

Electronic bridge process in $^{229}\text{Th}^+$

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We have studied the effect of atomic electrons on the nuclear transition from the isomeric ^{229m}Th state to the ground ^{229g}Th state in $^{229}\text{Th}^+$ due to the electronic bridge process. The exact value of the nuclear transition frequency is unknown so far; therefore, we have developed a formalism that can be used for any nuclear transition frequency. We have calculated positions of several high-lying even-parity states which are not presented in experimental atomic spectra databases. We have found their energy levels and g factors.

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I. INTRODUCTION

The energy splitting of the ground-state doublet of the ^{229}Th nucleus is only several electron volts [1]. At the same time the exact value of the frequency for the transition from the isomeric ^{229m}Th state to the ground ^{229g}Th state is unknown. Experiments give values of this frequency ω_N ranging from 3.5 ± 1.0 eV [2] to 7.6 ± 0.5 eV [3]. The measurements of the lifetime of the isomeric state performed by different experimental groups lead to values which differ from each other by many orders of magnitude (see, e.g., [4,5]).

As was noted in [6] the nuclear transition from the isomeric state to the ground state is of a great interest since it makes it possible to build a very precise nuclear clock. This transition is very sensitive to hypothetical temporal variation of the fundamental constants [7].

The triply ionized ^{232}Th was recently laser cooled [8]. Further, this experimental group plans to investigate the nuclear transition between the isomeric and the ground state in a cold $^{229}\text{Th}^{3+}$ ion. Another experimental group [9] plans to use the ion $^{229}\text{Th}^+$ to study the nuclear ^{229m}Th – ^{229g}Th transition.

In our previous work [10] we considered the $^{229}\text{Th}^{3+}$ ion and calculated the transition probability of the ^{229}Th nucleus from its lowest energy isomeric state ^{229m}Th to the ground state ^{229g}Th due to the electronic bridge (EB) process. In this paper we consider the more complicated three-valence ion $^{229}\text{Th}^+$. In our approach we do not fix the value of the nuclear transition frequency. Hence, the result obtained here can be applied for any value of ω_N .

The paper is organized as follows. In Sec. II we briefly discuss the general formalism describing the EB process. In Sec. III we describe the method of calculation of the properties of Th^+ . Section IV is devoted to the results of calculations and Sec. V contains concluding remarks. Atomic units ($\hbar = |e| = m_e = 1$ and the speed of light $c = 137$) are used throughout.

II. GENERAL FORMALISM

A derivation of the equation for the probability of the EB process, Γ_{EB} , is given in detail in [10]. For this reason we will repeat here only the main features of the formalism.

The EB process can be represented by the two Feynman diagrams in Fig. 1. In the following we assume that the initial

i and the final f electronic states are of opposite parity and fixed. A real photon which is emitted or absorbed is the electric dipole photon. The EB process can be effectively treated as the electric dipole $i \rightarrow f$ transition of the electron accompanied by the nuclear transition from its isomeric state to the ground state.

Because the exact value of the nuclear transition frequency is unknown we do not fix it in our calculation. Using the experimental data we suggest that most probably the real value of ω_N is between 2 and 8 eV. The general expression for Γ_{EB} we used for calculation of the EB process for $^{229}\text{Th}^{3+}$ can be simplified for $^{229}\text{Th}^+$. This is due to the spectrum of Th^+ being much denser than the spectrum of Th^{3+} . As a result, for any nuclear transition frequency ω_N lying between 2 and 8 eV we can find an atomic transition from the initial state i to the definite intermediate state n whose frequency will be very close to ω_N . Assuming the resonance character of the EB process we arrive at the following expression for Γ_{EB} [10]:

$$\Gamma_{\text{EB}} \approx \frac{4}{9} \left(\frac{\omega}{c} \right)^3 \frac{|\langle I_g || \mathcal{M}_1 || I_m \rangle|^2}{(2I_m + 1)(2J_i + 1)} G_1, \quad (1)$$

where \mathcal{M}_1 is the magnetic dipole nuclear moment and $|I_g\rangle$ and $|I_m\rangle$ are the ground nuclear state and the isomeric nuclear state ($I_g = 5/2^+$, [633] Nilsson state and $I_m = 3/2^+$, [631] Nilsson state); J_i is the electron total angular momentum of the initial state, ω is the real photon frequency determined from the law of conservation of energy as $\omega = \varepsilon_i - \varepsilon_f + \omega_N$ (where ε_k is the atomic energy), and G_1 can be approximated by

$$G_1 \approx \frac{1}{2J_n + 1} \left| \frac{\langle \gamma_f J_f || D || \gamma_n J_n \rangle \langle \gamma_n J_n || \mathcal{T}_1 || \gamma_i J_i \rangle}{\omega_{in} + \omega_N} \right|^2. \quad (2)$$

Here \mathcal{T}_1 is the electronic magnetic-dipole hyperfine coupling operator. The total hyperfine coupling Hamiltonian H_{HFI} may be represented as

$$H_{\text{HFI}} = \sum_{\lambda} \mathcal{M}_1^{\lambda} \mathcal{T}_{1\lambda}. \quad (3)$$

The operator D is the electric dipole moment operator, $\omega_{in} \equiv \varepsilon_i - \varepsilon_n$, and γ_k encapsulates all other electronic quantum numbers. The explicit expressions for the matrix elements of the operators \mathcal{T}_1 and D are given in our paper [10]. If we

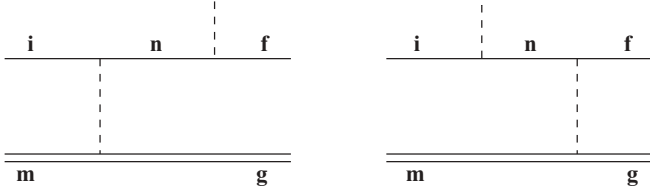


FIG. 1. Feynman diagrams of the EB process. The single and double solid lines relate to the electronic and the nuclear transitions, correspondingly. The dashed line is the photon line.

introduce the quantity

$$R_n \equiv |\langle \gamma_f J_f || D || \gamma_n J_n \rangle \langle \gamma_n J_n || T_1 || \gamma_i J_i \rangle|^2 \quad (4)$$

then Eq. (2) can be rewritten as

$$G_1 \approx \frac{1}{2J_n + 1} \frac{R_n}{(\omega_{in} + \omega_N)^2}. \quad (5)$$

In Eqs. (2)–(5) the electronic state $|\gamma_n J_n\rangle$ is assumed to be fixed. This state should be chosen to meet two conditions: 1. $-\omega_{in} \approx \omega_N$ and 2. if the first condition is fulfilled for two atomic states we should take the state for which R_n is larger. The second condition is important because in certain cases the coefficients R_n for two neighboring energy levels differ by several orders of magnitude.

In Ref. [10] we used the dimensionless quantity β_{M1} defined as the ratio of the probability of the EB process, Γ_{EB} , to the probability of the $M1$ radiative nuclear $m \rightarrow g$ transition, Γ_N :

$$\beta_{M1} = \frac{\Gamma_{EB}}{\Gamma_N} \approx \left(\frac{\omega}{\omega_N} \right)^3 \frac{G_1}{3(2J_i + 1)}. \quad (6)$$

It is reasonable to choose the ground state ($6d^2 7s$) $J = 3/2$ as the initial state i and consider the lowest lying odd-parity state ($5f 7s^2$) $J = 5/2$ as the final state f . Thus, the intermediate atomic states contributing to G_1 are even-parity states and our purpose is to calculate the coefficients R_n for all even-parity states whose transition frequencies to the ground state are between 2 and 8 eV. Then, using Eqs. (5) and (6) we can find the quantities G_1 and β_{M1} , correspondingly, for any ω_N lying between 2 and 8 eV.

III. METHOD OF CALCULATION

We consider Th^+ as the atom with three valence electrons above the closed-shell core $[1s^2, \dots, 6p^6]$. We employ the approach combining the configuration-interaction (CI) method in the valence space with many-body perturbation theory (MBPT) for core polarization effects. In the following we refer to this combined approach as the CI + MBPT method [11].

At the first stage we have solved the Dirac-Hartree-Fock (DHF) equations [12] in the V^{N-3} approximation. This means that the DHF equations were solved self-consistently for the core electrons. After that we determined the $5f$, $6d$, $7p$, $7s$, and $8s$ orbitals from the frozen-core DHF equations. The virtual orbitals were determined with the help of a recurrent procedure [13]. The one-electron basis set included $1s$ – $18s$, $2p$ – $17p$, $3d$ – $16d$, and $4f$ – $15f$ orbitals on the CI stage.

TABLE I. The low-lying energy levels in the range from 18119 to 40644 cm^{-1} (from 2 to 5 eV) in the CI + MBPT approximation, g factors, and the coefficients R_n (in a.u.). Δ is the difference between the energies of the ground state and the excited state. The notation $y[x]$ means $y \times 10^x$. The theoretical values are compared with the experimental data.

| Conf. | J | Δ (Expt.) ^a | Δ (Calc.) | g (Expt.) ^a | g (Calc.) | R_n |
|------------|-----|-------------------------------|------------------|--------------------------|-------------|-------|
| $6d^2 7s$ | 3/2 | 0 | 0 | 0.639 | 0.712 | 9[-2] |
| $6d^3$ | 3/2 | 18 119 | 21 351 | 0.93 | 0.887 | 4[-3] |
| $6d^3$ | 5/2 | 20 159 | 23 731 | 1.19 | 1.198 | 2[-3] |
| $6d^3$ | 5/2 | 22 106 | 26 005 | 0.92 | 0.931 | 3[-3] |
| $6d^3$ | 3/2 | 25 382 | 29 632 | 1.25 | 1.242 | 2[-7] |
| $5f 7s 7p$ | 5/2 | 26 489 | 26 971 | 0.776 | 0.747 | 5[-3] |
| $5f^2 7s$ | 3/2 | 26 762 | 27 561 | 0.4 | 0.480 | 1[-3] |
| $5f^2 7s$ | 5/2 | 27 594 | 28 396 | 0.963 | 0.975 | 1[-6] |
| $5f 7s 7p$ | 3/2 | 27 631 | 28 082 | 0.625 | 0.518 | 3[-2] |
| $6d^3$ | 3/2 | 28 011 | 32 348 | 0.717 | 0.841 | 1[-6] |
| $6d^3$ | 5/2 | 28 026 | 32 764 | 1.13 | 0.975 | 1[-4] |
| $5f 7s 7p$ | 5/2 | 28 824 | 29 367 | 0.987 | 0.993 | 2[-1] |
| $5f^2 7s$ | 5/2 | 29 346 | 30 440 | 0.935 | 0.933 | 1[-5] |
| $5f 6d 7p$ | 5/2 | 31 259 | 31 973 | 0.781 | 0.903 | 2[-3] |
| $5f 7s 7p$ | 5/2 | 31 754 | 32 554 | 0.948 | 0.997 | 4[-3] |
| $5f 6d 7p$ | 3/2 | 32 959 | 34 051 | 0.874 | 0.834 | 2[-4] |
| $5f^2 7s$ | 5/2 | 33 731 | 34 891 | 1.031 | 1.014 | 3[-2] |
| $5f^2 7s$ | 3/2 | 34 019 | 35 306 | 0.823 | 0.910 | 4[-2] |
| $5f^2 7s$ | 5/2 | 34 175 | 35 727 | 0.986 | 1.095 | 1[-2] |
| $5f 7s 7p$ | 5/2 | 34 544 | 34 732 | 1.003 | 0.965 | 2[-2] |
| $5f 7s 7p$ | 3/2 | 35 021 | 35 535 | 1.042 | 1.001 | 2[-3] |
| $5f 6d 7p$ | 5/2 | 35 741 | 37 326 | 0.954 | 0.996 | 8[-3] |
| $5f^2 6d$ | 5/2 | 36 066 | 36 864 | 0.887 | 0.834 | 6[-2] |
| $5f^2 7s$ | 3/2 | 36 329 | 38 069 | 1.615 | 1.636 | 4[-6] |
| $5f 6d 7p$ | 5/2 | 37 465 | 39 615 | 1.048 | 0.958 | 3[-3] |
| $5f^2 7s$ | 3/2 | 37 542 | 38 787 | 1.003 | 0.870 | 1[-2] |
| $5f 7s 7p$ | 3/2 | 37 822 | 39 376 | 1.15 | 0.942 | 1[-2] |
| $5f 7s 7p$ | 5/2 | 37 945 | 38 975 | 0.893 | 0.987 | 3[-2] |
| $5f^2 7s$ | 5/2 | 38 105 | 38 653 | 1.172 | 0.918 | 3[-2] |
| $5f^2 6d$ | 3/2 | 38 372 | 40 194 | 1.200 | 1.295 | 1[-3] |
| $5f 6d 7p$ | 5/2 | 38 729 | 40 305 | 1.255 | 1.177 | 3[-4] |
| $5f^2 7s$ | 3/2 | 38 757 | 40 937 | 0.935 | 0.903 | 2[-4] |
| $5f 6d 7p$ | 3/2 | 38 836 | 39 919 | 1.013 | 1.046 | 2[-4] |
| $5f 6d 7p$ | 5/2 | 38 864 | 40 386 | 0.967 | 1.076 | 4[-6] |
| $5f 6d 7p$ | 3/2 | 39 151 | 40 336 | 0.739 | 0.823 | 4[-3] |
| $5f 7s 7p$ | 5/2 | 39 367 | 40 679 | 1.140 | 1.277 | 7[-3] |
| $5f 6d 7p$ | 5/2 | 39 701 | 41 000 | 1.090 | 1.177 | 2[-3] |
| $5f 6d 7p$ | 5/2 | 40 216 | 41 967 | 1.024 | 0.941 | 2[-3] |
| $5f 7s 7p$ | 3/2 | 40 223 | 41 738 | 0.738 | 0.887 | 7[-4] |
| $5f 7s 7p$ | 3/2 | 40 278 | 41 890 | 0.705 | 0.595 | 7[-4] |
| $5f^2 6d$ | 5/2 | 40 644 | 42 229 | 0.856 | 0.979 | 1[-3] |

^aReference [16].

The configuration spaces for even-parity and odd-parity states were formed as follows. The main configuration of the ground state is $6d^2 7s$. We formed the configuration space for the even-parity states by allowing single, double, and triple excitations from the $6d^2 7s$ configuration to the $7s$ – $13s$, $7p$ – $12p$, $6d$ – $11d$, and $5f$ – $10f$ shells. The main configuration of the lowest lying odd-parity state is $5f 7s^2$. The configuration space for the odd-parity levels was formed by single, double, and triple excitations from the $5f 7s^2$ configuration to the $7s$ – $13s$, $7p$ – $12p$, $6d$ – $11d$, and $5f$ – $10f$ shells. Inclusion of

TABLE II. The low-lying energy levels in the range from 40924 to 64000 cm^{-1} (from 5 to 8 eV) in the CI+MBPT approximation, g factors, and the coefficients R_n (in a.u.). Δ is the difference between the energies of the ground state and the excited state. The notation $y[x]$ means $y \times 10^x$.

| Conf. | J | Δ (Expt.) ^a | Δ (Calc.) | g (Expt.) ^a | g (Calc.) | R_n |
|-------------------|-------|-------------------------------|------------------|--------------------------|-------------|-------|
| $5f6d7p$ | $5/2$ | 40 1924 | 42 449 | 0.988 | 1.063 | 3[-3] |
| $5f6d7p$ | $3/2$ | 40 992 | 42 501 | 1.036 | 1.037 | 3[-5] |
| $5f7s7p$ | $5/2$ | 41 328 | 42 747 | 1.101 | 0.957 | 1[-4] |
| $5f^26d$ | $3/2$ | 41 677 | 43 943 | 1.220 | 1.264 | 1[-6] |
| $5f^26d$ | $3/2$ | 41 937 | 43 236 | 1.095 | 1.088 | 1[-4] |
| $5f^26d + 5f6d7p$ | $5/2$ | 42 337 | 44 239 | 1.15 | 1.041 | 7[-4] |
| $5f^26d + 5f6d7p$ | $5/2$ | 42 352 | 44 305 | 1.126 | 1.237 | 5[-4] |
| $5f^26d + 5f6d7p$ | $5/2$ | 43 097 | 44 716 | 0.982 | 0.995 | 2[-3] |
| $5f^26d + 5f6d7p$ | $5/2$ | 43 228 | 44 876 | 1.153 | 1.135 | 1[-6] |
| $5f^26d$ | $3/2$ | 43 245 | 45 161 | 1.08 | 1.107 | 1[-5] |
| $5f^26d + 5f6d7p$ | $5/2$ | 43 772 | 45 900 | 1.04 | 0.985 | 3[-3] |
| $5f6d7p$ | $3/2$ | 43 808 | 45 544 | 1.211 | 1.271 | 1[-5] |
| $5f^26d$ | $3/2$ | 44 301 | 46 287 | 1.342 | 1.357 | 1[-5] |
| $5f^26d + 5f6d7p$ | $5/2$ | 44 389 | 46 283 | 1.158 | 1.087 | 1[-3] |
| $5f^26d + 5f6d7p$ | $5/2$ | 44 553 | 46 775 | 1.182 | 1.224 | 2[-6] |
| $5f^26d$ | $3/2$ | 44 890 | 46 742 | 1.346 | 0.960 | 3[-5] |
| $5f^26d + 5f6d7p$ | $5/2$ | 45 190 | 46 928 | 0.674 | 0.729 | 4[-5] |
| $5f6d7p$ | $3/2$ | 45 306 | 46 994 | 0.6 | 0.910 | 8[-4] |
| $5f^26d + 5f6d7p$ | $5/2$ | 45 611 | 47 310 | 1.075 | 1.076 | 1[-8] |
| $5f^26d + 5f6d7p$ | $5/2$ | 45 800 | 47 877 | 1.3 | 1.249 | 5[-4] |
| $5f6d7p$ | $3/2$ | 46 264 | 47 778 | 0.891 | 0.936 | 2[-3] |
| $5f6d7p$ | $3/2$ | 46 396 | 48 554 | | 1.268 | 1[-4] |
| $5f^26d + 5f6d7p$ | $5/2$ | 46 581 | 48 439 | 1.018 | 1.058 | 2[-3] |
| $5f^26d + 5f6d7p$ | $5/2$ | 46 603 | 48 616 | 1.112 | 1.135 | 2[-4] |
| $5f^26d + 5f6d7p$ | $5/2$ | 46 903 | 48 835 | 1.143 | 1.147 | 1[-3] |
| $5f^26d$ | $3/2$ | 46 936 | 49 401 | 0.956 | 0.567 | 6[-4] |
| $5f6d7p$ | $3/2$ | 47 149 | 49 137 | 1.09 | 1.316 | 1[-4] |
| $5f^26d + 5f6d7p$ | $5/2$ | 47 324 | 49 355 | 1.189 | 1.231 | 1[-4] |
| $5f^26d$ | $3/2$ | 47 870 | 50 324 | | 0.849 | 4[-4] |
| $5f^26d + 5f6d7p$ | $5/2$ | 48 321 | 50 553 | | 1.155 | 2[-4] |
| $5f^26d + 5f6d7p$ | $5/2$ | 48 492 | 50 633 | | 1.025 | 2[-4] |
| $5f6d7p$ | $3/2$ | 48 690 | 50 924 | 0.922 | 1.079 | 2[-5] |
| $5f^26d$ | $3/2$ | 48 818 | 50 749 | 0.956 | 0.727 | 2[-4] |
| $5f^26d + 5f6d7p$ | $5/2$ | 49 069 | 51 463 | | 1.061 | 4[-7] |
| $5f6d7p$ | $3/2$ | 49 415 | 51 692 | 1.003 | 1.213 | 1[-6] |
| $5f^26d + 5f6d7p$ | $5/2$ | 49 873 | 51 941 | | 1.054 | 5[-4] |
| $5f^26d + 5f6d7p$ | $5/2$ | 50 664 | 52 964 | | 1.207 | 2[-4] |
| $5f6d7p$ | $3/2$ | 50 735 | 52 761 | 1.36 | 1.585 | 1[-7] |
| $5f6d7p$ | $3/2$ | 50 908 | 53 760 | 1.3 | 0.852 | 3[-4] |
| $5f^26d + 5f6d7p$ | $3/2$ | 51 025 | 54 511 | 1.270 | 1.286 | 2[-5] |
| $5f^26d + 5f6d7p$ | $5/2$ | 51 363 | 54 363 | | 1.271 | 3[-4] |
| $5f6d7p$ | $3/2$ | 51 676 | 54 796 | | 1.069 | 3[-4] |
| $5f^26d + 5f6d7p$ | $5/2$ | 51 865 | 54 851 | | 1.031 | 1[-3] |
| $5f^26d + 5f6d7p$ | $5/2$ | 51 936 | 55 511 | | 1.279 | 1[-3] |
| $5f6d7p$ | $3/2$ | 52 307 | 55 562 | | 1.036 | 2[-3] |
| $5f6d7p$ | $3/2$ | 52 736 | 57 665 | | 1.246 | 3[-3] |
| $5f^26d + 5f6d7p$ | $5/2$ | 53 845 | 56 279 | | 1.253 | 1[-4] |
| $5f^26d + 5f6d7p$ | $5/2$ | 54 494 | 57 274 | | 1.198 | 2[-3] |
| $5f6d7p$ | $3/2$ | 54 922 | 58 868 | | 1.102 | 6[-6] |
| $5f6d7p$ | $3/2$ | 56 235 | 59 107 | | 0.884 | 2[-5] |
| $5f^26d + 5f6d7p$ | $5/2$ | 56 391 | 58 037 | | 1.446 | 1[-4] |
| $6d^28s$ | $3/2$ | | 58119 | | 0.645 | 6[-3] |
| $6d^28s$ | $5/2$ | | 58 301 | | 1.073 | 2[-2] |
| $5f^26d + 5f6d7p$ | $5/2$ | | 59 731 | | 0.932 | 1[-1] |
| $6d7s8s$ | $3/2$ | | 59 808 | | 1.092 | 3[-3] |

TABLE II. (*Continued.*)

| Conf. | J | Δ (Expt.) ^a | Δ (Calc.) | g (Expt.) ^a | g (Calc.) | R_n |
|-------------------|-------|-------------------------------|------------------|--------------------------|-------------|-------|
| $5f6d7p$ | $3/2$ | | 60 287 | | 1.167 | 1[-3] |
| $6d7s8s$ | $5/2$ | | 60 416 | | 1.205 | 2[-2] |
| $5f6d7p$ | $5/2$ | | 60 462 | | 1.216 | 1[-3] |
| $6d7s8s$ | $3/2$ | | 61 763 | | 0.784 | 1[-6] |
| $5f^26d$ | $5/2$ | | 61 996 | | 1.183 | 9[-5] |
| $6d^28s$ | $5/2$ | | 62 345 | | 0.937 | 2[-5] |
| $6d7s8s$ | $3/2$ | | 62 927 | | 0.839 | 9[-4] |
| $6d^27d$ | $5/2$ | | 63 308 | | 0.857 | 2[-4] |
| $6d^27d$ | $3/2$ | | 63 381 | | 1.079 | 1[-6] |
| $6d^27d$ | $3/2$ | | 63 729 | | 0.928 | 3[-5] |
| $6d^28s + 6d7s8s$ | $5/2$ | | 63 955 | | 1.065 | 7[-5] |

^aReference [16].

all possible (up to triple) excitations is important, especially for high-lying states. It allows us to take into account most completely the configuration interaction for all considered states.

In the CI+MBPT method, the energies and the wave functions are determined from the eigenvalue equation in the model space of the valence electrons,

$$H_{\text{eff}}(E_p)|\Phi_p\rangle = E_p|\Phi_p\rangle, \quad (7)$$

where the effective Hamiltonian is defined as

$$H_{\text{eff}}(E) = H_{\text{FC}} + \Sigma(E). \quad (8)$$

Here H_{FC} is the relativistic three-electron Hamiltonian in the frozen-core approximation and $\Sigma(E)$ is the energy-dependent core-polarization correction.

Together with the effective Hamiltonian H_{eff} we introduce the effective electric-dipole operator D_{eff} and the operator $(T_1)_{\text{eff}}$ acting in the model space of valence electrons. These operators were obtained within the relativistic random-phase approximation (RPA) [14,15], which describes a shielding of the externally applied electric field by the core electrons. The RPA sequence of diagrams was summed to all orders of the perturbation theory.

To solve the RPA equations and to calculate diagrams for the effective Hamiltonian and the effective operators D and T_1 we used a different basis set. The core orbitals in this basis set are the same as before, but the number of virtual orbitals is much larger. On the whole, it consisted of $1s-22s$, $2p-22p$, $3d-22d$, $4f-22f$, and $5g-16g$ orbitals.

IV. RESULTS AND DISCUSSION

We start the discussion of the results with the following remark: The spectrum of Th^+ is very complicated. As is seen from the experimental data [16], on the one hand, the states belonging to different configurations strongly interact with each other and LS coupling is not valid (even approximately) for this ion. On the other hand, it is not a chaotic system. Respectively, the methods of statistical physics are not applicable. Such an ‘‘intermediate’’ type of coupling makes the calculations of the properties of Th^+ rather difficult.

As we have already mentioned in Sec. II, we consider the following transition: $6d^27s (J = 3/2) \xrightarrow{T_1} n \xrightarrow{E1}$

$5f7s^2 (J = 5/2)$. According to Eqs. (2)–(5) only intermediate states n with $J_n = 3/2$ and $J_n = 5/2$ contribute to the probability of the EB process for this transitions.

In Tables I and II we presented the calculated values of the energy levels with $J_n = 3/2$ and $J_n = 5/2$ and also g factors and the coefficients R_n obtained with use of Eq. (4) for the most interesting frequency range from 2 to 8 eV. In Table I we present the results for the atomic frequencies from 2 to 5 eV and in Table II (which is a continuation of Table I) the data are listed for the frequencies from 5 to 8 eV. The results for the energy levels and g factors were obtained in the CI+MBPT approximation. The values of the coefficients R_n were found in the frame of the CI+MBPT+RPA approach.

As is seen from the tables basically the agreement between the experimental and the calculated energy levels is satisfactory. For the majority of the levels presented in Tables I and II the agreement is at the level of several percent. The largest difference between the experimental and the theoretical values is for the states belonging to the $6d^3$ configuration, where it reaches 15%. At the same time the g factors for these states were reproduced rather well. This means that the configuration interaction was taken into account correctly.

The energy levels with total angular momenta $J = 3/2$ and $J = 5/2$ lying higher than 56391 cm^{-1} are not identified experimentally. In our work we have determined several new high-lying energy levels with $J = 3/2$ and $5/2$. In the first rows of Tables I and II we indicate the configurations that give the largest contributions to these states according to our calculation.

As we have already mentioned the configuration mixture is strong for all states starting from the ground state. Sometimes we were unable to reproduce correctly the configuration interaction. In such cases the theoretical g factors differ from the experimental g factors and, respectively, the accuracy of calculation of R_n for such states is poorer.

As follows from Tables I and II the coefficients R_n change from 10^{-7} to 10^{-1} . This is not surprisingly if we note that the initial state $6d^27s$ and the final state $5f7s^2$ differ from each other by two electrons while T_1 and D are the one-electron operators. For this reason the $i \rightarrow n \rightarrow f$ transition occurs only by the configuration interaction. In a case when the

TABLE III. The nuclear transition frequency ω_N (given in eV and in cm^{-1}) along with the configuration, the total angular momentum J , and the transition frequency with respect to the ground state (ω_{res}) for the resonance state mainly contributing to G_1 , listed with the coefficients R_n (in a.u.), G_1 (in a.u.), and β_{M1} .

| ω_N | | Resonance state | | | | | |
|------------|------------------|-------------------|-------|--|-------|--------|--------------|
| eV | cm^{-1} | Conf. | J | ω_{res} (cm^{-1}) | R_n | G_1 | β_{M1} |
| 3.5 | 28 231 | $5f7s7p$ | $5/2$ | 28 824 | 0.2 | 4570 | 225 |
| 5.5 | 44 363 | $5f^26d + 5f6d7p$ | $5/2$ | 44 389 | 0.001 | 11 880 | 720 |

intermediate state n is characterized by configurations that open two strong one-electron $6d^27s \rightarrow n$ and $n \rightarrow 5f7s^2$ transitions, R_n turn out to be large. Due to the complexity of the energy level spectrum of Th^+ the accuracy of the calculation of the coefficients R_n is not high. We would consider these values as an order-of-magnitude estimate.

To illustrate how the developed formalism works we consider two possible values of the nuclear frequency, $\omega_N = 3.5$ eV [2] and $\omega_N = 5.5$ eV [17], as reported by two experimental groups in the mentioned papers. In Table III we present the values of the relevant quantities.

For $\omega_N = 3.5$ eV $\approx 28\,231$ cm^{-1} the resonance contribution to Γ_{EB} comes from the atomic state $J = 5/2$ at $28\,824$ cm^{-1} belonging to the configuration $5f7s7p$. We chose this state because the transition frequency ω_{res} from this state to the initial state i (the ground state) is close to ω_N and the coefficient R_n is largest. Knowing from Table I the coefficient R_n for this state and using Eqs. (5) and (6) we can easily find the quantities G_1 and β_{M1} for the transition $6d^27s$ ($J = 3/2$) $\xrightarrow{T_1}$ $5f7s7p$ ($J = 5/2$) $\xrightarrow{E1}$ $5f7s^2$ ($J = 5/2$). In a similar way G_1 and β_{M1} can be obtained for $\omega_N = 5.5$ eV.

Comparing the coefficients β_{M1} obtained for $\omega_N = 3.5$ eV and $\omega_N = 5.5$ eV we see that they are of the order of 10^2 – 10^3 . We note that in the case of $\omega_N = 5.5$ eV the difference ($\omega_{\text{res}} - \omega_N$) is only 26 cm^{-1} while $R_n = 0.001$ is rather small. For $\omega_N = 3.5$ eV the difference ($\omega_{\text{res}} - \omega_N$) ~ 600 cm^{-1} but the coefficient $R_n = 0.2$ is two orders of magnitude larger than that for $\omega_N = 3.5$ eV. The latter occurs because the resonance energy level whose frequency is close to $\omega_N = 3.5$ eV belongs to the configuration $5f7s7p$. Hence, there is a strong $5f7s7p$ ($J = 5/2$) $\xrightarrow{E1}$ $5f7s^2$ ($J = 5/2$) transition. Due to an admixture of the configuration $6d^27s$ to the configuration $5f7s7p$ the amplitude of the $6d^27s$ ($J = 3/2$) $\xrightarrow{T_1}$

$5f7s7p$ ($J = 5/2$) transition is not small. As a result, the coefficient R_n is large.

The case of $\omega_N = 7.6$ eV [3] requires special attention. The problem is that the atomic energy levels are not identified experimentally in the region of 7.5 eV and, consequently, we cannot compare the theoretical energy levels with the experimental energy levels. As we previously mentioned, the theoretical accuracy is at the level of several percent. Thus at present we are unable to reliably predict the position of the resonance energy level and, consequently, the coefficient β_{M1} . For this reason experimental investigations and identification of the energy levels in the frequency region ~ 7.5 eV would be very useful. Once these tasks are completed the coefficient β_{M1} can be easily determined.

V. CONCLUSION

To conclude, we have found several high-lying even-parity states with total angular momenta $J = 3/2$ and $J = 5/2$ that are not identified in the atomic spectra database [16]. We have determined the energy levels and the g factors of these states.

We have calculated the coefficients R_n determined by Eq. (4) for the even-parity states lying between 2 and 8 eV. When the nuclear transition frequency ω_N is exactly known and the atomic energy levels are experimentally identified, we can find, using R_n , the coefficients G_1 , β_{M1} , and the probability of the EB process.

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