# Calculation of parity and time invariance violation in the radium atom

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Parity ($P$) and time ($T$) invariance violating effects in the Ra atom are strongly enhanced due to close states of opposite parity, the large nuclear charge $Z$ and the collective nature of $(P,T)$-odd nuclear moments. We have performed calculations of the atomic electric dipole moments (EDM) produced by the electron EDM and the nuclear magnetic quadrupole and Schiff moments. We have also calculated the effects of parity nonconservation produced by the nuclear anapole moment and the weak charge. Our results show that as a rule the values of these effects are much larger than those considered so far in other atoms (enhancement is up to $10^5$ times).

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## I. INTRODUCTION

The lower energy levels of radium corresponding to configurations of different parity have very close energies. This leads to a strong enhancement of the various parity ($P$) and time ($T$) invariance violating effects. In our previous paper [1] we considered the states $7s6d\ ^3D_2$ with $E=13\,993.97$ cm$^{-1}$ and $7s7p\ ^3P_1$ with $E=13\,999.38$ cm$^{-1}$, which are separated by a very small interval of $\sim 5$ cm$^{-1}$ ($\sim 10^{-3}$ eV). Simple estimates showed that the effects of nuclear $P$- and $T$-odd moments such as the magnetic quadrupole moment (MQM), the Schiff moment (SM), and the anapole moment (AM) are many times larger than in all atomic systems considered before. In the present paper we present more accurate calculations of these and other parity and time invariance nonconserving effects in those states of the radium atom where the effects are large. We use a relatively simple *ab initio* approximation to perform the calculations. The approximation is a reasonable compromise between the simplicity of the calculations and the accuracy of the results. It is based on relativistic Hartree-Fock (RHF) and configuration interaction (CI) methods. A minimum number of basis states are used at the CI stage of the calculations. However, important many-body effects, such as polarization of the atomic core by an external field and correlations between core and valence electrons, are included in the calculations of single-electron matrix elements. To control the accuracy of the calculations we also calculated hyperfine-structure intervals and lifetimes of lower states of radium and its lighter analog barium.

Our calculations confirm the estimates done in the previous work [1] and show that the value of most $P$- and $T$-odd effects in radium is much higher than in other atoms considered before. The parity nonconserving (PNC) electric dipole transition $E1$ amplitude between the ground and $^3D_1$ even states is about $E_{PNC}\approx 0.8\times 10^{-9}(Q_W/N)iea_0$, which is 100 times larger than the measured PNC amplitude in cesium [2], about five times larger than the corresponding amplitude in francium [3], and has the same order of magnitude as the PNC amplitude in ytterbium [4]. The enhancement of the electron electric dipole moment (EDM) in the $^3D_1$ state of Ra is about 5400, which is again many times larger than corresponding values for the ground states of Fr (910) and Au (260) [5]. The transition amplitude between the ground and $^3D_2$ even states induced by the nuclear anapole moment is about $10^{-9}ea_0$, which is more than $10^3$ times larger than a similar amplitude in Cs [2]. Also, the EDM of the Ra atom in the $^3D_2$ state induced by the nuclear Schiff and magnetic quadrupole moments is strongly enhanced. This enhancement arises from two sources. First, nuclear SM and MQM moments are strongly enhanced in reflection asymmetric radium nuclei [6,7]. Second, electron matrix element is strongly enhanced due to close states of opposite parity. Both contributions (SM and MQM) are about $10^{-19}\eta e$ cm ($\eta$ is the dimensionless constant of the $(P\text{-},T)$-odd nucleon-nucleon interaction). This is again about $10^5$ times larger than the EDM of the Hg atom which currently gives the best limit on $\eta$ [8]. All this makes radium a very promising candidate for the experimental study of $P$- and $T$-odd forces by means of atomic physics.

## II. METHOD

We use relativistic Hartree-Fock (RHF) and configuration interaction (CI) methods to construct two-electron wave functions of the ground and lower excited states of barium and radium. The calculations start from the RHF method for a closed-shell system corresponding to the ground state configuration ($6s^2$ for Ba and $7s^2$ for Ra). Since $nsnp$ and $ns(n-1)d$ configurations, with $n=6$ for Ba and $n=7$ for Ra, do not correspond to a closed-shell system, we calculate $p$ and $d$ basis states in a model HF potential. For example, to calculate $7p$ and $6d$ states of Ra, we keep all other states frozen, remove the contribution of one $7s$ electron from the direct HF potential and use this potential to calculate the required states. The same procedure applies for Ba. Thus we have five single-electron basis states for the CI calculations $(ns_{1/2},np_{1/2},np_{3/2},(n-1)d_{3/2},(n-1)d_{5/2})$. It turns out, however, that this simple CI approximation significantly overestimates the relative value of spin-orbit intervals for the odd-parity states and underestimates it for the even-parity states. This affects the accuracy of the calculation of $P$- and $T$-odd effects because most of them involve transitions with a change of spin which are sensitive to the value of the relativistic effects. We found that the spin-orbit intervals are sensitive to the screening of the Coulomb interaction be-

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TABLE I. Energies and hyperfine-structure constants of lower excited states of $^{137}$Ba ($I=3/2$ $\mu=0.937\,365$) and $^{213}$Ra ($I=1/2$, $\mu=0.6133$).

| | | Energies ($cm^{-1}$) | | hfs const $A$ (MHz) | |
|---|---|---|---|---|---|
| Atom | State | Calc. | Expt. [17] | Calc. | Expt. [18] |
| Ba | $6s5d\ ^3D_1$ | 9225 | 9034 | −632 | −520.5 |
| | $^3D_2$ | 9346 | 9216 | 357 | 415.9 |
| | $^3D_3$ | 9554 | 9596 | 504 | 456.6 |
| | $^1D_2$ | 12 147 | 11 395 | −26 | −82.18 |
| | $6s6p\ ^3P_0$ | 12 203 | 12 226 | | |
| | $^3P_1$ | 12 577 | 12 637 | 1233 | 1150.59 |
| | $^3P_2$ | 12 464 | 13 514 | 878 | |
| | $^1P_1$ | 18 042 | 18 060 | −48 | −109.2 |
| Ra | $7s7p\ ^3P_0$ | 12 971 | 13 078 | | |
| | $^3P_1$ | 13 926 | 13 999 | 8058 | |
| | $^3P_2$ | 16 660 | 16 689 | 4637 | |
| | $^1P_1$ | 21 033 | 20 716 | −1648 | −2315 |
| | $7s6d\ ^3D_1$ | 13 893 | 13 716 | −4108 | |
| | $^3D_2$ | 14 042 | 13 994 | 1749 | |
| | $^3D_3$ | 14 299 | 14 707 | 2744 | |
| | $^1D_2$ | 17 750 | 17 081 | −320 | |

tween two external electrons (recall that Coulomb integrals contribute to the spin-orbit splitting due to the difference between the single-particle radial wave functions belonging to different components of the single-particle doublets). To improve the quality of the wave functions we introduce fitting factors $f_k$ to the Coulomb interaction in the CI calculations ($k$ is the multipolarity of the Coulomb interaction). It was found that multiplying all Coulomb integrals of multipolarities 0, 1, and 2 by factors $f_0=0.7$, $f_1=0.75$, $f_2=0.9$ significantly improves the energies and fine structure intervals of lower odd and even states of barium and radium. These factors simulate the effect of the screening of the Coulomb interaction between valence electrons and core electrons. They also compensate to some extent the effect of the incompleteness of the basis set.

To calculate values other than energy, such as the effect of electron interaction with photons and nuclear $P$- and $T$-odd fields, we also include core polarization effects [direct and exchange random-phase approximation (RPA)-type corrections] and core-valence correlation effects (the Brueckner-type correlation corrections). These two effects are very important for the considered states of radium. Indeed, consider mixture of the $^3D_J$ and $^3P_{J'}$ states by the $P$- and $T$-odd interaction $W$. Corresponding dominant configurations

TABLE II. Single-electron matrix elements of the $P$- and $T$-odd interactions for radium (presented reduced matrix elements of an electron part of the Hamiltonian as specified in the table; see Appendix for details). All values are in atomic units.

| | Approximation | | Even or |
|---|---|---|---|
| Matrix element | RHF[a] | RHF+RPA+$\Sigma$[b] | odd[c] |
| | Spin-independent PNC interaction, $H=\rho(r)\gamma_5$ | | |
| $\langle 7s_{1/2}\|H\|7p_{1/2}\rangle$ | −2769 | −3832 | odd |
| $\langle 7p_{3/2}\|H\|6d_{3/2}\rangle$ | 0.004 | −146.8 | odd |
| | Nuclear anapole moment, $H=\vec{\alpha}\rho(r)$ | | |
| $\langle 7s_{1/2}\|H\|7p_{1/2}\rangle$ | −503 | −577 | odd |
| $\langle 7s_{1/2}\|H\|7p_{3/2}\rangle$ | −0.508 | 20.26 | even |
| $\langle 7p_{1/2}\|H\|6d_{3/2}\rangle$ | −0.024 | −66.29 | even |
| $\langle 7p_{3/2}\|H\|6d_{3/2}\rangle$ | 0.0006 | −29.99 | odd |
| $\langle 7p_{3/2}\|H\|6d_{5/2}\rangle$ | 0 | 11.71 | even |
| | Electron dipole moment, $H=(\beta-1)\boldsymbol{\Sigma}\mathbf{E}$ | | |
| $\langle 7s_{1/2}\|H\|7p_{1/2}\rangle$ | 12.06 | 17.05 | even |
| $\langle 7p_{3/2}\|H\|6d_{3/2}\rangle$ | 0.556 | 2.082 | even |
| | Nuclear Schiff moment, $H=4\pi\boldsymbol{\nabla}\rho(r)$ | | |
| $\langle 7s_{1/2}\|H\|7p_{1/2}\rangle$ | −44 400 | −63 027 | even |
| $\langle 7s_{1/2}\|H\|7p_{3/2}\rangle$ | −32 550 | −56 730 | odd |
| $\langle 7p_{1/2}\|H\|6d_{3/2}\rangle$ | −1497 | 1873 | odd |
| $\langle 7p_{3/2}\|H\|6d_{3/2}\rangle$ | −0.03 | 2767 | even |
| $\langle 7p_{3/2}\|H\|6d_{5/2}\rangle$ | −0.07 | 8163 | even |
| | Nuclear magnetic quadrupole moment, $H=A_{mk}$ | | |
| $\langle 7s_{1/2}\|H\|7p_{3/2}\rangle$ | 17.28 | 25.06 | odd |
| $\langle 7p_{1/2}\|H\|6d_{3/2}\rangle$ | 2.831 | 2.933 | odd |
| $\langle 7p_{1/2}\|H\|6d_{5/2}\rangle$ | −0.2017 | 6.631 | even |
| $\langle 7p_{3/2}\|H\|6d_{5/2}\rangle$ | 0.5389 | 4.011 | odd |

[a]Relativistic Hartree-Fock.

[b]Core polarization and core-valence correlation interaction are included.

[c]Even means that $\langle i\|H\|j\rangle=\langle j\|H\|i\rangle$; odd means that $\langle i\|H\|j\rangle=-\langle j\|H\|i\rangle$.

TABLE III. $E1$-transition amplitudes for Ba and Ra ($|\langle i\|d_z\|j\rangle|a_0$).

| Transition | | Ba | | Ra | |
|---|---|---|---|---|---|
| $i$ | $j$ | Amplitude | Frequency $\epsilon_i-\epsilon_j$ (a.u.) | Amplitude | Frequency $\epsilon_i-\epsilon_j$ (a.u.) |
| $^3P_0$ | $^3D_1$ | 2.3121 | 0.014 73 | 3.0449 | −0.002 904 |
| $^3P_1$ | $^1S_0$ | 0.4537 | 0.057 58 | 1.0337 | 0.063 79 |
| $^3P_1$ | $^3D_1$ | 2.0108 | 0.016 41 | 2.6389 | 0.001 292 |
| $^3P_1$ | $^3D_2$ | 3.4425 | 0.015 59 | 4.4399 | 0.000 0247 |
| $^3P_1$ | $^1D_2$ | 0.1610 | 0.005 66 | 0.0467 | −0.014 04 |
| $^3P_2$ | $^3D_1$ | 0.5275 | 0.020 42 | 0.7166 | 0.013 54 |
| $^3P_2$ | $^3D_2$ | 2.024 | 0.019 59 | 2.7283 | 0.012 28 |
| $^3P_2$ | $^3D_3$ | 4.777 | 0.017 85 | 6.3728 | 0.009 027 |
| $^3P_2$ | $^1D_2$ | 0.1573 | 0.009 66 | 0.1499 | −0.001 790 |
| $^1P_1$ | $^1S_0$ | 5.236 | 0.082 29 | 5.4797 | 0.094 39 |
| $^1P_1$ | $^3D_1$ | 0.1047 | 0.041 13 | 0.4441 | 0.031 89 |
| $^1P_1$ | $^3D_2$ | 0.4827 | 0.040 30 | 1.188 | 0.030 63 |
| $^1P_1$ | $^1D_2$ | 1.047 | 0.030 37 | 2.4053 | 0.016 56 |

($7s6d$ and $7s7p$) can only be mixed by a $\langle 7p|W|6d\rangle$ matrix element. However, this matrix element is extremely small in the Hartree-Fock approximation. This is because the electron interaction with $P$- and $T$-odd nuclear moments is localized in the vicinity of the nucleus where the $d$ electron does not penetrate due to the centrifugal barrier. On the other hand, the polarization of the electron core by these moments produces a long-range correction $\delta V$ to the HF potential which effectively renormalizes the interaction of an external electron with the nucleus. The corresponding matrix element $\langle 7p|W+\delta V|6d\rangle$ is not small even in the case of the $p$-$d$ transition due to the long range of the renormalized interaction $W+\delta V$. Note that $\langle 7s|W|7p\rangle$ matrix elements also contribute to the mixture of the $^3D_J$ and $^3P_{J'}$ states due to the configuration interaction. Thus there is an interference of several factors: the $s$-$p$ matrix elements are large but their contribution is suppressed due to the smallness of the configuration mixing. The $p$-$d$ matrix elements are considerably smaller (although not negligible) but they appear in the dominating configurations. It cannot be said in advance which transitions are more important and as we see from our calculations there are cases when $s$-$p$ transitions dominate over $p$-$d$ and vice-versa (see below). The Bruckner-type correlation corrections (the correlation corrections to the single-electron wave functions) are also important, since they increase the density of an external electron on the nucleus by $\sim$30% (see, e.g., Ref. [9]).

The full scale inclusion of the core polarization and correlation effects into the CI calculations (see, e.g., Ref. [10]) lies beyond the framework of this research. We adopted a simplified approach in which the corresponding corrections are calculated for the single-particle matrix elements. The relative values of the renormalization of the matrix elements by the core polarization and core-valence correlations have been extrapolated from accurate calculations of the core polarization and Bruckner-type correlation corrections for the radium positive ion. $Ra^+$ has a simple electronic structure — one electron above closed shells — and the corresponding procedures are well defined for it [11].

TABLE IV. Single-electron contributions to the two-electron matrix element $\langle ^3P_1\|H\|^3D_2\rangle$. Blank space means no contribution due to selection rules. Zero means very small contribution. Same units as in Table II.

| Transition | $H=-e\mathbf{r}$[a] | $H=\boldsymbol{\alpha}\rho(r)$[b] | $H=4\pi\nabla\rho(r)$[c] | $H=A_{mk}$[d] |
|---|---|---|---|---|
| $7s_{1/2}$-$7p_{1/2}$ | −0.3677 | 58.78 | 6421 | |
| $7p_{1/2}$-$7s_{1/2}$ | 0.0215 | 3.431 | −375 | |
| $7s_{1/2}$-$7p_{3/2}$ | −0.1306 | −0.515 | 1441 | −1.565 |
| $7p_{3/2}$-$7s_{1/2}$ | −0.0585 | 0.230 | 645 | −0.289 |
| $7p_{1/2}$-$6d_{3/2}$ | 0.0020 | 0.029 | −1 | −0.003 |
| $6d_{3/2}$-$7p_{1/2}$ | 3.856 | −54.08 | −1528 | −1.848 |
| $7p_{1/2}$-$6d_{5/2}$ | | | | 0 |
| $6d_{5/2}$-$7p_{1/2}$ | | | | −2.032 |
| $7p_{3/2}$-$6d_{3/2}$ | 0.0004 | 0.006 | −1 | |
| $6d_{3/2}$-$7p_{3/2}$ | −0.2470 | 3.522 | 325 | |
| $7p_{3/2}$-$6d_{5/2}$ | 0 | 0 | 0 | 0 |
| $6d_{5/2}$-$7p_{3/2}$ | 1.364 | 2.442 | −1702 | −0.736 |
| Total | 4.4399 | 13.85 | 5226 | −6.473 |

[a]For $E1$ transition amplitude.
[b]For anapole moment contribution.
[c]For Schiff moment contribution.
[d]For Magnetic quadrupole moment contribution.

To check our method and the accuracy of our results, we calculated the hyperfine-structure (hfs) constants of $^{213}$Ra and $^{137}$Ba. The results for the energies and hfs constants are presented in Table I. One can see that even for this very simple CI approximation the accuracy of the energies and fine structure intervals is very good. The accuracy of the hfs constants is also good for the most important states $^3D_2$ and $^3P_1$. Table II shows the effect of the core polarization (RPA) and Bruckner-type correlations ($\Sigma$) on the single-electron matrix elements. One can see that these effects play a crucial role in the $p$-$d$ matrix elements. However, their contribution to the $s$-$p$ matrix elements is also very important.

## III. PARITY VIOLATION IN $7S^2 \rightarrow 7S6D$ TRANSITIONS

### A. Spin-independent parity nonconservation

The Hamiltonian $H_{PNC}$ of the interaction of an electron with the nuclear weak charge $Q_W$ [formula (A6) in the Appendix] mixes states of the same total momentum $J$ and opposite parity. Thus electric dipole transitions between states of initially equal parity become possible. In particular, the transition between the ground state $^1S_0$ and the excited $^3D_1$ state is enhanced due to the closeness of the opposite parity state $^3P_1$. The dominating contribution to this transition is given by

$$E_{PNC} = \frac{\langle 7s^2\,{}^1S_0|d_z|7s7p\,{}^3P_1\rangle\langle 7s7p\,{}^3P_1|H_{PNC}|7s6d\,{}^3D_1\rangle}{E(^3D_1)-E(^3P_1)}. \quad (1)$$

TABLE V. Parity nonconserving $E1$-transition amplitude induced by nuclear anapole moment.

| $I$ | $F$ | $F'$ | $\langle d_z \rangle$ (units $10^{-10}\kappa_a iea_0$) $^1S_0$-$^3D_1$ | $^1S_0$-$^3D_2$ |
|---|---|---|---|---|
| 0.5 | 0.5 | 1.5 | 2.05 | −20.3 |
| 1.5 | 1.5 | 0.5 | −0.58 | 5.7 |
| | 1.5 | 1.5 | −1.4 | 13.8 |
| | 1.5 | 2.5 | 1.3 | −12.9 |

Apart from the enhancement, there are several suppression factors in Eq. (1). First, the electric dipole matrix element is small because of a change of spin. It is three to five times smaller than most of those amplitudes which do not change atomic spin (see Table III). Second, in the matrix element of the PNC interaction, leading configurations produce only the $p_{3/2}$-$d_{3/2}$ single-electron matrix element which is small. It is not zero mostly due to core polarization. However, it is about 25 times smaller than the $s_{1/2}$-$p_{1/2}$ matrix element. The latter contributes to the PNC amplitude due to configuration mixing. Our calculations show that the contribution of the $s$-$p$ transition to the PNC amplitude is about seven times larger than the contribution of the $p$-$d$ transition. In spite of some suppression, the final answer is quite large:

$$^{225}\mathrm{Ra}: \; E_{PNC} = 0.77 \times 10^{-9} (Q_W/N) iea_0, \tag{2}$$

$$^{223}\mathrm{Ra}: \; E_{PNC} = 0.76 \times 10^{-9} (Q_W/N) iea_0. \tag{3}$$

This is 100 times larger than the measured PNC amplitude in cesium [2] and about five times larger than the corresponding amplitude in francium [3]. Even radium isotopes have close values of the amplitudes (approximately, the effect is proportional to the number of neutrons $N$).

### B. Anapole moment

The Hamiltonian of the electron interaction with the nuclear anapole moment is presented in the Appendix, Eq. (A9). Similar to the spin-independent PNC interaction, it mixes states of opposite parity and leads to nonzero $E1$-transition amplitudes between states of initially equal parity. However, it can also mix states with $\Delta J = 1$ and it depends on the nuclear spin, so that its contribution to transitions between different hyperfine structure components are different. The corresponding expression is very similar to Eq. (1). However, dependence on the hyperfine structure must be included [see formula (A12) in the Appendix for details]. This amplitude is proportional to the $\langle {}^3P_1 \| \vec{\alpha} \rho(r) \| {}^3D_2 \rangle$ matrix element. Contributions of different single-electron transitions into this matrix element are presented in Table IV. Note the strong cancellation between terms corresponding to $s$-$p$ and $p$-$d$ transitions. This means that an accurate inclusion of the core polarization and core-valence correlation effects is very important indeed, as has been discussed above. We believe that the fitting of the energies helps to stabilize this matrix element similar to the case of the $E1$-transition amplitude.

The results for $^1S_0$-$^3D_1$ and $^1S_0$-$^3D_2$ transitions are presented in Table V. Note that the contribution of the anapole moment to the PNC amplitude (3) can be measured by comparing the amplitudes between different hyperfine-structure components similar to what was done for cesium [2]. However, it may be much more efficient to measure the effect of the anapole moment in the $^1S_0$-$^3D_2$ transition because it is about 10 times larger due to the small energy denominator and because the nuclear spin independent PNC interaction does not contribute to this amplitude at all due to the large change of the total electron angular momentum $\Delta J = 2$.

## IV. ATOMIC ELECTRIC DIPOLE MOMENTS

### A. Electron EDM

An electron electric dipole moment interacting with an atomic field mixes states with the same total momentum $J$ and opposite parity. As a result, an atomic EDM appears. The EDM of radium in the $^3D_1$ state is strongly enhanced due to the closeness of the opposite parity state $^3P_1$. In an approximation when only the mixture of the closest states is included, the EDM is given by

$$d = 2 \frac{\langle 7s6d\,{}^3D_1 | -e\mathbf{r} | 7s7p\,{}^3P_1 \rangle \langle 7s7p\,{}^3P_1 | H_{EDM} | 7s6d\,{}^3D_1 \rangle}{E(^3D_1) - E(^3P_1)}. \tag{4}$$

Calculations using formulas from the Appendix give the following result:

$$d = 5370 d_e. \tag{5}$$

Note that a very strong enhancement is caused by the small energy denominator $E(^3D_1) - E(^3P_1) = 0.001\,292$ a.u.

### B. Schiff moment

Electron interaction with the nuclear Schiff moment also produces an atomic EDM. The EDM of Ra caused by the Schiff moment is strongly enhanced in the $^3D_2$ state. Its value is approximately given by

$$d_z = 2 \frac{\langle 7s6d\,{}^3D_2 | d_z | 7s7p\,{}^3P_1 \rangle \langle 7s7p\,{}^3P_1 | H_{SM} | 7s6d\,{}^3D_2 \rangle}{E(^3D_2) - E(^3P_1)}. \tag{6}$$

A more detailed formula which includes the dependence of Eq. (6) on the hyperfine structure is presented in the Appen-

dix, Eq. (A19).

Table IV shows single-electron contributions to the $\langle {}^3P_1\|H_{SM}\|{}^3D_2\rangle$ matrix element. Note that $s$-$p$ transitions strongly dominate here. However, the contribution of the $p$-$d$ transitions is not negligible and should be included for accurate results. Calculated values of the radium EDM induced by the Schiff moment are presented in Table VI.

### C. Magnetic quadrupole moment

Electron interaction with the nuclear MQM can also produce an EDM of an atom. However, in contrast with the case of the Schiff moment, the MQM of isotopes where the nuclear spin $I<1$ (like $^{225}$Ra, where $I=1/2$) is zero. The EDM of Ra in the $^3D_2$ state is given by a formula similar to Eq. (6):

$$d_z = 2\frac{\langle 7s6d\,{}^3D_2|d_z|7s7p\,{}^3P_1\rangle\langle 7s7p\,{}^3P_1|H_{MQM}|7s6d\,{}^3D_2\rangle}{E({}^3D_2)-E({}^3P_1)}. \tag{7}$$

Again, more detailed formula can be found in the Appendix, Eq. (A24).

Table IV shows single-electron contributions to the $\langle {}^3P_1\|A_{mk}\|{}^3D_2\rangle$ matrix element. Note that in contrast to the cases of the Schiff and anapole moments, $p$-$d$ transitions dominate over $s$-$p$ transitions in this matrix element. For the anapole moment these two types of transitions contribute almost equally, while for the Schiff moment $s$-$p$ transitions dominate. Note that $s$-$p$ transitions appear due to configuration mixing only, while contribution of the $p$-$d$ transitions is extremely small if core polarization is not included. This indicates once more that even for a rough estimation of the time or parity invariance violating effects in Ra an inclusion of the appropriate many-body effects is essential. Calculated values of the radium EDM induced by the magnetic quadrupole moment are presented in Table VII.

## V. LIFETIMES

To plan experimental measurements of space and time invariance violation in radium it is important to know the lifetimes of the states of interest. Apart from that, comparison of the calculated and experimental lifetimes can serve as a good test of the method used for calculation of $P$- and $T$-invariance violation since the same dipole transition amplitudes contribute in either case. As far as we know, none of the radium lifetimes have been measured so far. On the other hand, some experimental data is available for barium. Therefore we calculated lifetimes of lower states of both atoms. Results for dipole transition amplitudes are presented in Table III and the corresponding lifetimes are in Table VIII.

For the purpose of the present work, the most important states of radium are $^3P_1$, $^3D_1$, and $^3D_2$ states. The decay rate of the $^3P_1$ state is strongly dominated by the $^3P_1$-$^1S_0$ transition. Transitions to the $^3D_1$ and $^3D_2$ states are suppressed due to small frequencies. The $^3P_1$-$^1S_0$ dipole transition amplitude involves a change of the atomic spin and therefore is sensitive to the value of the relativistic effects. This makes the amplitude numerically unstable. This probably explains the poor agreement between different calculations (see Table VIII). However, we believe that the fitting of the fine structure which we have done for Ba and Ra (see Sec. II) brings the amplitude close to the correct value. This is supported by similar calculations for barium. The $^3P_1$-$^1S_0$ amplitude contributes 38% to the decay rate of the $^3P_1$ state of barium. Good agreement between calculated and experimental lifetimes of this state (see Table VIII) means that all transition amplitudes, including the $^3P_1$-$^1S_0$ amplitude, are calculated quite accurately.

The lifetime of the $^3D_1$ state of Ra is determined by the $^3D_1$-$^3P_0$ transition which is numerically stable. The lifetime of this state calculated by us is in good agreement with the estimations done by Budker and DeMille [12].

The $^3D_2$ state of radium is a metastable state. It decays only via electric quadrupole ($E2$) transition to the ground state. Calculations similar to the electric dipole transitions show that the lifetime of this state in the absence of external

TABLE VI. EDM of Ra atom in the $^3D_2$ state induced by nuclear Schiff moment.

| $I$ | $F$ | $d_z$ (a.u.) | | $d_z(ecm)$ |
|---|---|---|---|---|
| 0.5 | 1.5 | $-0.94\times10^8 S$ | $-0.19\times10^{-11}\eta$ [a] | $-0.36\times10^{-19}\eta$ |
| 1.5 | 0.5 | $-0.16\times10^8 S$ | $-0.42\times10^{-11}\eta$ [b] | $-0.80\times10^{-19}\eta$ |
| 1.5 | 1.5 | $-0.30\times10^9 S$ | $-0.81\times10^{-11}\eta$ [b] | $-0.15\times10^{-18}\eta$ |
| 1.5 | 2.5 | $-0.28\times10^9 S$ | $-0.76\times10^{-11}\eta$ [b] | $-0.14\times10^{-18}\eta$ |

[a]Nuclear Schiff moment $S$ is assumed to be $S=400\times10^8\,\eta e$ fm$^3$ [6].
[b]$S=300\times10^8\,\eta e$ fm$^3$ [6].

TABLE VII. EDM of $^{223}$Ra isotope ($I=3/2$) in the $^3D_2$ state induced by nuclear magnetic quadrupole moment.

| $F$ | $d_z$ [a] | $d_z$ [b] |
|---|---|---|
| 0.5 | $1344Mm_e$ | $7.4\times10^{-20}\eta e$ cm |
| 1.5 | $1292Mm_e$ | $7.0\times10^{-20}\eta e$ cm |
| 2.5 | $-806Mm_e$ | $-4.4\times10^{-20}\eta e$ cm |

[a]In terms of nuclear magnetic quadrupole moment $M$.
[b]$M$ is assumed to be $M=10^{-19}(\eta/m_p)\ e$ cm [7], where $m_p$ is the proton mass.

TABLE VIII. Lifetimes of lower short-living states of Ba and Ra.

| Atom | State | Lower states to decay to via $E1$ transitions | Lifetime | |
|---|---|---|---|---|
| | | | This work | Other data |
| Ba | $^3P_0$ | $^3D_1$ | 2.83 $\mu$s | |
| | $^3P_1$ | $^1S_0, ^3D_1, ^3D_2, ^1D_2$ | 1.37 $\mu$s | 1.2 $\mu$s[a] |
| | $^3P_2$ | $^3D_1, ^3D_2, ^3D_3, ^1D_2$ | 1.41 $\mu$s | |
| | $^1P_1$ | $^1S_0, ^3D_1, ^3D_2, ^1D_2$ | 9.1 ns | 8.5 ns[a] |
| Ra | $^3P_1$ | $^1S_0, ^3D_1, ^3D_2$ | 505 ns | 420 ns,[b] 250 ns[c] |
| | $^3P_2$ | $^3D_1, ^3D_2, ^3D_3$ | 74.6 ns | |
| | $^3D_1$ | $^3P_0$ | 617 $\mu$s | 800 $\mu$s[d] |
| | $^1D_2$ | $^3P_1, ^3P_2$ | 38 ms | |
| | $^1P_1$ | $^1S_0, ^3D_1, ^3D_2, ^1D_2$ | 5.5 ns | |

[a]Reference [19].
[b]Reference [20].
[c]Reference [21].
[d]Estimation, Ref. [12].

fields is about 15 sec. However, measurements of the atomic EDM involve placing the atoms in a strong electric field. It is important to know how the lifetimes of the $^3D_2$ and $^3D_1$ states of Ra are affected by this field. The electric field mixes states of different parity and $\Delta J = 0, \pm 1$. If only an admixture of the nearest state is taken into account, the amplitude which determines the decay rate of a $^3D_J$ state is given by

$$A = \frac{\langle ^1S_0|d_z\mathcal{E}|^3P_1\rangle\langle ^3P_1|d_z|^3D_J\rangle}{E(^3P_1) - E(^3D_J)}. \tag{8}$$

Where $\mathcal{E}$ is the electric field. This leads to the following decay rates:

$$W(^3D_2) = 0.21\mathcal{E}^2, \tag{9}$$

$$W(^3D_1) = 0.25\times 10^{-4}\mathcal{E}^2. \tag{10}$$

For an electric field of 10 kV/cm, the lifetime of the $^3D_2$ state is 30 $\mu$s, while the lifetime of the $^3D_1$ state is 240 ms. This latter result is in good agreement with estimations done by Budker and DeMille [12]. Note that the state $^3D_2$, with maximal or minimal possible projection of the total momentum on the direction of the electric field ($M = \pm 2$), cannot be mixed by this field with the $^3P_1$ state. Therefore its lifetime is much less affected.

## VI. CONCLUSION

The radium atom turns out to be a very promising candidate for the study of time and space invariance violating effects. All such effects considered in this paper are strongly enhanced due to the high value of the nuclear charge $Z$ and the closeness of the opposite parity states of the atom. Moreover, the contribution of different mechanisms to the time and space invariance violating effects can be studied separately if measurements are performed for different states and different isotopes of the radium atom. For example, the atomic EDM induced by the electron EDM is strongly enhanced in the $^3D_1$ state, while contributions of the nuclear Schiff and magnetic quadrupole moments are strongly enhanced in the $^3D_2$ state. On the other hand, the magnetic quadrupole moment is zero for isotopes with nuclear spin $I = 1/2$, like $^{225}$Ra, while the Schiff moment for these isotopes is not zero.

Calculations of the space and time invariance violating effects in radium reveal the importance of relativistic and many-body effects. The accuracy achieved in the present work is probably 20–30%. However, a further improvement in accuracy is possible if such a need arises from the progress in measurements.

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## APPENDIX: WAVE FUNCTIONS AND MATRIX ELEMENTS

### 1. Radium wave functions

Two-electron wave functions of the ground ($^1S_0$) and three excited ($^3P_1$, $^3D_1$, and $^3D_2$) states of radium used in this work for the calculation of space and time invariance violation have the following form:

$$|7s^2\,J=0,\ L=0,\ M=0\rangle=-0.9757|7s_{1/2,-1/2}7s_{1/2,1/2}\rangle-0.1150|7p_{1/2,-1/2}7p_{1/2,1/2}\rangle-0.0752(|7p_{3/2,-3/2}7p_{3/2,3/2}\rangle$$
$$-|7p_{3/2,-1/2}7p_{3/2,1/2}\rangle)+0.0658(|6d_{3/2,-3/2}6d_{3/2,3/2}\rangle-|6d_{3/2,-1/2}6d_{3/2,1/2}\rangle)$$
$$+0.0702(|6d_{5/2,-5/2}6d_{5/2,5/2}\rangle-|6d_{5/2,-3/2}6d_{5/2,3/2}\rangle+|6d_{5/2,-1/2}6d_{5/2,1/2}\rangle), \tag{A1}$$

$$|7s7p\,J=1,\ L=1,\ M=1\rangle=-0.9010|7s_{1/2,1/2}7p_{1/2,1/2}\rangle-0.3537|7s_{1/2,-1/2}7p_{3/2,3/2}\rangle+0.2042|7s_{1/2,1/2}7p_{3/2,1/2}\rangle$$
$$-0.0976|7p_{1/2,-1/2}6d_{3/2,3/2}\rangle+0.0563|7p_{1/2,1/2}6d_{3/2,1/2}\rangle+0.0512|7p_{3/2,-1/2}6d_{3/2,3/2}\rangle$$
$$-0.0591|7p_{3/2,1/2}6d_{3/2,1/2}\rangle+0.0512|7p_{3/2,3/2}6d_{3/2,-1/2}\rangle-0.0018|7p_{3/2,-3/2}6d_{5/2,5/2}\rangle$$
$$+0.0014|7p_{3/2,-1/2}6d_{5/2,3/2}\rangle-0.0010|7p_{3/2,1/2}6d_{5/2,1/2}\rangle+0.0006|7p_{3/2,3/2}6d_{5/2,-1/2}\rangle, \tag{A2}$$

$$|7s6d\,J=1,\ L=2,\ M=1\rangle=-0.8660|7s_{1/2,-1/2}6d_{3/2,3/2}\rangle+0.5000|7s_{1/2,1/2}6d_{3/2,1/2}\rangle+0.0002|6d_{3/2,-3/2}6d_{5/2,5/2}\rangle$$
$$-0.0001|6d_{3/2,-1/2}6d_{5/2,3/2}\rangle+0.0001|6d_{3/2,1/2}6d_{5/2,1/2}\rangle-0.0001|6d_{3/2,3/2}6d_{5/2,-1/2}\rangle$$
$$-0.0021|7p_{1/2,-1/2}7p_{3/2,3/2}\rangle-0.0012|7p_{1/2,1/2}7p_{3/2,1/2}\rangle, \tag{A3}$$

$$|7s6d\,J=2,\ L=2,\ M=2\rangle=-0.8087|7s_{1/2,1/2}6d_{3/2,3/2}\rangle-0.5366|7s_{1/2,-1/2}6d_{5/2,5/2}\rangle+0.2400|7s_{1/2,1/2}6d_{5/2,3/2}\rangle$$
$$-0.0084|6d_{3/2,1/2}6d_{3/2,3/2}\rangle-0.0059|6d_{3/2,-1/2}6d_{5/2,5/2}\rangle+0.0053|6d_{3/2,1/2}6d_{5/2,3/2}\rangle$$
$$-0.0032|6d_{3/2,3/2}6d_{5/2,1/2}\rangle-0.0068|6d_{5/2,-1/2}6d_{5/2,5/2}\rangle+0.0091|6d_{5/2,1/2}6d_{5/2,3/2}\rangle$$
$$+0.0130|7p_{1/2,1/2}7p_{3/2,3/2}\rangle+0.0038|7p_{3/2,1/2}7p_{3/2,3/2}\rangle. \tag{A4}$$

We use the following form for the single-electron wave function:

$$\psi(\mathbf{r})_{jlm}=\frac{1}{r}\begin{pmatrix} f(r)\Omega(\mathbf{r}/r)_{jlm} \\ i\alpha g(r)\tilde{\Omega}(\mathbf{r}/r)_{jlm}\end{pmatrix}. \tag{A5}$$

Here $\alpha=1/137.036$ is the fine structure constant, $\tilde{\Omega}(\mathbf{r}/r)_{jlm}=-(\vec{\sigma}\cdot\mathbf{n})\Omega(\mathbf{r}/r)_{jlm}$.

#### 2. Spin-independent weak interaction

The Hamiltonian of the spin-independent weak interaction of an electron with the nucleus is given by [13]

$$H_{PNC}=-\frac{G}{2\sqrt{2}}\rho(r)Q_W\gamma_5, \tag{A6}$$

where $G=2.222\,55\times10^{-14}$ a.u. is the Fermi constant, $\rho$ is the nuclear density $(\int\rho dV=1)$, $Q_W\approx-N+Z(1-4\sin^2\theta_W)$ is the nuclear weak charge, and $\gamma_5$ is a Pauli matrix. The matrix element of Eq. (A6) with wave functions (A5) has the form

$$\langle j_1l_1m_1|H_{PNC}|j_2l_2m_2\rangle=-i\frac{G}{2\sqrt{2}}Q_WR_{PNC}\delta_{j_1j_2}\delta_{l_1\tilde{l}_2}\delta_{m_1m_2}, \tag{A7}$$

$R_{PNC}=\alpha\int\rho(f_1g_2-g_1f_2)dr$ is the radial integral,

$\tilde{l}=2j-l$.

However, it is often more convenient to express Eq. (A7) in the form

$$\langle j_1l_1m_1|H_{PNC}|j_2l_2m_2\rangle=(-1)^{j_1-m_1}\begin{pmatrix} j_1 & 0 & j_2 \\ -m_1 & 0 & m_2\end{pmatrix}\times(-i)\alpha\frac{G}{2\sqrt{2}}Q_WC_{PNC}R_{PNC}, \tag{A8}$$

$C_{PNC}=\sqrt{2j_1+1}\,\delta_{j_1j_2}\delta_{l_1\tilde{l}_2}$ is the angular coefficient for the reduced matrix element.

#### 3. Anapole moment

The Hamiltonian of the interaction of an electron with the nuclear anapole moment has the form [14]

$$H_{AM}=\frac{G}{\sqrt{2}}\frac{(\mathbf{I}\cdot\vec{\alpha})}{I(I+1)}K\kappa_a\rho(r), \tag{A9}$$

where $I$ is the nuclear spin, $K=(I+\frac{1}{2})(-1)^{I+1/2-l}$, $l$ is the orbital momentum of the outermost nucleon, $\kappa_a$ is a dimensionless constant proportional to the strength of the nucleon-nucleon PNC interaction [15]. The matrix elements of the Hamiltonian (A9) between the many-electron states of the atoms depend on the hyperfine structure (see, e.g., Ref. [22])

$$\langle IJ'F|H_{AM}|IJF\rangle=\frac{G}{\sqrt{2}}\frac{K\kappa_a}{I(I+1)}(-1)^{F+I+J'}\begin{Bmatrix} I & I & 1\\ J & J' & F\end{Bmatrix}\times\sqrt{I(I+1)(2I+1)}\langle J'\|\vec{\alpha}\rho(r)\|J\rangle, \tag{A10}$$

$\mathbf{F}=\mathbf{I}+\mathbf{J}$, where $\mathbf{J}$ is the atomic total momentum.

The electron part of the operator (A9) is $\vec{\alpha}\rho(r)$. Its single-electron matrix elements over states (A5) have a form

$$\langle j_1 l_1 m_1|\vec{\alpha}\rho(r)|j_2 l_2 m_2\rangle=(-1)^{j_1-m_1}\begin{pmatrix} j_1 & 1 & j_2\\ -m_1 & q & m_2\end{pmatrix}\times(C_{1AM}R_{1AM}+C_{2AM}R_{2AM}), \tag{A11}$$

$$C_{1AM}=(-1)^{j_1+l_2+1/2}\sqrt{6(2j_1+1)(2j_2+1)}\begin{Bmatrix} \frac{1}{2} & j_1 & l_2\\ j_2 & \frac{1}{2} & 1\end{Bmatrix}\delta_{\tilde{l}_1 l_2},$$

$$C_{2AM}=(-1)^{j_1+l_1+3/2}\sqrt{6(2j_1+1)(2j_2+1)}\begin{Bmatrix} \frac{1}{2} & j_1 & l_1\\ j_2 & \frac{1}{2} & 1\end{Bmatrix}\delta_{l_1\tilde{l}_2},$$

$$R_{1AM}=-4\pi\alpha\int g_1 f_2 dr,$$

$$R_{2AM}=-4\pi\alpha\int f_1 g_2 dr.$$

The dominating contribution to the $z$ component of the parity nonconserving electric dipole transition amplitude between the $^1S_0$ and $^3D_1$ states of Ra induced by the anapole moment is given by

$$E1_{PV}=(-1)^{F-f}\begin{pmatrix} F & 1 & F'\\ -f & 0 & f\end{pmatrix}(-1)^{4F'+J+J'+2I+1}\times\frac{G}{\sqrt{2}}K\kappa_a\sqrt{\frac{2I+1}{I(I+1)}}\sqrt{(2F+1)(2F'+1)}\times\begin{Bmatrix} J' & I & F'\\ F & 1 & J\end{Bmatrix}\begin{Bmatrix} I & I & 1\\ J & J' & F'\end{Bmatrix}\times\frac{\langle 7s^2\|E1\|7s7p\rangle\langle 7s7p\|\vec{\alpha}\rho(r)\|7s6d\rangle}{E_{7s6d}-E_{7s7p}}. \tag{A12}$$

Here $\mathbf{F}=\mathbf{I}+\mathbf{J}$, $f=\min(F,F')$.

#### 4. Electron EDM

The Hamiltonian of the interaction of the electron EDM $d_e$ with the atomic electric field $\mathbf{E}$ has the form [13]

$$H_{EDM}=-d_e\beta(\mathbf{\Sigma}\cdot\mathbf{E}), \tag{A13}$$

where

$$\beta=\begin{pmatrix} 1 & 0\\ 0 & -1\end{pmatrix},\quad \mathbf{\Sigma}=\begin{pmatrix} \vec{\sigma} & 0\\ 0 & \vec{\sigma}\end{pmatrix},\quad \mathbf{E}=-\boldsymbol{\nabla}V(\mathbf{r}).$$

The atomic EDM induced by Eq. (A13) can be calculated as an average value of the operator of the dipole moment over states mixed by an operator similar to Eq. (A13):

$$H'_{EDM}=-d_e(\beta-1)(\mathbf{\Sigma}\cdot\mathbf{E}). \tag{A14}$$

Its single-electron matrix elements have a form

$$\langle j_1 l_1 m_1|H'_{EDM}|j_2 l_2 m_2\rangle=(-1)^{j_1-m_1}\begin{pmatrix} j_1 & 0 & j_2\\ -m_1 & 0 & m_2\end{pmatrix}d_e C_{EDM}R_{EDM}, \tag{A15}$$

$$C_{EDM}=\sqrt{2j_1+1}\,\delta_{j_1 j_2}\delta_{l_1\tilde{l}_2},$$

$$R_{EDM}=2\alpha^2\int g_1\frac{dV}{dr}g_2 dr.$$

Note that the selection rules and the angular coefficients are the same as for the spin independent weak interaction (A6), while the radial integrals are different.

#### 5. Schiff moment

The Hamiltonian of the interaction of an electron with the nuclear Schiff moment has the form [16]

$$H_{SM}=4\pi\mathbf{S}\cdot\boldsymbol{\nabla}\rho(r), \tag{A16}$$

$\mathbf{S}=S\mathbf{I}/I$, $S$ is Schiff moment. Many-electron matrix elements of Eq. (A16) depend on the hyperfine structure similar to Eq. (A9):

$$\langle IJ'F|H_{SM}|IJF\rangle=(-1)^{F+I+J'}\begin{Bmatrix} I & I & 1\\ J & J' & F\end{Bmatrix}\times S\sqrt{\frac{I(I+1)(2I+1)}{I}}\langle J'\|4\pi\boldsymbol{\nabla}\rho(r)\|J\rangle. \tag{A17}$$

The electron part of the operator (A16) is $4\pi\boldsymbol{\nabla}\rho(r)$. Its single-electron matrix elements over states (A5) have the form

$$\langle j_1 l_1 m_1|4\pi\boldsymbol{\nabla}\rho(r)|j_2 l_2 m_2\rangle = (-1)^{j_1-m_1}\begin{pmatrix} j_1 & 1 & j_2 \\ -m_1 & q & m_2 \end{pmatrix} C_{SM} R_{SM}, \tag{A18}$$

$$C_{SM} = (-1)^{j_2+3/2}\sqrt{(2j_1+1)(2j_2+1)} \times \begin{pmatrix} j_1 & j_2 & 1 \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} \xi(l_1+l_2+1),$$

$$\xi(x) = \begin{cases} 1, & \text{if } x \text{ is even} \\ 0, & \text{if } x \text{ is odd} \end{cases},$$

$$R_{SM} = -4\pi \int (f_1 f_2 + \alpha^2 g_1 g_2)\frac{d\rho}{dr} dr.$$

The EDM of Ra induced by the nuclear Schiff moment for a particular hyperfine-structure component of the $^3D_2$ state is approximately given by

$$d_z = 2\begin{pmatrix} F & 1 & F \\ -F & 0 & F \end{pmatrix}(-1)^{2F+2I+J+J'}\begin{Bmatrix} J' & I & F \\ F & 1 & J \end{Bmatrix}\begin{Bmatrix} I & I & 1 \\ J & J' & F \end{Bmatrix}\sqrt{\frac{(I+1)(2I+1)}{I}}(2F+1) \times S\frac{\langle 7s6d\,^3D_J\|E1\|7s7p\,^3P_{J'}\rangle\langle 7s7p\,^3P_{J'}\|4\pi\boldsymbol{\nabla}\rho(r)\|7s6d\,^3D_J\rangle}{E_{7s6d}-E_{7s7p}}. \tag{A19}$$

**6. Magnetic quadrupole moment**

The Hamiltonian of the interaction of an electron with the nuclear magnetic quadrupole moment has the form [16]

$$H_{MQM} = -\frac{M}{4I(2I-1)} t_{mk} A_{mk},$$

$$t_{mk} = I_m I_k + I_k I_m - \frac{2}{3}\delta_{km} I(I+1), \tag{A20}$$

$$A_{mk} = \epsilon_{nim}\alpha_n \partial_i \partial_k \frac{1}{r}.$$

Its many-electron matrix element is

$$\langle IJ'F|H_{MQM}|IJF\rangle = \frac{3M}{8I(2I-1)}\sqrt{5(2F+1)(2I+3)(I+1)(2I+1)I(2I-1)}\begin{Bmatrix} 2 & 2 & 0 \\ J' & I & F \\ J & I & F \end{Bmatrix}\langle J'\|A_{mk}\|J\rangle. \tag{A21}$$

The single-electron matrix elements of the operator $A_{mk}$ have the form

$$\langle j_1 l_1 m_1|A_{mk}|j_2 l_2 m_2\rangle = (-1)^{j_1-m_1}\begin{pmatrix} j_1 & 2 & j_2 \\ -m_1 & q & m_2 \end{pmatrix} \times (C_{1MQM}+C_{2MQM})R_{MQM}, \tag{A22}$$

$$C_{1MQM} = (-1)^{j_2-1/2}\frac{4}{3}\sqrt{(2j_1+1)(2j_2+1)} \times \begin{pmatrix} j_1 & j_2 & 2 \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} \xi(l_1+l_2+1),$$

$$C_{2MQM} = (-1)^{j_1+j_2+l_2+1} 4 \times \sqrt{5(2j_1+1)(2j_2+1)(2l_1+1)(2l_2+1)} \times \begin{pmatrix} l_1 & 1 & l_2 \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} 1 & l_1 & l_2 \\ 2 & j_1 & j_2 \\ 1 & \frac{1}{2} & \frac{1}{2} \end{Bmatrix},$$

$$R_{MQM} = \alpha \int F(r)(g_1 f_2 + f_1 g_2) dr,$$

where

$$F(r)=\begin{cases} r/r_N^4, & \text{if } r\leqslant r_N \\ 1/r^3, & \text{if } r>r_N \end{cases},$$

$r_N$ – nuclear radius.

The EDM of Ra induced by the nuclear MQM for a particular hyperfine-structure component of the $^3D_J$ state is approximately given by

$$d_z=2\begin{pmatrix} F & 1 & F \\ -F & 0 & F \end{pmatrix}(-1)^{F+I+J}(2F+1)^{3/2}\frac{3\sqrt{5}}{4}M\sqrt{\frac{(2I+3)(I+1)(2I+1)}{I(2I-1)}}\begin{Bmatrix} J' & I & F \\ F & 1 & J \end{Bmatrix}$$
$$\times\begin{Bmatrix} 2 & 2 & 0 \\ J & I & F \\ J' & I & F \end{Bmatrix}\frac{\langle 7s6d\,^3D_J\|E1\|7s7p\,^3P_{J'}\rangle\langle 7s7p\,^3P_{J'}\|A_{mk}\|7s6d\,^3D_J\rangle}{E_{7s6d}-E_{7s7p}}. \tag{A23}$$

For the case of the EDM in the $^3D_2$ state, $J'=1$, $J=2$ in Eq. (A23).


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