Relativistic configuration interaction plus linearized-coupled-cluster calculations of U^{2+} energies, g factors, transition rates, and lifetimes

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Relativistic CI+linearized coupled-cluster calculations of U^{2+} energies, g-factors, transition rates and lifetimes

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Excitation energies, term designations, g-factors, transition rates and lifetimes of U^{2+} are determined using a relativistic configuration interaction (CI) + linearized coupled-cluster (LCC) approach. The CI-LCC energies are compared with CI+many-body-perturbation-theory (MBPT) and available experimental energies. Close agreement has been found with experiment, within hundreds of cm^{-1}. In addition, lifetimes of higher levels have been calculated for comparison with three experimentally measured lifetimes, and close agreement was found within the experimental error. CI-LCC calculations constitute a benchmark test of the CI+all-order method in complex relativistic systems such as actinides and their ions with many valence electrons. The theory yields many energy levels, g-factors, transition rates, and lifetimes of U^{2+} that are not available from experiment. The theory can be applied to other multi-valence atoms and ions, which would be of interest to many applications.

I. INTRODUCTION

Atomic properties of actinides, such as energy levels, are needed in many applications, from nuclear forensic to industrial uses to quantum chemistry calculations. In particular, energies of actinide ions are needed for calibration of model potentials in chemical calculations of molecules containing actinide atoms used to reduce large full Hilbert space [1, 2]. In addition to being of practical interest, actinides are an intriguing research subject, since they are considered among the most complex atoms that pose several challenges. First, relativistic effects are important and have to be treated consistently. Second, actinides have many valence electrons, including those in the f-shell, that generate a very large number of possible states, and valence-valence interactions between these states have to be treated in all orders, for example with the configuration-interaction (CI) method. Finally, valence-core interactions are also strong, as will be evident below from differences between experimental and 2nd order many-body perturbation theory (MBPT) single-electron energies in U^{5+} ion, and the CI+2nd-order MBPT approach can be inaccurate. Thus more elaborate approaches, such as CI+all-order, may be required. The study of the U^{2+} ion is important for developing theory for more complex actinide ions since the valence CI space contains only configurations with four elections in our method and can still be saturated. From point of view of testing the theory, many experimental U^{2+} energy levels are available to gauge the precision of the theory; in addition, substantial gaps in experimental data exist that can be filled with the theoretical calculations, provided theory is proved satisfactory.

Because of the aforementioned challenges, there were no reliable *ab initio* or semi-empirical calculations of U^{2+} energy levels reported in the literature. An early attempt to estimate a few energy levels was made by Brewer [3] using trends in energies of different actinide atoms. It was estimated that the ground state was the odd $5f^3 6d\ ^5L_6$ and the first even state $5f^4\ ^5I_4$ had energy 1000 ± 1000 cm^{-1} from the ground state. Considering the uncertainty, either of these states could have been the ground state. Palmer and Engleman [4] used the predictions by Brewer[3] to assign labels to two lowest states: $5f^3 6d$ $(^4I)^5L_6$ to the ground state and $5f^3 6d\ (^4I)^5K_5$ to the next odd state. Experimentally many actinide ions are difficult to deal with and the available data are generally limited to only energy levels. Few data for transition rates or lifetimes are available for actinides. Spectroscopic measurements of lines in discharges, where different stages of ionicity coexist and many levels are simultaneously excited, were converted to energy levels using a fitting procedure. The assignment of labels was done using parametric method following the Slater-Condon method [5, 6]. Apart from the problem of level identification, some effort was focused on calculations of ionization potentials with approach of model potentials and pseudopotentials [7, 8], which are widely used in quantum chemistry. As it is evident from the literature search, data for multiple-charge actinide ions is scarce, and there is a great need for developing an *ab initio* approach, such as described in this paper.

Recently, atomic properties of the neutral thorium and its ions were evaluated by Safronova *et al.* [9]. Excitation energies, term designations, and g factors of Th, Th$^+$, and Th^{2+} were determined using a relativistic hybrid configuration-interaction (CI) plus linearized coupled-cluster methods (LCC)[10]. The results were compared with other theoretical and experimental values where available.

The neutral Th and Th-like Uranium have similar electronic structure: a radon core ([Xe]$4f^{14}5d^{10}6s^26p^6$ where [Xe]$=1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s^25p^6$) and four valence electrons. The ground state of neutral thorium is $6s^27s^2\ ^3F_2$; its experimental energies are compiled in the recently updated website [11]. In the case of Th-like uranium, U^{2+}, the experimental data are quite old and less complete [4, 12]. The $5f^4\ ^5F_4$ level was determined to be the ground state of U^{2+} [12], but level identification was not presented and only odd-parity states were referenced. The low-lying valence configurations of Th and Th-like U are very different, with dominant even configurations being $6s^27s^2$ and $6d^37s$ in Th and $5f^4$ and $5f^26d^2$ in Th-like uranium. Large correlation effects for systems with nf electrons were discussed by Safronova *et al.* [13]. For example, the correction due to high partial waves is largely determined by a number of nf electrons in a configuration [13].

In the present paper, we evaluate energies of U^{2+}using the CI+LCC approach. The energies of odd and even-parity complex states with $J = 0$-7 were evaluated. Each complex includes 12 states, that gives together 192 states. Electric multipole matrix elements (E1, E2, and E3) and magnetic multipole matrix elements (M1, M2, and M3) were calculated. We use these matrix elements to evaluate transition rates, oscillator strengths, and lifetimes.

II. CI+MPBT APPROACH

It is known that it is important to consider valence-valence interactions using the non-perturbative configuration-interaction (CI) method, while weaker valence-core interactions can be included using pseudo-potentials or many-body perturbation theory. Recently, we have studied the Si atom [14], which has corrections beyond the 2nd order quite small, much smaller than missing corrections from incomplete valence-valence CI space. However, in the current case of U^{2+}, it appears that the 2nd order is not sufficient, with errors from the omission of higher-order corrections on the order 1,000 cm^{-1}. In the present study, we find that by scaling correlation corrections, especially the single-electron part with $l = 0$, much better agreement can be achieved. Thus we include CI-scaled MBPT energies for comparison with experiment and CI-LCC calculations.

A CI-MBPT method developed for open shell atoms with multiple valence electrons is used in the current calculations (see for example [15]). The effective CI-MBPT Hamiltonian for U^{2+} is split into two parts:

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

The one-electron contribution

$$h_1 = c\alpha \cdot \mathbf{p} + (\beta - 1)mc^2 - Ze^2/r + V^{N-4} + \Sigma_1 \tag{2}$$

in addition to the V^{N-4} 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 2nd-order MBPT. The two electron Hamiltonian is

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

where Σ_2 is the term accounting for Coulomb interaction screening arising from the presence of the core [17]. In the CI-MBPT calculations, the screening is calculated to the 2nd order.

To understand the valence-core effects, we compared monovalent U VI energies calculated with the 2nd-order MBPT and the LCC method with experiment in Table I. As expected, the agreement with experiment is better for the LCC method. More specifically, the accuracy for the $7s$ and $7p$ states is worse than 1,000 cm^{-1} in the case of MBPT, while the LCC method gives deviations less than 1,000 cm^{-1}, except for the $7p_{3/2}$ state. Since low-lying U^{2+} levels do not contain substantial contributions from the $7p$ states, it is expected that the accuracy of the CI-LCC approach for these levels would be on the order of 500 cm^{-1}. In the case of the CI-MBPT, because the contribution from the $7s$ state is significant and the error of MBPT for this state is as large as 3,000 cm^{-1}, the expected accuracy of CI-MBPT will be on the order of 1,000 cm^{-1}. To amend this, we introduced scaling factors in front of Σ_1 in our calculations to correct single-valence MBPT energies and Σ_2 to correct Coulomb screening to higher orders. We find, indeed, that results improve substantially, especially after scaling of Σ_1 for the s wave to account for 7s state energy shift, and the agreement approaches that for the CI-LCC method.

III. CI+LCC METHOD

In the CI + LCC approach introduced in [20], corrections to the effective Hamiltonian Σ_1 and Σ_2 are calculated using a modified version of the linearized coupled-cluster (all-order) method with single and double excitations (LCCSD) described in [21, 22]. As a result, the effective Hamiltonian contains dominant core and core-valence correlation corrections to all orders. The main issue it to efficiently calculate the LCC correction to $\Sigma_2(ijkl)$.

The implementation of this approach proceeds as follows:
(1) The 2nd-order corrections Σ_1 and Σ_2 to the effective Hamiltonian are calculated in the same way as in the CI+MBPT method.
(2) The single-double (SD) LCC calculations are carried out for Rn-like U^{6+} core with 24 subshells. Single and double excitations are allowed from *all* 24 core subshells.
(3)Using the core LCC results, the single -double (SD) core-valence calculations are carried out for 21 valence states: $7s-9s$, $7p_{1/2}-9p_{1/2}$, $7p_{3/2}-9p_{3/2}$, $6d_{3/2}-8d_{3/2}$,

TABLE I: Comparison of U^{5+} 2nd-order MBPT and LCC energy levels with theoretical [18] and experimental [12] results.

Level	Expt.	2nd-MBPT	Diff.	LCC	Diff.	Ref. [18]	Diff.
$5f_{5/2}$	0	0	0	0	0	0	
$5f_{7/2}$	7609	7914	-306	7481	128	7611	-2
$6d_{3/2}$	91000	90165	835	90593	407	91502	-502
$6d_{5/2}$	100511	100347	163	99841	670	101056	-545
$7s_{1/2}$	141447	138422	3025	141103	344	141118	329
$7p_{1/2}$	193340	191308	2032	192508	832	196146	2806
$7p_{3/2}$	215886	214328	1558	213197	2689	217482	-1596

$6d_{5/2} - 8d_{5/2}$, $5f_{5/2} - 7f_{5/2}$ and $5f_{7/2} - 7f_{7/2}$. Core excitations were also allowed from *all* 24 core subshells. The LCC method is modified to exclude valence diagram that will be later accounted for by the CI. This part of the calculation produces the Σ_1 and $\Sigma_2(ijva)$ quantities, where i and j can be any excited state, a are core states and v are the 21 states on the above list.
(4) The $\Sigma_2(ijvw)$ correction to the CI Hamiltonian are calculated, with w also taken from the above valence list. We have tested that restricting the LCC calculation to 21 valence electrons results in sufficient numerical accuracy. We note that the remaining $\Sigma_2(ijkl)$ elements are still corrected in 2nd order. More details of the CI+LCC approaches are described in [20].All of 2nd-order and the LCC calculations include partial waves with $l = 0 - 6$.
(5) The CI method [23] is then used to treat valence-valence correlations, with the CI code modified to include effective Hamiltonian constructed as described above. The CI space includes configurations with four valence electrons in our approach and is constructed as described, for example, in [24]. Briefly, we start with $5f^4$, $5f^36d$, $5f^37s$, $5f^37p$, $6d^25f^2$, and $6d5f^27s$ configurations and allow up to two replacements of any of the configuration electrons to the set of $13s12pdfg$ orbitals to construct the configurations for the CI calculation.

The CI+LCC method was used to evaluate properties of atomic systems with two to four valence electrons [25–31]. This method was also used to calculate atomic properties of the superheavy elements No, Lr and Rf by Dzuba *et al.* [32]. The $7s^2$ and $7snl$ states were considered for nobelium atom, the $7s^26d$, and $7s7p6d$ states were considered for lawrencium atom, and the $7s^26d^2$, $7s^27p6d$ and $7s7p6d^2$ states were considered for rutherfordium atom [32].

The CI+LCC method was used to calculate energies in Ce, Ce$^+$, La, Ce^{2+}, and La$^+$, respectively [13] and to study various correlation corrections in these systems. The difference between neutral and low-ionized systems were considered. The ground states in Ce^{2+} and La$^+$ are $4f^2 \, ^3H_4$ and $5d^2 \, ^3D_2$ instead of the usual the $ns^2 \, ^1S_0$ ground state in Pb^{2+} [25], in Tl$^+$ [26], and in Si^{2+} [27].

IV. RESULTS

A. Excitation energies in U^{2+}

Excitation energies for the lowest states of U^{2+} are presented in Tables II and III. To save space, we list results in Table II only for 96 states instead of 192 states that we included in our calculations. We presented results for $J = 4, 5, 6$, and 7 even and odd-parity states in Table II. The results are ordered by energy within each J for both even and odd states. Since the ground state is odd $J = 6$ state in our calculations, we list $J = 6$ set of odd states first, and list $J = 4, 5, 7$ odd results below.

The g-factors were also evaluated and compared non-relativistic values of g-factors given by Eq. (4) for identification of the LS terms

$$g_{\mathrm{nr}} = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}, \quad (4)$$

where J is total angular momentum of the atom, L is its angular momentum and S is the spin ($\mathbf{J} = \mathbf{L} + \mathbf{S}$).

Our results give odd ground state, $5f^36d \, ^3K_6$, instead of the even $5f^4 \, ^5I_4$ state listed as a ground state in [12]. The energy level of the $5f^4 \, ^5I_4$ level relative our ground $5f^36d \, ^3K_6$ state is 1846 cm^{-1}. Table II data are all counted from the ground $5f^36d \, ^3K_6$ state. In order to provide comparison with [12] in Table III, we count the energies of odd and even states from the corresponding lowest levels, $5f^4 \, ^5I_4$ for even-parity states and $5f^36d \, ^3K_6$ for odd-parity states. We added 210 cm^{-1} to the odd states to align theoretical and experimental levels with respect to $5f^36d \, ^3K_6$ level.

Our and Ref. [12] assignments of configurations and LSJ values are shown in separate columns. Some of the energy levels listed in Ref. [12] are only identified by the total angular momentum J and not by a complete LSJ term designation. Such designations are always approximate and sometimes ambiguous, as in cases of strong configuration mixing.

The $5f^4$, $5f^26d^2$ and $5f^36d$, $5f^37s$ are dominant configuration for even- and odd-parity states, respectively, among the considered levels.

We find that CI+LCC calculations are in very good agreement with experiment (see Table III) considering the complexity of this ion for theory. More specifically,

TABLE II: CI+LCC excitation energies (cm^{-1}) and g-factors of the lowest states of U^{2+} Th-like. Non-relativistic values of g-factors (g_{nr}) are given by Eq.(4).

Conf.	Term	g-factors		Energy	Conf.	Term	g-factors		Energy
		nr	Present				nr	Present	
Odd-parity states					Even-parity states				
$5f^3 6d$	$^3K_6$	0.857	0.745	0	$5f^4$	$^5I_4$	0.600	0.639	1846
$5f^3 6d$	$^5K_6^a$	0.905	0.921	4524	$5f^4$	$^1G_4$	1.000	1.001	10298
$5f^3 6d$	$^5K_6^b$	0.905	0.985	7787	$5f^4$	$^3F_4$	1.250	1.225	14103
$5f^3 7s$	$^5I_6$	1.071	1.055	8364	$5f^4$	$^3G_4^a$	1.050	1.049	15890
$5f^3 6d$	$^1I_6$	1.000	1.008	11880	$5f^4$	$^5G_4^a$	1.150	1.123	19102
$5f^3 6d$	$^5I_6^a$	1.071	1.053	12735	$5f^2 6d^2$	$^3H_4^a$	0.800	0.811	19276
$5f^3 7s$	$^3I_6$	1.024	1.020	12955	$5f^4$	$^3G_4^b$	1.050	1.048	20792
$5f^3 6d$	$^5I_6^b$	1.071	1.071	14601	$5f^4$	$^5G_4^b$	1.150	1.175	22870
$5f^3 6d$	$^3H_6$	1.167	1.152	14998	$5f^4$	$^5G_4^c$	1.150	1.115	24491
$5f^3 6d$	$^3I_6$	1.024	1.033	16404	$5f^2 6d^2$	$^3H_4^b$	0.800	0.877	25481
$5f^3 6d$	$^5H_6$	1.214	1.223	17772	$5f^4$	$^5G_4^d$	1.150	1.089	26277
$5f^3 7s$	$^5H_6$	1.214	1.204	20496	$5f^4$	$^3G_4^c$	1.050	1.068	26792
$5f^3 7s$	$^5I_4$	0.600	0.625	3430	$5f^4$	$^5I_5^a$	0.900	0.907	4791
$5f^3 6d$	$^3H_4^a$	0.800	0.777	6406	$5f^4$	$^3G_5^a$	1.200	1.209	13939
$5f^3 6d$	$^3H_4^b$	0.800	0.760	8021	$5f^4$	$^5G_5$	1.267	1.260	16779
$5f^3 6d$	$^5H_4$	0.900	0.904	8692	$5f^4$	$^3G_5^b$	1.200	1.152	18681
$5f^3 6d$	$^1G_4$	1.000	1.020	12066	$5f^4$	$^5I_5^b$	0.900	0.922	20037
$5f^3 7s$	$^5H_4$	0.900	0.938	14563	$5f^2 6d^2$	$^5K_5^a$	0.667	0.761	22250
$5f^3 7s$	$^3F_4$	1.250	1.235	16247	$5f^4$	$^5H_5$	1.100	1.092	23803
$5f^3 7s$	$^5G_4^a$	1.150	1.135	18308	$5f^2 6d^2$	$^5I_5$	0.900	0.942	24088
$5f^3 7s$	$^5G_4^b$	1.150	1.123	20031	$5f^2 6d^2$	$^3I_5$	0.833	0.886	26484
$5f^3 7s$	$^3G_4^a$	1.050	1.043	20649	$5f^4$	$^3H_5^a$	1.033	1.059	26652
$5f^3 7s$	$^3G_4^b$	1.050	1.094	22110	$5f^4$	$^3H_5^a$	1.033	1.044	27856
$5f^3 7s$	$^3G_4^c$	1.050	1.078	23126	$5f^2 6d^2$	$^1H_5$	1.000	1.017	28574
$5f^3 6d$	$^5K_5$	0.667	0.726	565	$5f^4$	$^5I_6$	1.071	1.056	7441
$5f^3 7s$	$^3I_5^a$	0.833	0.887	4415	$5f^4$	$^3K_6^a$	0.857	0.875	14059
$5f^3 6d$	$^3I_5$	0.833	0.890	6782	$5f^2 6d^2$	$^3K_6$	0.857	0.781	17963
$5f^3 7s$	$^3I_5^b$	0.833	0.870	8431	$5f^4$	$^5H_6$	1.214	1.240	19152
$5f^3 6d$	$^1H_5$	1.000	0.929	9943	$5f^4$	$^3H_6$	1.167	1.176	21212
$5f^3 6d$	$^1H_5^a$	1.000	1.004	11598	$5f^2 6d^2$	$^5I_6$	1.071	1.056	22974
$5f^3 6d$	$^3H_5$	1.033	1.077	12590	$5f^4$	$^3K_6^b$	0.857	0.875	24397
$5f^3 6d$	$^1H_5^b$	1.000	1.009	13218	$5f^4$	$^3I_6$	1.024	1.024	26200
$5f^3 7s$	$^5H_5$	1.100	1.120	14498	$5f^2 6d^2$	$^1I_6$	1.000	1.002	27060
$5f^3 6d$	$^3G_5$	1.200	1.165	15875	$5f^2 6d^2$	$^5K_6$	0.905	0.934	27476
$5f^3 6d$	$^5H_5$	1.100	1.097	17867	$5f^4$	$^1I_6$	1.000	0.979	29103
$5f^3 7s$	$^5G_5$	1.267	1.264	18932	$5f^2 6d^2$	$^3I_6$	1.024	1.037	29407
$5f^3 6d$	$^3L_7$	0.875	0.918	4136	$5f^4$	$^3I_7$	1.143	1.142	9769
$5f^3 6d$	$^3K_7$	1.018	1.039	8061	$5f^4$	$^1K_7$	1.000	0.973	15546
$5f^3 6d$	$^5I_7^a$	1.179	1.151	11898	$5f^4$	$^3L_7$	0.875	0.950	20868
$5f^3 6d$	$^1K_7$	1.000	0.975	12584	$5f^2 6d^2$	$^3L_7$	0.875	0.932	23126
$5f^3 6d$	$^5K_7$	1.054	1.039	13569	$5f^4$	$^5K_7^a$	1.054	1.097	23764
$5f^3 6d$	$^3I_7$	1.143	1.144	15495	$5f^2 6d^2$	$^3K_7$	1.018	1.019	28042
$5f^3 7s$	$^3I_7$	1.143	1.109	16414	$5f^4$	$^3K_7$	1.018	1.024	29918
$5f^3 7s$	$^3I_7$	1.143	1.127	17054	$5f^2 6d^2$	$^3I_7$	1.143	1.114	31000
$5f^3 6d$	$^5I_7^b$	1.179	1.178	18514	$5f^4$	$^5K_7^b$	1.054	1.042	31419
$5f^3 6d$	$^3I_7$	1.143	1.110	20398	$5f^4$	$^5K_7^c$	1.054	1.053	31898
$5f^3 7s$	$^3K_7$	1.018	1.021	21482	$5f^2 6d^2$	$^5K_7$	1.054	1.081	34670
$5f^3 7s$	$^1K_7$	1.000	0.970	23987	$5f^2 6d^2$	$3K_7$	1.018	1.012	35556

TABLE III: Excitation energies (cm^{-1}) of U^{2+} evaluated using the CI+LCC approach are compared with compilation from Refs. [12]. The LCC energies for the odd-parity states in Table II and in similar way CI-MBPT energies are shifted by 210 cm^{-1} to facilitate comparison with the original experimental data. CI-2nd-order MBPT calculations are done for odd states to evaluate theoretical accuracy of the CI-LCC approach, which is on the order of few 100 cm^{-1}, except for $J = 3$ odd states. Even states have very limited experimental data, so the comparison there not only serve to test theoretical accuracy, but also to fill in the gaps in the experimental data.

Conf. Present	Term Present	CI+LCC	CI+2nd	Exp.[12]	Dev.	Conf.+Term [12]	Conf. Present	Term Present	CI+LCC	[12]	Conf.+Term
			Odd-parity states					Even-parity states			
$5f^36d$	$^3G_3^a$	4303	6162	4611	-98	$5f^36d\ ^5H$	$5f^4$	$^5I_4$	0	0	$5f^4\ ^5I_4$
$5f^36d$	$^3G_3^b$	9108	9882	8569	749	$5f^36d$	$5f^4$	$^1G_4$	8438		
$5f^36d$	$^3F_3$	10677	12525	9186	1701	$5f^36d$	$5f^4$	$^3F_4$	12243		
$5f^36d$	$^3G_3^c$	12956	12906	11948	1218	$5f^36d$	$5f^4$	$^3G_4^a$	14030		
$5f^37s$	$^5G_3^b$	17105		17058	257	$5f^36d$	$5f^4$	$^5G_4^b$	21010	24249	4
$5f^37s$	$^3D_3$	25548					$5f^4$	$^3G_4^c$	24932	24935	4
$5f^37s$	$^5I_4$	3640	2771	3745	105	$5f^37s\ ^5I$	$5f^4$	$^5I_5^a$	2932	3037	$5f^4\ ^5I_5$
$5f^36d$	$^3H_4^a$	6616	6721	6286	540	$5f^36d\ ^5I$	$5f^4$	$^3G_5^a$	12080		
$5f^36d$	$^3H_4^b$	8231	8478	7894	547	$5f^36d$	$5f^4$	$^5G_5$	14919		
$5f^36d$	$^5H_4$	8902	10284	9113	-1	$5f^36d$	$5f^4$	$^3G_5^b$	16821		
$5f^37s$	$^5H_4$	14773	13022	14669	314	$5f^36d\ (4)5$	$5f^26d^2$	$^5K_5^a$	20390		
$5f^37s$	$^5G_4^a$	18518					$5f^26d^2$	$^5I_5$	22228	23531	$5f^26d^2\ 5$
$5f^37s$	$^3G_4^b$	22320					$5f^4b$	$^3H_5$	25996	25611	5
$5f^36d$	$^5K_5$	775	1133	885	100	$5f^36d\ ^5K$	$5f^4$	$^5I_6$	5582	5719	$5f^4\ ^5I_6$
$5f^37s$	$^3I_5^a$	4625	4040	4718	117	$5f^37s\ ^5I$	$5f^4a$	$^3K_6$	12199		
$5f^36d$	$^3I_5$	6782	7959	7288	-86	$5f^36d$	$5f^26d^2$	$^3K_6$	16104		
$5f^37s$	$^3I_5^b$	8641	8130	8816	35	$5f^37s\ ^3I$	$5f^4$	$^5H_6$	17293		
$5f^36d$	$^1H_5$	10153	9840	9864	499	$5f^36d\ ^5I$	$5f^4$	$^3H_6$	19353	19417	$5f^26d^2\ ^5L_6$
$5f^36d$	$^3H_5$	12800	12535	13024	-14	$5f^36d\ (5)4$	$5f^4b$	$^3K_6$	22537		
$5f^36d$	$^1H_5^b$	13428	13964	13192	446	$5f^36d\ (5)4$	$5f^4$	$^3I_6$	24340	24539	$5f^26d^2\ 6(7)$
$5f^37s$	$^5H_5$	14708	14769	14669	249	$5f^36d\ (4)5$	$5f^26d^2$	$^1I_6$	25201		
$5f^36d$	$^3G_5$	16085	15310	15008	1287	$5f^36d\ (4)5$	$5f^26d^2$	$^5K_6$	25616		
$5f^36d$	$^5H_5$	18077	16750	17250	1037	$5f^36d\ (4)5$	$5f^4$	$^1I_6$	27243		
$5f^37s$	$^5G_5$	19142	18154	18510	842	$5f^36d\ (5)6$	$5f^26d^2$	$^3I_6$	27548		
$5f^36d$	$^3K_6$	210	210	210	210	$5f^36d\ ^5L_6$	$5f^4$	$^3I_7$	7910		
$5f^36d$	$^5K_6^a$	4734	4670	4940	4	$5f^36d\ ^5K_6$	$5f^4$	$^1K_7$	13687		
$5f^36d$	$^5K_6^b$	7997	7716	7894	313	$5f^36d\ 6$	$5f^4$	$^3L_7$	19008		
$5f^37s$	$^5I_6$	8574	9150	8778	6	$5f^37s\ ^5I_6$	$5f^26d^2$	$^3L_7$	21266		
$5f^36d$	$^1I_6$	12090	12359	12210	90		$5f^4a$	$^5K_7$	21905		
$5f^36d$	$^5I_6^a$	12945	12628	12636	519	$5f^36d\ ^5I$	$5f^26d^2$	$^3K_7$	26182	25507	$5f^26d\ ^5L_7$
$5f^36d$	$^5H_6$	17982	18321	18510	-318	$(5)6$	$5f^26d^2$	$^5K_7$	32810		
$5f^37s$	$^5H_6$	20706	20197	20689	227	$(5)6$	$5f^26d^2$	$^3K_7$	33696	33993	7(6)
$5f^36d$	$^3L_7$	4346	4556	4504	52	$5f^36d\ ^5L_7$					
$5f^36d$	$^3K_7$	8271	8481	8437	44	$5f^36d\ ^5K_7$					
$5f^36d$	$^5I_7^a$	12108	12318	12025	293	$5f^37s\ ^5I_7$					

in most cases for odd states, the deviation was a few 100 cm^{-1} out of 10,000 cm^{-1}, but four levels had the differences exceeding 1,000 cm^{-1}. The experimental data for even states are fairly incomplete; nevertheless, because of large spacing between theoretical levels and established accuracy for the odd states, the comparison can be also done for even levels, confirming the experimental levels. In addition, the CI-LCC calculations provide many missing energy levels. This information can be used for the experimental search of these levels and for the analysis of lifetimes requiring branching ratios data. The deviation from experiment in even states is more or less similar.

Levels with unusually large deviations might need additional theoretical and experimental verification.

The CI-MBPT method requires adjustments of scaling factors in front of Σ_1 and to less extent in front of Σ_2 to approach the accuracy of the LCC approach, with the most important being the adjustment of the s-wave correction of Σ_1, as we have already discussed it. The comparison with CI-MBPT calculations serves two purposes. One is to understand the strength of valence-core interactions needed to estimate theoretical accuracy. Second, it is important to answer the question whether the CI-MBPT method, as much simpler and now available as

TABLE IV: Wavelengths (λ in Å), multipole matrix elements $Z_{\mathrm{M1}}^{\mathrm{CI+LCC}}$, $Z_{\mathrm{E2}}^{\mathrm{CI+LCC}}$, and $Z_{\mathrm{M3}}^{\mathrm{CI+LCC}}$ in a.u. and transition rates A_r^{M1}, A_r^{E2}, and A_r^{M3} (in s^{-1}) evaluated using the CI+LCC approach. The numbers in brackets represent powers of 10.

Conf.	Term	Conf.	Term	λ	$Z_{\mathrm{M1}}^{\mathrm{CI+LCC}}$	$Z_{\mathrm{E2}}^{\mathrm{CI+LCC}}$	$Z_{\mathrm{M3}}^{\mathrm{CI+LCC}}$	A_r^{M1}	$A_r^{\mathrm{E2}}/A_r^{\mathrm{M1}}$	$A_r^{\mathrm{M3}}/A_r^{\mathrm{M1}}$
$5f^4$	$^5G_4^c$	$5f^4$	$^5G_4^d$	55960	0.150	1.347	3.093	3.84[-04]	1.1[-03]	6.7[-18]
$5f^4$	$^5G_4^c$	$5f^4$	$^3G_4^c$	43459	0.029	0.704	0.096	3.03[-05]	1.3[-02]	4.8[-19]
$5f^26d^2$	$^3H_4^a$	$5f^4$	$^3G_4^c$	13305	0.029	0.923	3.570	1.10[-03]	2.3[-01]	7.3[-14]
$5f^4$	$^3F_4$	$5f^4$	$^5G_4^b$	11406	0.011	0.706	10.316	2.37[-04]	1.4[+00]	8.3[-12]
$5f^4$	$^1G_4$	$5f^26d^2$	$^3H_4^a$	11138	0.389	1.023	2.290	3.29[-01]	2.3[-03]	3.5[-16]
$5f^4$	$^3F_4$	$5f^4$	$^5G_4^c$	9626	0.064	0.737	0.921	1.40[-02]	5.8[-02]	3.7[-15]
$5f^4$	$^1G_4$	$5f^4$	$^3G_4^b$	9528	0.088	0.421	0.985	2.68[-02]	1.0[-02]	2.4[-15]
$5f^4$	$^3G_4^a$	$5f^4$	$^3G_4^c$	9173	0.282	0.419	5.538	3.10[-01]	1.1[-03]	8.4[-15]
$5f^4$	$^3F_4$	$5f^26d^2$	$^3H_4^b$	8788	0.055	0.585	1.206	1.36[-02]	6.0[-02]	1.2[-14]
$5f^4$	$^1G_4$	$5f^4$	$^5G_4^b$	7954	0.105	1.266	2.976	6.53[-02]	9.6[-02]	3.1[-14]
$5f^4$	$^3F_4$	$5f^4$	$^3G_4^c$	7881	0.073	0.101	2.499	3.24[-02]	1.3[-03]	4.7[-14]
$5f^4$	$^1G_4$	$5f^4$	$^5G_4^c$	7046	0.061	0.406	0.647	3.22[-02]	3.7[-02]	7.0[-15]
$5f^4$	$^1G_4$	$5f^26d^2$	$^3H_4^b$	6586	0.032	1.212	0.130	1.05[-02]	1.4[+00]	1.4[-15]
$5f^4$	$^1G_4$	$5f^4$	$^5G_4^d$	6258	0.050	0.102	1.702	3.06[-02]	4.4[-03]	1.2[-13]
$5f^4$	$^1G_4$	$5f^4$	$^3G_4^c$	6063	0.068	0.833	3.607	6.28[-02]	1.7[-01]	3.2[-13]
$5f^4$	$^5I_4$	$5f^4$	$^5G_4^a$	5805	0.033	0.729	1.808	1.73[-02]	5.9[-01]	4.0[-13]
$5f^4$	$^5I_4$	$5f^26d^2$	$^3H_4^a$	5746	0.006	1.438	2.485	5.12[-04]	8.1[+01]	2.7[-11]
$5f^4$	$^5I_4$	$5f^4$	$^5G_4^b$	4763	0.047	0.162	1.031	6.04[-02]	2.2[-02]	1.5[-13]
$5f^4$	$^5I_4$	$5f^26d^2$	$^3H_4^b$	4236	0.006	0.268	0.449	1.64[-03]	4.0[+00]	2.4[-12]
$5f^4$	$^5I_4$	$5f^4$	$^3G_4^c$	4013	0.045	0.233	1.257	9.56[-02]	6.8[-02]	4.6[-13]

TABLE V: Excitation energies (cm^{-1}), wavelengths (λ in Å) , dipole matrix elements $Z^{\mathrm{CI+LCC}}$ in a.u., oscillator strengths f in arbitrary units, and transition rates (A_r in s^{-1}) evaluated using the CI+LCC approach. The numbers in brackets represent powers of 10.

Conf.	Term	Conf.	Term	Energies in cm^{-1}			λ	$Z^{\mathrm{CI+LCC}}$	gf	gA_r
Low level		Upper level		Low	Upper	ΔE	Å	a.u.	arbitrary	s^{-1}
$5f^4$	$^5I_4$	$5f^36d$	$^5H_3$	1846	13056	11210	8921	1.90650	0.1238	1.037[7]
$5f^4$	$^5I_6$	$5f^36d$	$^5H_5$	7441	17855	10414	9602	2.17260	0.1493	1.080[7]
$5f^36d$	$^3K_6$	$5f^26d^2$	$^3K_6$	0	17963	17963	5567	1.47800	0.1192	2.565[7]
$5f^36d$	$^3K_6$	$5f^26d^2$	$^5K_5^a$	0	22250	22250	4494	1.47350	0.1467	4.846[7]
$5f^36d$	$^5K_5$	$5f^26d^2$	$^5K_5^a$	553	22250	21697	4609	1.43010	0.1348	4.233[7]
$5f^36d$	$^3L_7$	$5f^26d^2$	$^3L_7$	4124	23126	19002	5263	1.60390	0.1485	3.576[7]
$5f^36d$	$^5K_6^a$	$5f^26d^2$	$^5I_5$	4511	24088	19577	5108	0.85588	0.0436	1.114[7]
$5f^36d$	$^3L_7$	$5f^4$	$^3K_6$	4124	24397	20273	4933	0.76973	0.0365	1.000[7]
$5f^36d$	$^3L_7$	$5f^26d^2$	$^1I_6$	4124	27060	22936	4360	0.89745	0.0561	1.969[7]
$5f^36d$	$^5K_6^a$	$5f^26d^2$	$^1I_6$	4511	27060	22549	4435	0.71342	0.0349	1.182[7]
$5f^36d$	^3L	$5f^26d^2$	$^5K_6$	4124	27476	23352	4282	1.37940	0.1350	4.909[7]
$5f^36d$	$^5K_6^a$	$5f^26d^2$	$^5K_6$	4511	27476	22965	4354	1.01970	0.0725	2.552[7]
$5f^36d$	$^3K_7$	$5f^26d^2$	$^3K_7$	8049	28042	19993	5002	1.00590	0.0614	1.638[7]
$5f^36d$	$^5K_6^b$	$5f^26d^2$	$^1H_5$	7775	28574	20799	4808	1.23680	0.0966	2.789[7]
$5f^36d$	$^3K_7$	$5f^26d^2$	$^3I_7$	8049	31000	22951	4357	0.68950	0.0331	1.165[7]
$5f^36d$	$^3K_7$	$5f^4$	$^5K_7$	8049	31419	23370	4279	0.72833	0.0377	1.372[7]
$5f^36d$	$^3K_7$	$5f^4$	$^5K_7$	8049	31898	23849	4193	0.81787	0.0485	1.838[7]
$5f^36d$	$^5D_1$	$5f^26d^2$	$^5D_1$	9607	33609	24002	4166	0.62427	0.0284	1.092[7]
$5f^36d$	$^5G_2$	$5f^26d^2$	$^3D_1$	9070	37657	28587	3498	0.81754	0.0580	3.164[7]
$5f^36d$	$^3F_2^b$	$5f^26d^2$	$^3D_1$	12855	37657	24802	4032	0.60089	0.0272	1.116[7]

open source software [24], can be used for calculations of actinide properties. Although such calculations require adjustments of correlation corrections, such adjustments improve agreement and simplify identification. The situation is similar to that with the Cowan code; however, in contrast, the number of adjustable parameters is much smaller.

TABLE VI: Lifetimes $\tau^{\mathrm{CI+LCC}}$ (in ms), branching ratio, transition rates A_r (in s^{-1}), and reduced matrix elements $Z^{\mathrm{CI+LCC}}$ (in a.u.) for electric-dipole (E1) and transitions in U^{2+} ion evaluated in the CI+LCC approximation. The numbers in brackets represent powers of 10.

Conf. Level	Term	Conf. Lower level	Term	Conf. Upper level	Term	Energies (cm^{-1}) Lower	Upper	λ Å	$Z^{\mathrm{CI+all}}$ a.u.	$A_r^{\mathrm{CI+all}}$ s^{-1}	Branch. ratio	$\tau^{\mathrm{CI+all}}$ msec
$5f^4$	$^5I_6$	$5f^36d$	$^5Ka_6$	$5f^4$	$^5I_6$	4511	7441	34130	0.237	2.19[2]	0.66	3.009
		$5f^36d$	$^5K_5$	$5f^4$	$^5I_6$	553	7441	14518	0.040	8.28[1]	0.25	
$5f^36d$	$^3H_4^b$	$5f^4$	$^5I_4$	$5f^36d$	$^3H_4^b$	1846	8009	16226	1.330	9.32[4]	0.95	0.010
		$5f^4$	$^5I_5^a$	$5f^36d$	$^3H_4^b$	4791	8009	31075	0.770	4.44[3]	0.05	
$5f^37s$	$^3I_5^b$	$5f^4$	$^5I_5^a$	$5f^37s$	$^3I_5^b$	4791	8419	27563	0.130	1.48[2]	0.54	3.650
		$5f^4$	$^5I_4$	$5f^37s$	$^3I_5^b$	1846	8419	15214	0.049	1.26[2]	0.46	
$5f^4$	$^5F_1$	$5f^36d$	$_0$	$5f^4$	$^5F_1$	5165	9682	22139	0.079	3.92[2]	0.76	1.928
		$5f^36d$	$^5G_2$	$5f^4$	$^5F_1$	9070	9682	163399	0.905	1.27[2]	0.24	
$5f^4$	$^3I_7$	$5f^36d$	$^5K_6^b$	$5f^4$	$^3I_7$	7775	9769	50150	0.423	1.91[2]	0.64	3.364
		$5f^36d$	$^3K_7$	$5f^4$	$^3I_7$	8049	9769	58140	0.304	6.35[1]	0.21	
$5f^36d$	$^1H_5$	$5f^4$	$^5I_5^a$	$5f^36d$	$^1H_5$	4791	9931	19455	2.092	1.09[5]	0.86	0.008
		$5f^4$	$^5I_4$	$5f^36d$	$^1H_5$	1846	9931	12369	0.425	1.76[4]	0.14	
$5f^4$	$^1G_4$	$5f^36d$	$^3I_5$	$5f^4$	$^1G_4$	6769	10298	28337	0.736	5.36[3]	0.64	0.120
		$5f^36d$	$^3H_4^a$	$5f^4$	$^1G_4$	6393	10298	25608	0.308	1.27[3]	0.15	
$5f^37s$	$^5F_1$	$5f^4$	$^1D_2^a$	$5f^37s$	$^5F_1$	8591	11074	40274	0.086	7.67[1]	0.88	11.509
		$5f^4$	$^5F_1$	$5f^37s$	$^5F_1$	9682	11074	71839	0.075	1.02[1]	0.12	
$5f^4$	$^3F_3^a$	$5f^36d$	$^3H_4^a$	$5f^4$	$^3F_3^a$	6393	11312	20329	0.408	5.75[3]	0.52	0.090
		$5f^36d$	$^3G_3^a$	$5f^4$	$^3F_3^a$	4081	11312	13829	0.144	2.27[3]	0.21	0.090
		$5f^36d$	$^5H_4$	$5f^4$	$^3F_3^a$	8679	11312	37979	0.617	2.01[3]	0.18	
$5f^36d$	$^1H_5^a$	$5f^4$	$^5I_5^a$	$5f^36d$	$^1H_5^a$	4791	11586	14717	0.520	1.56[4]	0.67	0.043
		$5f^4$	$^5I_4$	$5f^36d$	$^1H_5^a$	1846	11586	10267	0.159	4.32[3]	0.19	
		$5f^4$	$^5I_6$	$5f^36d$	$^1H_5^a$	7441	11586	24125	0.507	3.37[3]	0.14	
$5f^4$	$^3F_2^a$	$5f^36d$	$^3G_3^a$	$5f^4$	$^3F_2^a$	4081	11601	13298	0.334	1.92[4]	0.81	0.042
		$5f^36d$	$^3G_3^b$	$5f^4$	$^3F_2^a$	8886	11601	36832	0.576	2.70[3]	0.11	
		$5f^36d$	$^5G_2$	$5f^4$	$^3F_2^a$	9070	11601	39510	0.478	1.50[3]	0.06	
$5f^37s$	$^1D_2$	$5f^4$	$^1D_2^a$	$5f^37s$	$^1D_2$	8591	11698	32185	0.081	8.02[1]	0.82	10.165
		$5f^4$	$^5F_1$	$5f^37s$	$^1D_2$	9682	11698	49603	0.074	1.82[1]	0.18	
$5f^36d$	$^1I_6$	$5f^4$	$^5I_6$	$5f^36d$	$^1I_6$	7441	11868	22589	0.345	1.61[3]	0.62	0.385
		$5f^4$	$^5I_5^a$	$5f^36d$	$^1I_6$	4791	11868	14130	0.114	7.16[2]	0.28	

B. Multipole matrix elements, transition rates, and lifetimes in Th-like U^{2+}

We evaluated 3024 E1, M2, and E3 matrix elements that included transitions between even-parity states with $J = 0 - J = 7$ and odd-parity states with $J = 0 - J = 7$. As we noted above, we calculated 12 even and odd parity states for each of the $J = 0 - 7$. Therefore, each set of matrix element calculations between J and J' sets includes 144 transitions, with 21 J-J' cases. We also evaluate multipole M1, E2, and M3 matrix elements for 64 transitions inside of even-parity ($5f^4 + 5f^26d^2$) sets of states. Such large number of transitions is needed for the evaluation of lifetimes.

Our CI + LCC results for the multipole matrix elements $Z^{\mathrm{CI+LCC}}$, oscillator strengths f, transition rates A_r, and lifetimes $\tau^{\mathrm{CI+LCC}}$ in Th-like U^{2+} are listed in

Tables IV, V, VI, and VII. Results for the effective multipole operator include random phase approximation (RPA) corrections. The code packages for the calculation of matrix elements and RPA correction to the matrix elements are the same for CI+MBPT and CI+LCC approaches and are described in detail in Ref. [24]. The expected accuracy for strong transitions, evaluated from the accuracy of transition energies, is on the order of 10%. The package has only length form output for the electric dipole transitions, so the difference between length and velocity forms cannot be used for testing the accuracy of the matrix elements.

The multipole A_r^{Ek} (E1, E2, and E3) and multipole A_r^{Mk} (M1, M2, and M3) transition probabilities (s^{-1}) are obtained in terms of matrix elements Z_{Ek} and Z_{Mk} (a.u.), and transition energies ΔE (a.u.) as

TABLE VII: Lifetimes $\tau^{\text{CI+LCC}}$ (in ms) and sum of transition rates $\sum A_r$ (in s^{-1}), for electric-dipole (E1) in U^{2+} ion evaluated in the CI+LCC approximation. The numbers in brackets represent powers of 10.

Conf.	Term	Energies	$\sum A_r^{\text{CI+all}}$	$\tau^{\text{CI+LCC}}$	Conf.	Term	Energies	$\sum A_r^{\text{CI+all}}$	$\tau^{\text{CI+LCC}}$
		Odd-parity states					Even-parity states		
$5f^3 6d$	$^3K_6$	0.0			$5f^4$	$^5I_4$	1846	2.89[+2]	3.46[+0]
$5f^3 6d$	$^5K_6^a$	4511			$5f^4$	$^1G_4$	10298	8.37[+3]	1.20[-1]
$5f^3 6d$	$^5K_6^b$	7775	2.63[+1]	3.81[+1]	$5f^4$	$^3F_4$	14103	4.03[+3]	2.48[-1]
$5f^3 7s$	$^5I_6$	8352	1.39[+0]	7.21[+2]	$5f^4$	$^3G_4^a$	15890	2.32[+4]	4.30[-2]
$5f^3 6d$	$^1I_6$	11868	2.60[+3]	3.85[-1]	$5f^4$	$^5G_4^a$	19102	2.82[+5]	3.55[-3]
$5f^3 6d$	$^5I_6^a$	12723	1.17[+5]	8.54[-3]	$5f^2 6d^2$	$^3H_4^a$	19276	1.61[+6]	6.20[-4]
$5f^3 7s$	$^3I_6$	12943	1.95[+4]	5.12[-2]	$5f^4$	$^3G_4^b$	20792	1.18[+5]	8.49[-3]
$5f^3 6d$	$^5I_6^b$	14589	5.06[+4]	1.98[-2]	$5f^4$	$^5G_4^b$	22870	1.63[+4]	6.15[-2]
$5f^3 6d$	$^3H_6$	14986	7.90[+3]	1.27[-1]	$5f^4$	$^5G_4^c$	24491	9.12[+4]	1.10[-2]
$5f^3 6d$	$^3I_6$	16392	5.97[+4]	1.68[-2]	$5f^2 6d^2$	$^3H_4^b$	25481	2.35[+6]	4.26[-4]
$5f^3 7s$	$^5I_4$	3418	6.06[+0]	1.65[+2]	$5f^4$	$^5Ia_5$	4791	2.74[+2]	3.65[+0]
$5f^3 6d$	$^3H_4^a$	6393	3.96[+4]	2.53[-2]	$5f^4$	$^3G_5^a$	13939	1.23[+4]	8.15[-2]
$5f^3 6d$	$^3H_4^b$	8009	9.77[+4]	1.02[-2]	$5f^4$	$^5G_5$	16779	1.09[+4]	9.17[-2]
$5f^3 6d$	$^5H_4$	8679	3.60[+4]	2.78[-2]	$5f^4$	$^3G_5^b$	18681	3.54[+4]	2.83[-2]
$5f^3 6d$	$^1G_4$	12054	2.37[+3]	4.23[-1]	$5f^4$	$^5Ib_5$	20037	8.11[+4]	1.23[-2]
$5f^3 7s$	$^5H_4$	14551	9.13[+3]	1.10[-1]	$5f^2 6d^2$	$^5K_5^a$	22250	9.04[+6]	1.11[-4]
$5f^3 7s$	$^3F_4$	16235	1.26[+3]	7.92[-1]	$5f^4$	$^5H_5$	23803	5.00[+5]	2.00[-3]
$5f^3 7s$	$^5G_4^a$	18296	6.58[+3]	1.52[-1]	$5f^2 6d^2$	$^5I_5$	24088	2.61[+6]	3.84[-4]
$5f^3 6d$	$^5K_5$	553			$5f^4$	$^5I_6$	7441	3.32[+2]	3.01[+0]
$5f^3 7s$	$^3I_5^a$	4403	3.74[+0]	2.68[+2]	$5f^4$	$^3K_6$	14059	1.75[+4]	5.72[-2]
$5f^3 6d$	$^3I_5$	6769	2.76[+2]	3.62[+0]	$5f^2 6d^2$	$^3K_6$	17963	2.43[+6]	4.11[-4]
$5f^3 7s$	$^3I_5^b$	8419	2.74[+2]	3.65[+0]	$5f^4$	$^5H_6$	19152	4.30[+4]	2.33[-2]
$5f^3 6d$	$^1H_5$	9931	1.28[+5]	7.84[-3]	$5f^4$	$^3H_6$	21212	4.56[+4]	2.19[-2]
$5f^3 6d$	$^1H_5^a$	11586	2.33[+4]	4.29[-2]	$5f^2 6d^2$	$^5I_6$	22974	7.41[+4]	1.35[-2]
$5f^3 6d$	$^3H_5$	12578	1.87[+4]	5.35[-2]	$5f^4 b$	$^3K_6$	24397	2.73[+6]	3.66[-4]
$5f^3 6d$	$^3L_7$	4124			$5f^4$	$^3I_7$	9769	2.97[+2]	3.36[+0]
$5f^3 6d$	$^3K_7$	8049	2.49[+1]	4.02[+1]	$5f^4$	$^1K_7$	15546	1.88[+4]	5.31[-2]
$5f^3 6d$	$^5I_7^a$	11886	7.94[+1]	1.26[+1]	$5f^4$	$^3L_7$	20868	3.36[+4]	2.97[-2]
$5f^3 6d$	$^1K_7$	12571	4.53[+2]	2.21[+0]	$5f^2 6d^2$	$^3L_7$	23126	3.04[+6]	3.30[-4]
$5f^3 6d$	$^5K_7$	13557	9.07[+3]	1.10[-1]	$5f^4 a$	$^5K_7$	23764	8.84[+4]	1.13[-2]

$$A_r^{Ek} = \frac{C^{(k)} [\Delta E]^{2k+1}}{(2J+1)} (Z_{Ek})^2, \ C^{(1)} = 2.14200 \times 10^{10}, \ C^{(2)} = 5.70322 \times 10^4, \ C^{(3)} = 7.71311 \times 10^{-2} \quad (5)$$

$$A_r^{Mk} = \frac{D^{(k)} [\Delta E]^{2k+1}}{(2J+1)} (Z_{Mk})^2, \ D^{(1)} = 2.85161 \times 10^5, \ D^{(2)} = 7.59260 \times 10^{-1}, \ D^{(3)} = 1.02683 \times 10^{-6}.$$

C. Multipole matrix elements and transition rates

In Table IV, we list wavelengths, multipole matrix elements $Z_{\text{M1}}^{\text{CI+LCC}}$, $Z_{\text{E2}}^{\text{CI+LCC}}$, and $Z_{\text{M3}}^{\text{CI+LCC}}$ and transition rates A_r^{M1}, A_r^{E2}, and A_r^{M3} evaluated using the CI+LCC approach. We evaluate 64 transitions between the even-parity states ($5f^4 + 5f^2 6d^2$), but list only 20 transitions in Table IV to save space. The E2/M1 and M3/E1 ratios of transition rates are shown in two last columns of Table IV. The ratios of $A_r^{\text{E2}}/A_r^{\text{M1}}$ are generally small, 10^{-3} - 10^{-2}. However, there are transitions with A_r^{E2} being larger than the A_r^{M1}. The $A_r^{\text{M3}}/A_r^{\text{M1}}$ ratio is much smaller than $A_r^{\text{E2}}/A_r^{\text{M1}}$, as expected, 10^{-19} - 10^{-11}.

In Table V, we list excitation energies, wavelengths, dipole matrix elements $Z^{\text{CI+LCC}}$, oscillator strengths f, and transition rates evaluated using the CI+LCC approach.

In Table V, we present results for 20 transitions among 3024 transitions that we considered. We choose transitions with the largest values of A_r. It should be noted that we evaluated also values of A_r for magnetic quadrupole M2 and electric octupole E3 transitions. We find that $A_r^{\text{M2}}/A_r^{\text{E1}}$ ratio is small, about 10^{-6}. The

TABLE VIII: Energy levels (cm^{-1}), g-factors, and lifetimes (ns) in U^{2+}. Non-relativistic values of g-factors (g_{nr}) are given by Eq. (4). The first column gives the dominant contribution for the configuration. Experimental lifetimes are taken from Ref. [19]. Energy levels are from the experimental compilation of Ref. [12].

| | Level | | g-factors | | Energies | | Conf. | Lifetimes | |
%	Conf.	Level	Present	nr	Present	Expt. [12]	Expt.[12]	Present	Expt [19]
36	$5f^2 6d^2$	$^5H_4$	0.898	0.900	28466	28922	$5f^2 6d^2\ ^5I$	97.5	104±10
45	$5f^4$	$^1G_4$	0.997	1.000	28695			167.	
37	$5f^2 6d7s$	$^5H_4$	0.875	0.900	28957	28773	$5f^2 6d7s\ ^5I$	65.0	
56	$5f^2 6d^2$	$^5H_4$	0.912	0.900	29349			73.0	
34	$5f^2 6d7s$	$^3G_4$	1.056	1.050	29617			307.	
36	$5f^2 6d^2$	$^5H_4$	0.904	0.900	30100	31469	$5f^2 6d^2$	58.6	41±3
62	$5f^2 6d^2$	$^3G_4$	1.074	1.050	30398			212.	
56	$5f^2 6d^2$	$^3G_4$	1.051	1.050	31183			117.	
35	$5f^2 6d7s$	$^5H_4$	0.950	0.900	31417	32020	$5f^2 6d7s$	310.	
38	$5f^2 6d^2$	$^1G_4$	0.993	1.000	31840			226.	
65	$5f^2 6d^2$	$^3G_4$	1.099	1.050	31994			233.	
49	$5f^2 6d^2$	$^3H_5$	1.027	1.033	30170			93.4	
33	$5f^2 6d7s$	$^1H_5$	0.972	1.000	30373			84.7	
38	$5f^2 6d^2$	$^5I_5$	0.960	0.900	31315			51.7	
62	$5f^2 6d^2$	$^1H_5$	1.001	1.000	31821	32511		79.8	
59	$5f^2 6d^2$	$^1H_5$	1.002	1.000	32028	32945	$5f^2 6d^2$	48.0	
32	$5f^2 6d7s$	$^5H_5$	1.077	1.100	32391	33237	$5f^2 6d7s$	162.	150±15
45	$5f^4$	$^1H_5$	0.972	1.000	32602			31.8	
65	$5f^2 6d^2$	$^1H_5$	1.008	1.000	32912	33546		70.2	
28	$5f^2 6d^2$	$^5H_5$	1.115	1.100	33536			34.2	
35	$5f^2 6d^2$	$^3H_5$	1.024	1.033	33876			13.4	
37	$5f^2 6d^2$	$^5H_5$	1.072	1.100	34216	34453		15.6	

A_r^{E3}/A_r^{E1} ratio is extremely small, about 10^{-16}, as expected and we did not include those transitions in Table V and other two tables with results for lifetimes and branching ratios.

D. Branching ratios and lifetimes in U^{2+}

In Table VI, we list lifetimes τ^{CI+LCC}, branching ratios, transition rates A_r, and reduced matrix elements Z^{CI+LCC} for electric-dipole transitions. We evaluate the results for 188 levels in Th-like U^{2+}, which excludes several metastable levels with no contributing E1 transitions, however, we show data in for only 12 levels Table VI for illustration

In order to determine the lifetimes listed in the last column of Table VI, we sum over all possible radiative transitions. The number of contributing transitions increases significantly for higher levels. For example, 8 transitions contribute to the lifetime of the relatively low-lying $5f^4\ ^3F_3$ state, $E(5f^4\ ^3F_3) = 11601$ cm^{-1}. However, only one transition, $5f^3 6d\ ^3G_3 - 5f^4\ ^3F_3$, contributes significantly, and the total contribution of other 7 transitions to the $5f^4\ ^3F_3$ lifetime is equal to 19%. The final values of τ^{CI+all} for 12 lowest-lying levels are listed in the last column of Table VI. The term designation for those levels are in the first column of Table VI.

In Table VII, we present results for other 92 E1 transitions for low-lying levels. In this table, we list lifetimes τ^{CI+LCC} (in ms) and sum of transition rates for 12 states odd-parity and even-parity states with $J = 4$ - 7. The largest value of the lifetime is about 721 ms for $5f^3 7s\ ^5I_6$ level with excitation energy equal to 8352 cm^{-1}. Unfortunately, we did not find any theoretical or experimental results to compare with our A_r and τ values for the low-lying states listed in Table VII.

We find only one work that reported lifetime measurements of U^{2+} [19], with data given for five levels. The corresponding excitation energies for these levels are in the higher range of $29000 - 37000$ cm^{-1}. In order to compare with the lifetimes listed in Ref. [19], we made additional calculation of energies and transition rates using the CI+LCC method with larger configuration sets. We evaluated energies for the 30 even-parity states with $J = 4$ and 5 to reach required higher energy levels. Results of our calculations are presented in Table VIII where we list energies and lifetimes in the interval of energies $28000 - 31000$ cm^{-1} and $30000 - 34000$ cm^{-1} for even-parity states with $J = 4$ and 5, respectively. As a result, we were able to compare our CI+LCC results with three lifetime values given in Ref. [19].

Energies of the levels quoted in Ref. [19] were taken from compilation of Ref. [12]. In order to be sure that our identification of levels in Table VIII is correct, we compare also our CI+LCC results with energies from Ref. [12]. Unfortunately, we found only few results, with missing full terms designation and only J being listed.

The theoretical lifetime 97.5 ns for the the $5f^2 6d^2$ level

with $J = 4$ agrees with experiment 104 ± 10 ns within the experimental precision. The difference in corresponding energies is about 1.5%. The theoretical lifetime for the $5f^2 6d7s$ $^5H_5$ level, 162 ns, also in agreement with the experiment, 150 ± 15 ns, while the difference in energies is larger, 2.5%. No term identification is given in [12] for this level. We find about 30% difference in the lifetime and 4.4% in the energy for the $5f^2 6d^2$ $^5H_4$ level.

In order to obtain these lifetimes, we sum transition rates for 36 odd-parity levels with $J = 3\text{-}5$ and the 36 odd-parity levels with $J = 4\text{-}6$. The branching ratios of the odd-parity states with $J = 3$, 4, and 5 are equal to 19.5%, 12.5%, and 68%, respectively, for the $5f^2 6d^2$ level with $J = 4$ (97.5 ns). For the $5f^2 6d7s$ level with $J = 5$ (162 ns), the branching ratios of the odd-parity states with $J = 4$, 5, and 6 are equal to 12.3%, 42.3%, and 45.5%, respectively.

V. CONCLUSIONS

In this paper, we calculated energy levels, g-factors, transition probabilities and lifetimes for U^{2+} ion. Results for energies and lifetimes are in good agreement with experiment, where available. We compared CI-LCC and CI-2nd-order MBPT calculations. CI-LCC results are in good agreement with experiment without any adjustable parameters, while CI-MBPT after scaling correlation corrections achieves similar agreement, except for even $J = 3$ levels. This paper is focused on CI-LCC calculations, and CI-MPBT results are presented to give an idea of valence-core effects and give an estimate of the theoretical accuracy. Both theoretical methods can be applied to other systems, for example U^+ and neutral U. CI-MPBT has an advantage of simplicity, but requires adjustments of correlation corrections. *Ab initio* CI-LCC method, on the other hand, is more accurate, but this method is more complicated and unlike CI-MBPT [24] its availability is limited.

VI. ACKNOWLEDGEMENTS

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