note that the first Σ_1 parameter differ from that in the case of J=1 even states. The standard deviation for energy is 360 cm^{-1}.

Level	Conf.	g-factor	E	Conf.	E	dE	g-factor	dg
#	NIST	NIST	NIST	CI-MBPT	CI-MBPT		CI-MBPT	
1	4f5d	0.542	21442	4f5d	21442	0	0.548	0.006
2	4f5d	1.431	22705	4f5d	22570	-135	1.443	0.012
3	5d6p	0.782	25973	5d6p	26005	32	0.715	-0.067
4	5d6p	0.876	27424	5d6p	27532	108	1.057	0.181
5	6s6p	1.267	28155	5d6p	28751	597	1.203	-0.064
6	4f5d	1.074	30353	4f5d	31231	878	1.039	-0.035
7	5d6p	1.492	32161	5d6p	32338	177	1.493	0.001
8	6s6p	0.999	45692	6s6p	45574	-118	1.002	0.003

it can generate a complete set of transitions, especially those outside the observable range. In general a consistent agreement of CI-MBPT with all listed experimental lifetimes can be observed, although for the two lowest states, the CI-MBPT theory gave larger deviation than the "HFR+FI+CP" theory of [10]. Excellent agreement can be observed for states with short lifetimes, as expected, since the corresponding decay channels are dominated by strong transitions which can be calculated more accurately. The current theory agrees most systematically with the LIF experiments of [7].

VIII. FINE TUNING 10 PARAMETERS VS. AB INITIO AND ONE-PARAMETER-VALUE OPTIMIZATION

The above results were presented for the case when 10 parameters were optimized after a good initial guess for 7 first parameters from La III ion energies. The seven parameters were optimized separately for each value of J of La III. Roughly 80% reduction is observed, which indicates that contributions beyond second order are quite small, so the theory presented above is almost *ab initio*, in contrast to Cowan's code approach, where the ab initio results substantially deviate from the correct values. The reduction of the second-order correction can be attributed to screening by core and can be roughly accounted for by setting all parameters used in CI-MBPT

TABLE VI: The CI-MBPT energies and g-factors for J=2 odd states of La II with comparison with NIST energies [21]. Theoretical and experimental (NIST) energies are given in cm^{-1} and are aligned for the first level. The optimized CI-MBPT Σ_1 and Σ_2 parameters are the following: 0.8052,0.8100,0.8100,0.8450,0.8550,0.8100,0.8150;0.9923,0.7593,1.4451. Note that the first Σ_1 parameter differ from that in the case of J=1 odd state. The standard deviation for energy is 38 cm^{-1}. The energies are very well reproduced as well as g-factors.

Level	Conf.	g-factor	E	Conf.	E	dE	g-factor	dg
#	NIST	NIST	NIST	CI-MBPT	CI-MBPT		CI-MBPT	
1	4f6s	0.664	14148	4f6s	14148	0	0.668	0.004
2	4f5d	0.754	17212	4f5d	17128	-83	0.744	-0.010
3	4f5d	0.923	18895	4f5d	18814	-82	0.934	0.011
4	4f5d	1.167	22106	4f5d	22064	-42	1.178	0.011
5	4f5d	1.459	23247	4f5d	23182	-65	1.456	-0.003
6	5d6p	0.887	24463	5d6p	24434	-29	0.886	-0.001
7	5d6p	0.825	26414	5d6p	26376	-38	0.820	-0.005
8	5d6p	1.168	27388	5d6p	27292	-96	1.169	0.001
9	6s6p	1.471	29498	6s6p	29368	-130	1.482	0.011
10	6s6p	1.494	33204	6s6p	33098	-106	1.496	0.002

TABLE VII: The CI-MBPT energies and g-factors for J=3 odd states of La II with comparison with NIST energies [21]. Theoretical and experimental (NIST) energies are given in cm^{-1} and are aligned for the first level. The optimized CI-MBPT Σ_1 and Σ_2 parameters are the following: 0.8046,0.8100,0.8100,0.8450,0.8550,0.8100,0.8150;0.9564,0.7357,0.8000. Note that only one Σ_1 parameter differs from that of J=2 odd state. The standard deviation for energy is 326 cm^{-1}.

Level	Conf.	g-factor	E	Conf.	E	dE	g-factor	dg
#	NIST	NIST	NIST	CI-MBPT	CI-MBPT		CI-MBPT	
1	4f6s	1.056	14375	4f6s	14375	0	1.065	0.009
2	4f6s	1.017	15774	4f6s	15883	109	1.019	0.002
3	4f5d	1.086	18236	4f5d	17977	-259	1.083	-0.003
4	4f5d	0.757	20403	4f5d	20119	-284	0.754	-0.003
5	4f5d	1.288	22537	4f5d	22641	104	1.309	0.021
6	4f5d	1.034	24523	4f5d	25317	795	1.021	-0.013
7	5d6p	1.088	26838	5d6p	26712	-126	1.089	0.001
8	5d6p	1.308	28315	5d6p	28202	-114	1.318	0.010
9	5d6p	1.005	32201	5d6p	32397	196	1.008	0.003

calculations to 0.8. More accurate optimization gave the following parameters and deviations: J=1 even, 0.82, 334 cm^{-1}; J=2 even, 0.815, 333 cm^{-1}; J=3, even, 0.83, 352 cm^{-1}; J=4, even, 0.81, 526 cm^{-1}; J=1 odd, 0.86, 430 cm^{-1}; J=2 odd, 0.82, 466 cm^{-1}; J=3 odd, 0.83, 524 cm^{-1}. It is quite remarkable that such agreement is obtained with essentially adjusting a single variable. However, when we considered the transition line strengths, the results presented above in tables have much better accuracy than the results from calculations using all 10 parameters set to single values, shown above, for example J=2 even to J=1 odd transition, in TableXIII. The ab initio values were quite off and not much correlated with experimental results.

IX. CONCLUSION

This paper presents accurate CI-MBPT calculations of La II transition line strengths, probabilities and lifetimes, consistent with available reliable experimental measurements. Ten adjustable parameters were introduced to improve energy levels. Seven parameters were estimated from energies of La III ion, and then fit led to sets of parameters which had 6 the same parameters and 4 different parameters for different J and parity of La II. Most parameters have meaningful values and as the result, the transitions were observed in systematic agreement with experiment. While the optimized parameters described above give the best agreement with experiment for line strengths, it is remarkable that it is possible to get quite accurate result by setting 10 parameters to the same value and optimizing this value for each J and par-

TABLE VIII: The comparison theoretical and NIST [21] line strengths for J=2 even J=1 odd transitions. For J=2 even states the parameters were chosen: 0.7600,0.8100,0.8100,0.8450,0.8550,0.8100,0.8150;0.8600,0.7163,0.7500, which give energy level error 261 cm^{-1} and for J=1 odd states the parameters were: 0.8159,0.81,0.81,0.845,0.855,0.81,0.815;1.0525,0.8707,2.000, which give energy level error 360 cm^{-1}. NIST accuracy labels: B+≤7%, B≤10%, C+≤18%, C≤25%.

# even	E even	# odd	E odd	S NIST	Acc. NIST	S CI-MBPT	dS/S
1	0	1	21441	0.87	B+	1.014	-17%
1	0	3	25973	4.5	B+	5.365	-19%
1	0	4	27423	3.10	B	1.872	40%
2	1394	1	21441	0.82	B+	0.684	17%
2	1394	2	22705	0.239	B	0.236	1%
2	1394	3	25973	1.49	B	1.462	2%
2	1394	4	27423	1.83	B	1.589	13%
3	2592	1	21441	0.78	B	0.785	-1%
3	2592	2	22705	1.15	B+	1.271	-11%
3	2592	3	25973	1.01	B	1.189	-18%
3	2592	4	27423	0.57	C	0.426	25%
4	6227	4	27423	0.96	B	1.435	-49%
5	10095	4	27423	3.9	C+	3.108	20%

TABLE IX: The comparison theoretical and NIST [21] line strengths for J=2 even J=2 odd transitions. For J=2 even states the parameters were chosen: 0.7600,0.8100,0.8100,0.8450,0.8550,0.8100,0.8150;0.8600,0.7163,0.7500, which give energy level error 261 cm^{-1} and for J=2 odd states the parameters were: 0.8052,0.8100,0.8100,0.8450,0.8550,0.8100,0.8150;0.9923,0.7593,1.4451, which give energy level error 38 cm^{-1}. NIST accuracy labels: B+≤7%, B≤10%, C+≤18%, C≤25%.

# even	E even	# odd	E odd	S NIST	Acc. NIST	S CI-MBPT	dS/S
1	0	3	18895	0.39	C+	0.381	2%
1	0	5	23247	0.37	B	0.294	21%
1	0	6	24463	11.5	B+	9.880	14%
2	1394	5	23247	1.25	B+	1.418	-13%
2	1394	6	24463	12.5	B+	14.240	-14%
2	1394	7	26414	11.3	B+	11.102	2%
3	2592	4	22106	2.39	B+	3.244	-36%
3	2592	5	23247	0.26	C+	0.450	-73%
3	2592	7	26414	7	B+	7.133	-2%
3	2592	8	27388	11	B	11.892	-8%

ity. The values for different J and parity are also quite close, around 0.8. It can be concluded that ab initio CI-2nd order MBPT results are almost correct, with 20% correction of the second-order contribution coming from the core screening or higher order corrections. However, due to strong mixing, even such small corrections are important to include to obtain reliable transition line strengths. It can be noted that another theoretical approach based on Cowan code with fitting and additional polarization potentials (HFR+FIT+CP) leads also to some agreement with experiment, since it takes into account similar effects as CI-MBPT: relativistic effects and core-polarization in valence-core interaction. The current CI-MBPT theory is not limited to La II and can be extended to other ions and atoms with strong valence-core interaction and relativistic effects. However, the accuracy for atoms with more valence electrons might be reduced since mixing coefficients become more sensitive to accuracy of calculations and it can become difficult to saturate contributions in valence-valence CI.

X. ACKNOWLEDGEMENT

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TABLE X: The comparison of theoretical and NIST [21] line strengths for J=2 even J=3 odd transitions. For J=2 even states the parameters were chosen: 0.7600,0.8100,0.8100,0.8450,0.8550,0.8100,0.8150;0.8600,0.7163,0.7500, which give energy level error 261 cm$^-$1 and for J=3 odd states the parameters were: 0.8046,0.8100,0.8100,0.8450,0.8550,0.8100,0.8150;0.9564,0.7357,0.8000, which give energy level error 326 cm$^-$1. NIST accuracy labels: B+$\leq$7%, B$\leq$10%, C+$\leq$18%, C$\leq$25%.

# even	E even	# odd	E odd	S NIST	Acc. NIST	S CI-MBPT	dS/S
1	0	3	18236	0.105	C+	0.087	17%
1	0	4	20403	2.97	B+	3.439	-16%
1	0	5	22537	0.063	C+	0.067	-7%
1	0	6	24523	0.232	C+	0.310	-33%
2	1394	4	20403	0.2	C+	0.182	9%
2	1394	5	22537	0.65	B+	0.611	6%
2	1394	6	24523	1.6	B+	2.110	-32%
2	1394	7	26838	6.2	B+	7.106	-15%
2	1394	8	28315	1.9	C+	1.549	18%
3	2592	3	18236	0.81	B	1.119	-38%
3	2592	6	24523	1.6	B+	3.019	-89%
3	2592	7	26838	18.2	B+	17.579	3%
3	2592	8	28315	6.7	C+	5.459	19%
4	6227	8	28315	3.8	C	4.230	-11%

TABLE XI: The comparison for some transition probabilities. "HFR+FIT+CP" theoretical transition probabilities that are based on fitting and core-polarization potential are taken from [10]; "Expt.1" are experimental values from [7]; "Expt.2" are taken from [12].Units are 10^7 s^{-1}.

Level				Theory				
Upper	Energy	Lower	Energy	CI-MBPT	HFR+FIT+CP	Theory[9]	Expt.1	Expt.2
5d6p $^3D_1$	25973	5d^2 $^3F_2$	0	6.35	3.58		5.30±0.30	
5d6p $^1D_2$	24463	5d^2 $^3F_2$	0	5.86	7.73		6.80±0.40	
5d6p $^1D_2$	24463	5d^2 $^1D_2$	1394	7.08	8.10		6.20±0.30	
5d6p $^1D_2$	24463	5d6s $^3D_1$	1895	3.10	2.85		3.03±0.17	
5d6p $^3D_2$	27388	5d^2 $^3F_2$	0	0.70				0.670±0.007
5d6p $^3D_2$	27388	5d^2 $^3F_3$	1016	9.60	11.3	10.7	9.90±0.60	9.94±0.09
5d6p $^3D_2$	27388	5d6s $^3D_1$	1895	2.71	5.59	6.75	3.10±0.40	2.72±0.03
5d6p $^3D_2$	27388	5d6s $^3D_2$	2592	7.35	4.51	7.18	6.80±0.50	6.58±0.06
5d6p $^3D_3$	28315	5d^2 $^1D_2$	1394	0.89				1.28±0.01
5d6p $^3D_3$	28315	5d6s $^3D_2$	2592	2.71	5.48	5.51	3.30±0.40	3.06±0.03
5d6p $^3D_3$	28315	5d^2 $^3P_2$	6227	1.31				1.04±0.01
5d6p $^3F_2$	26414	5d^2 $^3F_2$	0	0.27				0.88±0.01
5d6p $^3F_2$	26414	5d^2 $^3F_3$	1016	0.55				0.388±0.004
5d6p $^3F_2$	26414	5d^2 $^1D_2$	1394	7.05	6.41		7.20±0.40	6.58±0.06
5d6p $^3F_2$	26414	5d6s $^3D_1$	1895	7.12	5.66		7.00±0.40	6.08±0.06
5d6p $^3F_2$	26414	5d6s $^3D_2$	2592	3.91	6.52		3.81±0.20	4.08±0.04
5d6p $^3F_3$	26838	5d^2 $^3F_2$	0	0.17				0.079±0.001
5d6p $^3F_3$	26838	5d^2 $^1D_2$	1394	3.33	1.87		2.97±0.16	2.44±0.02
5d6p $^3F_3$	26838	5d6s $^3D_2$	2592	7.31	7.23	6.56	7.50±0.40	7.26±0.07
5d6p $^3F_3$	26838	5d^2 $^3P_2$	6227	0.054				0.0389±0.0004
6s6p $^3P_2$	33204	5d^2 $^1D_2$	1394	0.64				0.308±0.003
6s6p $^3P_2$	33204	5d6s $^3D_1$	1895	0.413				0.418±0.004
6s6p $^3P_2$	33204	5d6s $^3D_2$	2592	5.22				5.16±0.05
6s6p $^3P_2$	33204	5d6s $^3D_3$	3250	27.2				28.4±0.3
6s6p $^3P_2$	33204	5d^2 $^3P_1$	5718	1.04	1.08		3.13±0.19	0.596±0.06
6s6p $^3P_2$	33204	5d^2 $^3P_2$	6227	3.60				3.52±0.04

TABLE XII: The comparison for lifetimes, given in ns. Expt. CI-MBPT lifetimes are calculated with fit parameters given in the captions of the energy tables. Experimental lifetimes: LIF1 - [7]; LIF2 - ^{a} [3], ^{c} [4], ^{d}[5]; others ^{e} - [6]. Theory: ^{b}[9], ^{x}-HFR+FIT+CP [10]

Energy	CI-MBPT	LIF1	LIF2	others	Theory
17211.93	370	503±26	511±13^a		255^b,486^x
18895.41	327	489±24	573±21^c		303^b,477^x
22106.02	37.2	52.5±2.6	51.1±1.6^c		33.4^b,55.6^x
23246.93	48.6	56.1±2.8			72.8^x
24462.66	6.14	6.2±0.3	6.7±0.4^d		3.23^b, 5.34^x
27388.11	4.24	4.2±0.2	4.4±0.2^d		3.66^x
26414.01	5.24	5.3±0.3	5.8±0.3^d	5.6±0.5^e	3.5^b,5.03^x
29498.05	18.8	13.6±0.7			14.2^x
33204.41	2.63	2.8±0.2	2.6±0.2^d		2.44^x

TABLE XIII: Comparison of line strengths (S) calculated with CI-MBPT: fully optimized (A), all parameters constrained to be of the same value, which was optimized independently for J=2 even and J=1 odd (B), ab initio (C).

# even	E even	# odd	E odd	S NIST	Acc. NIST	S_A	S_B	S_C
1	0	1	21441	0.87	B+	1.014	0.95	0.12
1	0	3	25973	4.5	B+	5.365	4.51	1.24
1	0	4	27423	3.10	B	1.872	1.80	5.84
2	1394	1	21441	0.82	B+	0.684	1.13	0.14
2	1394	2	22705	0.239	B	0.236	0.23	0.08
2	1394	3	25973	1.49	B	1.462	1.11	1.14
2	1394	4	27423	1.83	B	1.589	2.50	1.88
3	2592	1	21441	0.78	B	0.785	0.36	0.11
3	2592	2	22705	1.15	B+	1.271	1.08	0.52
3	2592	3	25973	1.01	B	1.189	0.44	0.26
3	2592	4	27423	0.57	C	0.426	0.26	1.73
4	6227	4	27423	0.96	B	1.435	1.40	0.01
5	10095	4	27423	3.9	C+	3.108	2.95	0.01

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