Polarizabilities and tune-out wavelengths of the hyperfine ground states of ^{87,85}Rb

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The static and dynamic polarizabilities and the tune-out wavelengths of the ground state of Rb and the hyperfine ground states of ^{87,85}Rb have been calculated by using the relativistic configuration interaction plus core polarization (RCICP) approach. It is found that the first primary tune-out wavelengths of the $5s_{1/2}, F = 1,2$ states of ^{87}Rb are 790.018187(193) and 790.032602(193) nm, respectively, where the calculated result for the $5s_{1/2}, F = 2$ state is in good agreement with the latest high-precision measurement 790.032388(32) nm [R. H. Leonard *et al.*, Phys. Rev. A **92**, 052501 (2015)]. Similarly, the first primary tune-out wavelengths of the $5s_{1/2}, F = 2,3$ states of ^{85}Rb are 790.023515(218) and 790.029918(218) nm, respectively. Furthermore, the tune-out wavelengths for the different magnetic sublevels M_F of each hyperfine level F are also determined by considering the contributions of tensor polarizabilities.

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I. INTRODUCTION

If an atom is placed in an ac electromagnetic field, the energy shift due to the Stark effect can be written as

$$\Delta E \approx -\tfrac{1}{2}\alpha_d(\omega)F^2 + \cdots, \tag{1}$$

where $\alpha_d(\omega)$ is the dynamic dipole polarizability of the quantum state at frequency ω and F is the strength of the ac electromagnetic field. When the frequency ω is zero, $\alpha(0)$ is called static polarizability. When the frequency ω tends to a certain value, the dynamic polarizability goes to zero, and the corresponding wavelength is called the tune-out wavelength.

With the recent development of atomic manipulation and measurement in experimental optical traps, studies on the polarizabilities of atoms and ions have been of great interest. The knowledge of static polarizabilities can be used to evaluate the Stark effect [1] and the blackbody-radiation (BBR) shift [2], which are very important for determining the uncertainty of the atomic clock [3–5].

The tune-out wavelength was initially introduced by LeBlanc and Thywissen [6], and they discussed its application in multispecies atom traps. The atom trapped in the optical lattice is released, while the other atoms are still strongly trapped when the wavelength of the trapping laser is equal to the tune-out wavelength of the atom. In addition, high-precision measurement of the tune-out wavelength can be used to test atomic structure calculations [7]. Up to now, the tune-out wavelengths of Rb [8–10], K [7], and metastable states of He [11] have been measured in experiment. The longest tune-out wavelength of the ground state of K is measured with an uncertainty of 1.5 pm [7]. This experiment provides the most accurate determination of the ratio of the $4s$-$4p_{3/2}$ and $4s$-$4p_{1/2}$ line strengths of K, and the uncertainty is half as much as the theoretical uncertainty [12]. Recently, a tune-out wavelength of the $5s_{1/2}, F = 2$ state of ^{87}Rb was measured with an accuracy of about 30 fm [9] by using a condensate interferometer. This accuracy is better than the precision of other previously measured tune-out wavelengths [7,11,13,14]. The tune-out wavelength of the $5s_{1/2}, F = 1, M_F = 0$ magnetic sublevel of ^{87}Rb has also been measured with subpicometer accuracy by Schmidt *et al.* [8]. These experiments give some very good opportunities for testing the theories.

In this paper, the static and dynamic polarizabilities and tune-out wavelengths of the ground state of Rb and the hyperfine ground states of ^{87,85}Rb have been calculated by using the relativistic configuration interaction plus core polarization (RCICP) approach. First, the wave functions, energies, and transition matrix elements of the fine structure of Rb are computed. Then, combining the most accurate $5s$-$5p_J$ and $5s$-$6p_J$ matrix elements [9,14] with the RCICP results, the static and dynamic polarizabilities and three tune-out wavelengths of the $5s_{1/2}$ state are determined. Finally, after considering the hyperfine splittings, the dipole matrix elements between the hyperfine states, the static and dynamic polarizabilities, and the tune-out wavelengths of the hyperfine ground states of ^{87,85}Rb are also determined. In Sec. II, a brief description of the theoretical method is presented. In Secs. III and IV, the energies, matrix elements, static and dynamic polarizabilities, and tune-out wavelengths of the fine- and hyperfine-structure states are computed. In Sec. V, a few conclusions are pointed out. The units used in the present calculations are atomic units, in which the mass of an electron m_e and $\hbar$ have a numerical value of 1 and the speed of light is 137.0359991.

II. FORMULATION AND CALCULATIONS

The RCICP method is used in the present calculations. The details of the calculation method are similar to those reported in [15,16]. The starting point is the Dirac-Fock (DF) calculation for the Rb^+ ground state. The single-electron orbitals of the core are made up of the linear combinations of some analytical S-spinor basis functions, which were introduced by Grant and Quiney [17,18]. S spinors can be treated as relativistic generalizations of the Slater-type orbitals.

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TABLE I. The cutoff parameters $\rho_{\ell,j}$ of the polarization potential of Rb^+.

ℓ	J	$\rho_{\ell,j}$ (a.u.)
s	1/2	2.4254
p	1/2	2.3448
	3/2	2.3450
d	3/2	2.8047
	5/2	2.8222

The effective interaction potential of the valence electron with the core is written as

$$H = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta c^2 + V_{\rm core}(\boldsymbol{r}), \tag{2}$$

where $\boldsymbol{\alpha}$ and β are 4×4 matrices of the Dirac operator, $\boldsymbol{p}$ is the momentum operator, and c is the speed of light [18]. The core operator is

$$V_{\rm core}(\boldsymbol{r}) = -\frac{Z}{r} + V_{\rm dir}(\boldsymbol{r}) + V_{\rm exc}(\boldsymbol{r}) + V_p(\boldsymbol{r}). \tag{3}$$

The direct interaction $V_{\rm dir}(\boldsymbol{r})$ and exchange interaction $V_{\rm exc}(\boldsymbol{r})$ of the valence electron with the DF core are calculated without any approximation. The ℓ, j-dependent polarization potential V_p is semiempirical and can be written as

$$V_p(r) = -\sum_{k=1}^{3}\frac{\alpha_{\rm core}^{(k)}}{2r^{(2(k+1))}}\sum_{\ell,j} g_{k,\ell,j}^2(r)|\ell,j\rangle\langle\ell,j|. \tag{4}$$

Here, the factors $\alpha_{\rm core}^{(k)}$ are the static kth-order polarizabilities of the core electrons. In the present calculations, dipole polarizability is 9.076 a.u. [19], quadrupole polarizability is 35.41 a.u. [19], and octupole polarizability is 314 a.u. [20]. $g_{k,\ell,j}^2(r) = 1-\exp(-r^{[2(k+2)]}/\rho_{\ell,j}^{[2(k+2)]})$ is the cutoff function to make the polarization potential finite at the origin. The cutoff parameters $\rho_{\ell,j}$ that can be tuned to redo the energies of the ns,np_J,nd_J states are listed in Table I.

The effective Hamiltonian of the valence electron is diagonalized in a large L-spinor basis. L spinors can be treated as relativistic generalizations of the Laguerre-type orbitals [17,18]. This basis can be enlarged until completeness without any linear dependence problem.

III. RESULTS OF FINE STRUCTURE

A. Energies

Table II gives the present theoretical energy levels for a few low-lying excited states of Rb, which are compared with experimental energies from the National Institute of Standards and Technology (NIST) tabulation [21]. The polarization potential parameters $\rho_{\ell,j}$ are tuned to give the correct experimental energies of $5s, 5p_J, 4d_J$. Hence, the spin-orbit splittings of $5p_J$ and $4d_J$ are the same as experimental values. It is worth noting that the spin-orbit splittings of the $6p_J$,$7p_J$,$5d_J$, and $6d_J$ states are also very close to experimental values. For example, the spin-orbit splittings of $5p_J$ and $6p_J$ states are 0.0010825 and 0.0003536 hartree in theory, which are in good agreement with the experimental values of 0.0010826 and 0.0003532 hartree. The spin-orbit splittings of $4d_J$ and $5d_J$ states are 0.0000023 and 0.0000131 hartree in theory, which are also consistent with the experimental values of 0.0000020 and 0.0000135 hartree.

TABLE II. Theoretical and experimental energy levels (in hartrees) for a few low-lying excited states of Rb. The energies are given relative to the energy of the Rb^+ core. The experimental data come from the National Institute of Standards and Technology (NIST) tabulation [21].

State	J	Present	Experiment
$5s$	1/2	−0.1535067	−0.1535066
$5p$	1/2	−0.0961927	−0.0961927
	3/2	−0.0951102	−0.0951101
$4d$	5/2	−0.0653180	−0.0653178
	3/2	−0.0653157	−0.0653158
$6s$	1/2	−0.0616926	−0.0617762
$6p$	1/2	−0.0454285	−0.0454528
	3/2	−0.0450749	−0.0450996
$5d$	3/2	−0.0363087	−0.0364064
	5/2	−0.0362956	−0.0363929
$7s$	1/2	−0.0335803	−0.0336229
$4f$	7/2	−0.0314334	−0.0314329
	5/2	−0.0314333	−0.0314328
$7p$	1/2	−0.0266661	−0.0266809
	3/2	−0.0265057	−0.0265211
$6d$	3/2	−0.0227249	−0.0227985
	5/2	−0.0227150	−0.0227881
$8s$	1/2	−0.0211350	−0.0211596
$5f$	7/2	−0.0201079	−0.0201073
	5/2	−0.0201077	−0.0201072
$5g$	7/2	−0.0200232	−0.0200233
	9/2	−0.0200232	−0.0200233

B. Dipole matrix elements

Table III gives the reduced electric dipole ($E1$) matrix elements for a number of low-lying excited-state transitions of Rb. The matrix elements are calculated with a modified transition operator [30–32],

$$\boldsymbol{r} = \boldsymbol{r} - \left[1-\exp\left(\frac{-r^6}{\rho^6}\right)\right]^{1/2}\frac{\alpha_d \boldsymbol{r}}{r^3}. \tag{5}$$

The cutoff parameter ρ used in Eq. (5) is 2.5279 a.u., which is the average of the s, p, and d cutoff parameters (note the weighting of s is doubled to give it the same weighting as the two p and d orbitals). The present RCICP calculations are compared with the relativistic many-body perturbation theory all-order method (RMBPT all-order) [22,23] and the relativistic coupled cluster with single, double, and triple excitations (RCCSDT) calculations [24]. For the $5s$-$5p_J$ transitions, the differences among the present RCICP, RMBPT all-order, and RCCSDT theoretical results are not larger than 1%. The present RCICP results have good agreement with the average values of experiments [27–29] and the results of Leonard *et al.* [9]. For the $5s$-$6p_J$ transitions, the present RCICP results agree with some available results [14,23,24] very well, and the experimental values lie in the middle of the present RCICP results and other theoretical results.

TABLE III. Comparison of reduced electric dipole ($E1$) matrix elements (in a.u.) for the principal transitions of Rb with experimental results and other theoretical calculations.

Transition	RCICP	RMBPT all-order [22,23]	RCCSDT [24]	RCCSD [25]	Expt.
$5s$-$5p_{1/2}$	4.221(21)	4.253(34)	4.26(3)	4.26115	4.233(2)[a]
					4.2339(16) [9]
$5s$-$5p_{3/2}$	5.962(30)	6.003(48)	6.02(5)	6.01328	5.978(4)[a]
					5.9760(23) [9]
$5s$-$6p_{1/2}$	0.313(4)	0.333	0.342(2)		0.3235(9) [14]
$5s$-$6p_{3/2}$	0.513(5)	0.541	0.553(3)		0.5230(8) [14]
$6s$-$5p_{1/2}$	4.150(12)	4.145(10)	4.1187	4.144(3)	
$6s$-$5p_{3/2}$	6.052(17)	6.047(13)	6.0145	6.048(5)	
$6s$-$6p_{1/2}$	9.723(17)	9.721(24)	9.6839		
$6s$-$6p_{3/2}$	13.660(25)	13.647(34)	13.5918		
$4d_{3/2}$-$5p_{1/2}$	8.028(40)	8.037(43)	7.9802	8.07(2)	
$4d_{3/2}$-$5p_{3/2}$	3.625(18)	3.628(20)	3.6029	3.65(2)	
$4d_{3/2}$-$6p_{1/2}$	5.2257(87)	4.717			
$4d_{3/2}$-$6p_{3/2}$	2.2810(40)	2.055			
$4d_{5/2}$-$5p_{3/2}$	10.880(54)	10.889(58)	10.8149	10.96(4)	
$4d_{5/2}$-$6p_{3/2}$	6.846(12)	6.184			
$5d_{3/2}$-$5p_{1/2}$	1.297(56)	1.616	1.184(3)		
$5d_{3/2}$-$5p_{3/2}$	0.640(26)	0.787	0.59(2)		
$5d_{3/2}$-$6p_{1/2}$	18.209(98)	18.195(87)	18.1341		
$5d_{3/2}$-$6p_{3/2}$	8.2131(56)	8.205(27)	8.1778		
$5d_{5/2}$-$5p_{3/2}$	1.909(77)	2.334	1.76(3)		2.290(42) [26]
$5d_{5/2}$-$6p_{3/2}$	24.645(16)	24.621(80)	24.5410		
$4d_{3/2}$-$5f_{5/2}$	4.630(96)	4.614(39)	4.5951		
$4d_{5/2}$-$5f_{5/2}$	1.238(26)	1.234(10)	1.2287		
$4d_{5/2}$-$5f_{7/2}$	5.54(18)	5.518(45)	5.4948		
$5d_{3/2}$-$4f_{5/2}$	25.382(11)	25.357(56)	25.3138		
$5d_{5/2}$-$4f_{5/2}$	6.786(68)	6.779(14)	6.7677		
$5d_{5/2}$-$4f_{7/2}$	30.35(51)	30.316(64)	30.2657		
$\frac{\lvert\langle 5p_{3/2}\lvert\lvert D\rvert\rvert 5s_{1/2}\rangle\rvert^2}{\lvert\langle 5p_{1/2}\lvert\lvert D\rvert\rvert 5s_{1/2}\rangle\rvert^2}$	1.994(40)	1.992(65)	1.997(62)	1.99145	1.995(3)[a]
					1.99221(3) [9]

[a]These values are the average of several experiments [27–29] and are given by Leonard *et al.* [9].

The ratio of the line strengths, which are the square of electric dipole matrix elements of the $5s$-$5p_{1/2}$ and $5s$-$5p_{3/2}$ transitions, is also given in Table III. This ratio should exactly be 2.0 in the nonrelativistic limit. The deviation of this ratio comes from the slight differences of radial wave functions for the spin-orbit doublet arising from the small differences of energies [33]. The present RCICP ratio 1.994(40) is in excellent agreement with the average experimental value of 1.995(3), larger than the latest experimental ratio of 1.99221(3) which has been determined by the measurement of the tune-out wavelength and the experimental matrix element of $5s$-$5p_{1/2}$ of 4.233 [9]. So far none of the theoretical results are within the latest experimental error bar, but the RMBPT all-order result is the closest to this latest experimental ratio.

C. Polarizabilities of the ground state

The static scalar polarizability is written as

$$\alpha^{(k)}(0) = \sum_n \frac{f_{ni}^{(k)}}{\varepsilon_{ni}^2}, \tag{6}$$

where $f_{ni}^{(k)}$ is the oscillator strength and ε_{ni} is the excitation energy of the transition. The oscillator strength is defined as

$$f_{ni}^{(k)} = \frac{2|\langle L_i J_i \| r^k C^k(r) \| L_n J_n\rangle|^2 \varepsilon_{ni}}{(2k+1)(2J_n+1)}. \tag{7}$$

Table IV gives the present and some available theoretical and experimental dipole, quadrupole, and octupole polarizabilities of the $5s_{1/2}$ state of Rb. It is found that the

TABLE IV. The dipole $\alpha^{(1)}$, quadrupole $\alpha^{(2)}$, and octupole $\alpha^{(3)}$ polarizabilities (in a.u.) of the $5s_{1/2}$ state of Rb.

$5s_{1/2}$	$\alpha^{(1)}$	$10^{-3}\alpha^{(2)}$	$10^{-5}\alpha^{(3)}$
Present RCICP	317.05(3.10)	6.479(1)	2.381(44)
DFCP [34]	317.62	6.4810	2.3783
CICP [35]	315.7	6.480	2.378
RCCSD [36]	316.17		
RCCSD [37,38]	318.47/318.3(6)	6.491(18)	
MBPT-SD [39]	317.39		
RMBPT all-order [22,40]	316.4/322(4)	6.525(37)	2.374(16)
RMBPT [20]		6.520(80)	2.37
Expt. E × H [41]	319(6.1)		
Expt. [42]	318.79(1.42)		
Expt. [43]	320.1(6)		

present RCICP results agree with the DiracFock plus core polarization (DFCP) results [34] very well. The DFCP method is the same as the present RCICP method except that DFCP uses the B-spline basis. The RCICP dipole polarizability is larger than that calculated by the nonrelativistic configuration interaction plus core polarization (CICP) [35], RCCSD of Lim *et al.* [36], and the RMBPT all-order method [40] but smaller than the RCCSD result of Kaur *et al.* [37,38], the earlier relativistic many-body perturbation with single, double excitations (MBPT-SD) result [39], and the experimental values [41,42]. If the experimental electric dipole matrix elements of the $5s$-$5p_J$ transitions [9] are used in the calculation of polarizabilities, the static dipole polarizability of the $5s$ state is 318.743 a.u., which agrees with the experimental result [42] very well. So the differences in static dipole polarizabilities between experiments and the present results are mainly from the differences in the $5s$-$5p_J$ matrix elements. The latest experimental value [43], 320.1(6) a.u., is larger than most of the theoretical and other experimental values.

The present quadrupole and octupole polarizabilities of the $5s$ state are close to the results of CICP, RMBPT, RCCSD, and RMBPT all-order. The differences between the present RCICP calculations and other available results [20,22,35,37,38] are not more than 0.6%.

D. Tune-out wavelengths of the ground state

The dynamic dipole polarizabilities computed with the usual oscillator strength sum rules can be written as

$$\alpha^{(1)}(\omega) = \sum_n \frac{f_{ni}^{(1)}}{\varepsilon_{ni}^2 - \omega^2}. \tag{8}$$

The core polarizability is given by a pseudospectral oscillator strength distribution [35]. The distribution is derived from the single-particle energies of the Hartree-Fock core and is listed in Table V. Each separate (n,l) level is identified with one transition with a pseudo-oscillator strength that is equal to the number of electrons in the shell. The excitation energy is set by adding a constant to the Koopman energies and tuning the constant until the core polarizability is equal to the known core polarizability from the oscillator strength sum rules.

Table VI shows the present three tune-out wavelengths of the $5s_{1/2}$ state of Rb, which are compared with the RMBPT calculations and some available experiments. In the present calculations of dynamic polarizabilities, the matrix elements of $5s$-$5p_J$ and $5s$-$6p_J$ transitions are replaced by the most accurate experimental values [9,14]. There are two cases in which the tune-out wavelengths occur. The first case is when the tune-out wavelength exists between $np_{1/2}$ and the $np_{3/2}$ spin-orbit doublet, such as when the 790.02765-nm wavelength lies in the $5s$-$5p_J$ splitting and the 421.07565-nm wavelength lies in the $5s$-$6p_J$ splitting. The present tune-out wavelength, 790.02765 nm, is shorter than the early RMBPT result [12] by 0.007 nm but agrees with the latest RMBPT result, 790.0261(7) nm, very well. There are two experiments [10,13] investigating the longest available tune-out wavelength of the $5s$ state. The experiment of Lamporesi *et al.* [13], 790.018(2) nm agrees with the RMBPT and the present RCICP theoretical results very well. The experiment of Catani *et al.* [10], 789.85(1) nm, has a big difference from the available values [9,12,13] and the present RCICP calculation. The reason for this difference should be because the light is not linearly polarized in this experiment [10]. The present tune-out wavelength near 421 nm agrees with the RMBPT result [12] and the experimental result [14] perfectly. The second case is when the tune-out wavelength occurs when the wavelength is shorter than the $5s$-$np_{3/2}$ transition wavelength and longer than the $5s$-$(n+1)p_{1/2}$ transition wavelength, such as when the 423.02428-nm wavelength lies between $5p_{3/2}$ and $6p_{1/2}$. This tune-out wavelength also has good agreement with the experimental result [14] and the MBPT result [12].

TABLE V. Pseudospectral oscillator strength distribution for Rb^+. Transition energies ε_n are given in atomic units.

n	ε_n	f_n
1	551.524651	2.0
2	75.117766	2.0
3	12.201477	2.0
4	1.592215	2.0
5	67.974337	6.0
6	9.575915	6.0
7	0.878715	6.0
8	4.800593	10.0

TABLE VI. Tune-out wavelengths λ_{zero} (in nm) of the $5s_{1/2}$ state of Rb.

Transition	RCICP	RMBPT	Expt.
$5s$-$5p_{1/2}$	790.02765(20)	790.0261(7) [9] 790.034(7) [12]	789.85(1) [10] 790.018(2) [13]
$5s$-$5p_{3/2}$	423.02428(391)	423.05(8) [12]	423.018(7) [14]
$5s$-$6p_{1/2}$	421.07565(49)	421.08(3) [12]	421.075(2) [14]
$5s$-$6p_{3/2}$			

IV. RESULTS OF HYPERFINE STRUCTURE

A. Energies and reduced matrix elements

According to first-order perturbation theory, the energy for a hyperfine state $|LJIF\rangle$ is given [44,45] by

$$E = E_{NLJ} + W_F, \tag{9}$$

where E_{NLJ} is the energy of the unperturbed fine-structure state and W_F is the hyperfine interaction energy, which can be written as

$$W_F = \frac{1}{2}AR + B\frac{\frac{3}{2}R(R+1) - 2I(I+1)J(J+1)}{2I(2I-1)2J(2J-1)}, \tag{10}$$

where A and B are hyperfine-structure constants and it is usual to give the A and B coefficients in megahertz, where 1.0 MHz $= 1.519829903 \times 10^{-10}$ a.u.

$$R = F(F+1) - I(I+1) - J(J+1). \tag{11}$$

F is the total angular momentum of the hyperfine state, I is the nuclear spin ($I = 3/2$ for ^{87}Rb and $I = 5/2$ for ^{85}Rb), and J is the total angular momentum of the atomic state.

The hyperfine interaction energies of the different hyperfine levels of the $5s_{1/2}$,$5p_J$, and $6p_J$ states of ^{87,85}Rb are listed in

TABLE VII. The hyperfine interaction energies of the hyperfine states of ^{85}Rb and ^{87}Rb. The notation $a[b]$ means $a \times 10^b$. Hyperfine-structure constants are from other studies.

	J	A (MHz)	B (MHz)	F	W_F (a.u.)
		^{87}Rb, $I = 3/2$			
$5s$	1/2	3417.341307 [22]		1	−6.4922[−7]
				2	3.8953[−7]
$5p$	1/2	406.2 [22]		1	−7.7169[−8]
				2	4.6302[−8]
$5p$	3/2	84.845 [22]	12.52 [22]	0	−4.5978[−8]
				1	−3.4986[−8]
				2	−1.1098[−8]
				3	2.9489[−8]
$6p$	1/2	132.565 [22]		1	−2.5185[−8]
				2	1.5111[−8]
$6p$	3/2	27.700 [22]	3.593 [22]	0	−1.5036[−8]
				1	−1.1427[−8]
				2	−3.6080[−9]
				3	9.6225[−9]
		^{85}Rb, $I = 5/2$			
$5s$	1/2	1011.910813 [39]		2	−2.6914[−7]
				3	1.9224[−7]
$5p$	1/2	120.7 [39]		2	−3.2108[−8]
				3	2.2934[−8]
$5p$	3/2	25.038 [46]	26.011 [46]	1	−1.7218[−8]
				2	−1.2756[−8]
				3	−3.1143[−9]
				4	1.5248[−8]
$6p$	1/2	39.11 [39]		2	−1.0402[−8]
				3	7.4301[−9]
$6p$	3/2	8.25 [39]	8.40 [44]	1	−5.6891[−9]
				2	−4.2027[−9]
				3	−1.0156[−9]
				4	5.0211[−9]

Table VII. The hyperfine-structure constants A and B originate from other studies [22,39,44,46]. The energy shifts of the $5s_{1/2}$ state are about one or two orders of magnitude larger than those of the $5p_J$,$6p_J$ excited states. Similarly, the hyperfine splittings of the $np_{1/2}$ states are obviously larger than the splittings of the $np_{3/2}$ states.

The dipole matrix elements between the hyperfine states are calculated by using the Wigner-Eckart theorem. The transition matrix elements between the two hyperfine states $|n_i L_i J_i I F_i\rangle$ and $|n_g L_g J_g I F_g\rangle$ can be written as

$$\begin{aligned}&\langle L_g J_g I F_g \| r^k C^k(r) \| L_i J_i I F_i \rangle \\ &= (-1)^{I+J_g+F_i+k} \hat{F}_i \hat{F}_g \begin{Bmatrix} I & J_i & F_i \\ k & F_g & J_g \end{Bmatrix} \\ &\times \langle L_g J_g \| r^k C^k(r) \| L_i J_i \rangle, \end{aligned} \tag{12}$$

where $k = 1$ for a dipole transition and $\hat{F} = \sqrt{2F+1}$.

The absorption oscillator strength $f_{gi}^{(k)}$ for a transition from hyperfine state $g \to i$ is defined as

$$f_{gi}^{(k)} = \frac{2|\langle L_i J_i I F_i \| r^k C^k(r) \| L_g J_g I F_g \rangle|^2 \varepsilon_{gi}}{(2k+1)(2F_g+1)}. \tag{13}$$

TABLE VIII. The partial derivatives for the matrix elements of $5s$-$5p_J$ and $5s$-$6p_J$ transitions with respect to the initial- and final-state binding energies.

Transition	$\frac{\partial A}{\partial E_{5s}}$	$\frac{\partial A}{\partial E_j}$
$5s_{1/2}$-$5p_{1/2}$	31.070953	−1.800089
$5s_{1/2}$-$5p_{3/2}$	44.794208	−4.888183
$5s_{1/2}$-$6p_{1/2}$	−17.415952	136.505937
$5s_{1/2}$-$6p_{3/2}$	−23.446857	208.756559

In the present calculations, in order to consider energy-dependent correction of the matrix elements, the matrix elements are treated as parametric functions of their binding energies [16]. The functional form is

$$\begin{aligned}A_{ij}(E_i, E_j) \approx A_{ij}(E_{0,i}, E_{0,j}) &+ \frac{\partial A_{ij}}{\partial E_i}(E_i - E_{0,i}) \\ &+ \frac{\partial A_{ij}}{\partial E_j}(E_j - E_{0,j}), \end{aligned} \tag{14}$$

where $E_{0,i}$ and $E_{0,j}$ are the binding energies without any hyperfine splitting. The partial derivatives are evaluated by redoing the calculations with the slightly different polarization potentials and leading to the change in the reduced matrix elements. The partial derivatives of matrix elements are listed in Table VIII.

B. Dipole polarizabilities of the hyperfine ground states

The dynamic dipole polarizabilities are computed with the usual oscillator strength sum rules in Eq. (8), where the sum over n includes all allowable hyperfine-structure transitions. In the calculations of polarizabilities for the hyperfine states, the resonance transition energies of hyperfine levels of the $5s$,$5p_J$,$6p_J$ states are replaced by the experimental results [47]. The uncertainties of these resonance transition energies reach 3.8×10^{-8} eV.

The dipole polarizability also has a tensor component for states with $F > 1/2$. It can be written as

$$\begin{aligned}\alpha_{\mathrm{T}}^{(1)}(\omega) = 6&\left(\frac{5F_g(2F_g-1)(2F_g+1)}{6(F_g+1)(2F_g+3)}\right)^{1/2} \\ &\times \sum_i (-1)^{F_g+F_i} \begin{Bmatrix} F_g & 1 & F_i \\ 1 & F_g & 2 \end{Bmatrix} \frac{f_{gi}^{(1)}}{\varepsilon_{gi}^2 - \omega^2}. \end{aligned} \tag{15}$$

The dipole polarizabilities of the hyperfine levels can be calculated by the following equation [30]:

$$\alpha_{M_g}^{(1)}(\omega) = \alpha^{(1)}(\omega) + \alpha_T^{(1)}(\omega) \frac{3M_g^2 - F_g(F_g+1)}{F_g(2F_g-1)}. \tag{16}$$

Table IX gives the static scalar and tensor dipole polarizabilities of the hyperfine ground states of ^{87,85}Rb. There are no other theoretical or experimental results that can be directly compared with the values in Table IX. However, the hyperfine stark shift, which is the difference in scalar polarizabilities between the hyperfine states with the same (L, J) but different F quantum numbers, can be compared with other theoretical and experimental results. Table X gives the

TABLE IX. The scalar $\alpha^{(1)}$ and tensor $\alpha_T^{(1)}$ dipole polarizabilities of the hyperfine ground states of ^{87,85}Rb. The notation $a[b]$ means $a \times 10^b$.

	State	F	$\alpha^{(1)}$ (a.u.)	$\alpha_T^{(1)}$ (a.u.)
^{87}Rb	$5s_{1/2}$	1	318.699491	1.5883[−5]
	$5s_{1/2}$	2	318.709441	−8.8203[−5]
^{85}Rb	$5s_{1/2}$	2	318.702958	2.0494[−5]
	$5s_{1/2}$	3	318.707444	−4.0621[−5]

differences in scalar and tensor polarizabilities of the hyperfine ground states of ^{87,85}Rb in atomic units. There are some studies of the hyperfine Stark shifts of ^{87,85}Rb [31,48–51] that are often reported as the Stark shift coefficients k, with units of $(\mathrm{Hz}/(\mathrm{V/m})^2$. These units are converted into atomic units by multiplying 0.4018778×10^8 [30]. The present hyperfine Stark shift of ^{87}Rb is slightly smaller than the relativistic configuration interaction plus many-body perturbation (RCI + MBPT) [48] and the relativistic linearized coupled-cluster with single, double, and partially triple contributions (RLCCSDT) [49] and larger than the perturbation theory [31]. This value is also between the experimental value [50] by Mowat *et al.* and the experimental value [51] by Dallal and Ozeri. The present hyperfine Stark shift of ^{85}Rb is larger than perturbation theory [31] and the experimental value [50].

The tensor polarizabilities of the hyperfine states do not exceed 10^{-4} a.u. in magnitude. The tensor polarizability of the $F = 1$ ground state of ^{87}Rb is positive, and that of the $F = 2$ ground state of ^{87}Rb is negative. The difference of the present tensor polarizabilities of the $F = 2$ and $F = 1$ ground states of ^{87}Rb is -1.0409×10^{-4} a.u., which is more negative than the experimental value of -0.8841×10^{-4} a.u. [51]. The difference between experiment and the present calculation is 1.568×10^{-5} a.u., which is larger than the experimental error bar of 1.045×10^{-5} a.u. The tensor polarizability of the $F = 2$ ground state of ^{85}Rb is positive, and that of the $F = 3$ ground state of ^{85}Rb is negative. The difference of tensor polarizabilities of the $F = 3$ and $F = 2$ ground states of ^{85}Rb is -6.1115×10^{-5} a.u. There are no other comparable theoretical and experimental data available at present.

The energy-dependent corrections of the dipole matrix elements play an important role in the calculation of dynamic polarizabilities. Omitting the matrix element correction results in hyperfine Stark shifts of about half these values, namely, 5.454×10^{-3} a.u. for ^{87}Rb and 2.423×10^{-3} a.u. for ^{85}Rb, respectively.

C. Tune-out wavelengths of the hyperfine ground states

1. ^{87}Rb

Hyperfine splittings lead to two new features in the tune-out wavelengths. One feature is that the splitting of the $5s_{1/2}$ state has resulted in two duplicate sets of tune-out wavelengths, that is, for the $F = 1$ and $F = 2$ hyperfine ground states. Another feature is that the hyperfine splittings of the $5p_{J,F}$ state have also resulted in the creation of additional tune-out wavelengths that arise from two adjacent hyperfine states. The hyperfine splitting of the $5p_{1/2}$ state has resulted in one additional tune-out wavelength, located between the $5p_{1/2}, F = 1$ and $5p_{1/2}, F = 2$ states. The hyperfine structure with regard to the $5p_{3/2}$ state brings two additional tune-out wavelengths, located between the three $5p_{3/2}, F = 1,2,3$ levels with allowed dipole transitions to the $5s_{1/2}, F = 2$ hyperfine state or between the three $5p_{3/2}, F = 0,1,2$ levels with allowed dipole transitions to the $5s_{1/2}, F = 1$ hyperfine state. There are several tune-out wavelengths that are defined as the primary tune-out wavelengths, which are the closest to the tune-out wavelengths calculated without the hyperfine splittings.

Table XI gives the tune-out wavelengths of the two hyperfine ground states of the $5s_{1/2}$ state of ^{87}Rb. These wavelengths are given to six digits after the decimal point to ensure that all the differences of the tune-out wavelengths are at least two digits. The longest tune-out wavelengths near 794 nm occur in the hyperfine splitting of the $5p_{1/2}$ state. These tune-out wavelengths are hard to detect due

TABLE X. The difference of scalar and tensor dipole polarizabilities of the hyperfine ground states of ^{87,85}Rb. The notation $a[b]$ means $a \times 10^b$.

Method	$\Delta\alpha^{(1)}$ (a.u.)
^{87}Rb: $\alpha^{(1)}(F = 2) - \alpha^{(1)}(F = 1)$	
Present RCICP	0.995[−2]
RCI + MBPT [48]	0.997(8)[−2]
RLCCSDT [49]	0.997(3)[−2]
Perturbation theory [31]	0.972[−2]
Expt. [50]	0.99(24)[−2]
Expt. [51]	0.9967(32)[−2]
^{85}Rb: $\alpha^{(1)}(F = 3) - \alpha^{(1)}(F = 2)$	
Present RCICP	4.486[−3]
Perturbation theory [31]	4.311[−3]
Expt. [50]	4.389(96)[−3]
^{87}Rb: $\alpha_T^{(1)}(F = 2) - \alpha_T^{(1)}(F = 1)$	
Present RCICP	−1.0409[−4]
Expt. [51]	−0.8841(1045)[−4]
^{85}Rb: $\alpha_T^{(1)}(F = 3) - \alpha_T^{(1)}(F = 2)$	
Present RCICP	−6.1115[−5]

TABLE XI. Tune-out wavelengths λ_{zero} (in nm) of the $5s_{1/2}, F = 1$ and $5s_{1/2}, F = 2$ states of ^{87}Rb. $\Delta\lambda$ (in nm) is the shift of the primary tune-out wavelengths compared to the tune-out wavelengths of the $5s$ state. Tune-out wavelengths are given to six digits after the decimal point.

$F = 1$		$F = 2$	
λ_{zero}	$\Delta\lambda(10^{-3})$	λ_{zero}	$\Delta\lambda(10^{-3})$
794.970633		794.984469	
790.018187	−9.46	790.032602	+4.95
780.233113		780.246852	
780.232827		780.246413	
423.021740	−2.42	423.025808	+1.46
421.670240		421.674241	
421.073131	−2.51	421.077158	+1.51
420.296547		420.300560	
420.296519		420.300519	

TABLE XIII. Tune-out wavelengths λ_{zero} (in nm) of the $5s_{1/2}, F = 2$ and $5s_{1/2}, F = 3$ states of ^{85}Rb. $\Delta\lambda$ (in nm) is the shift of the primary tune-out wavelengths compared to the tune-out wavelengths of the $5s$ state. Tune-out wavelengths are given to six digits after the decimal point.

$F = 2$		$F = 3$	
λ_{zero}	$\Delta\lambda(10^{-3})$	λ_{zero}	$\Delta\lambda(10^{-3})$
794.975393		794.981538	
790.023515	−0.41	790.029918	+2.27
780.237979		780.244089	
780.237860		780.243899	
423.023277	−1.00	423.025001	+0.72
421.671676		421.673454	
421.074607	−1.04	421.076392	+0.74
420.297985		420.299769	
420.297974		420.299750	

to the very small energy splittings of the hyperfine states. The second tune-out wavelengths near 790 nm are the first primary tune-out wavelengths, which lie between the excitation thresholds of the $5p_{1/2}$ and $5p_{3/2}$ states. The first primary tune-out wavelengths of the $5s_{1/2}, F = 1,2$ states are 790.018187 and 790.032602 nm, respectively. The present calculation, 790.032602 nm of the $5s_{1/2}, F = 2$ state, is larger than the latest experimental value of 790.032388(32) nm [9], and the difference is 0.000214 nm. This difference is still about 7 times larger than the experimental error bars. The tune-out wavelengths near 423 nm are other primary tune-out wavelengths, which lie between the excitation thresholds of the $5p_{3/2}$ and $6p_{1/2}$ states. Similarly, the tune-out wavelengths near 421.07 nm are also primary tune-out wavelengths, which lie between the excitation thresholds of the $6p_{1/2}$ and $6p_{3/2}$ states. These primary tune-out wavelengths of the $5s_{1/2}, F = 1$ state are shorter than the corresponding tune-out wavelengths of the $5s$ state of Rb, and those of the $5s_{1/2}, F = 2$ state are longer than the close tune-out wavelengths of the $5s$ state of Rb. The tune-out wavelengths near 780, 421.67, and 420.3 nm occur in the hyperfine splittings of the $5p_{3/2}, 6p_{1/2}$, and $6p_{3/2}$ states, respectively, which are also very hard to detect.

The tune-out wavelengths also depend on the magnetic sublevels if tensor polarizabilities are considered. The tune-out wavelengths associated with the different magnetic sublevels of the $5s_{1/2}, F$ states of ^{87}Rb are listed in Table XII. Compared with the tune-out wavelengths for the different magnetic sublevels of the same hyperfine ground state, the shifts in tune-out wavelengths due to tensor polarizabilities are less than 10^{-4} nm. Here, we focus on the fact that the difference of the first primary tune-out wavelengths for $M_F = \pm 1$ and $M_F = 0$ of the $5s_{1/2}, F = 1$ state is 9.1×10^{-5} nm. The first primary tune-out wavelength of the $M_F = 0$ sublevel of the $5s_{1/2}, F = 1$ state is 790.0181259 nm. It is a little shorter than the very recent experimental value of 790.01858(23) nm [8], and the difference is about 0.00045 nm, which is nearly 2 times larger than the experimental error bars. The first primary tune-out wavelengths for the $M_F = 0, M_F = \pm 1$, and $M_F = \pm 2$ sublevels of the $5s_{1/2}, F = 2$ state are 790.0326845, 790.0326434, and 790.0325203 nm, respectively. The differences in these tune-out wavelengths for any of the different magnetic sublevels do not exceed 1.7×10^{-4} nm.

2. ^{85}Rb

Table XIII gives the tune-out wavelengths of the $5s_{1/2}, F = 2$ and $5s_{1/2}, F = 3$ states of ^{85}Rb. Table XIV gives the tune-out wavelengths for the different magnetic sublevels. All analyses

TABLE XII. Tune-out wavelengths λ_{zero} (in nm) of the different magnetic sublevels of the $5s_{1/2}, F = 1$ and $5s_{1/2}, F = 2$ states of ^{87}Rb. Tune-out wavelengths are given to seven digits after the decimal point.

$F = 1$		$F = 2$		
$M_F = -1,1$	$M_F = 0$	$M_F = -2,2$	$M_F = -1,1$	$M_F = 0$
794.9705853	794.9707284	794.9846000	794.9844029	794.9843373
790.0182169	790.0181259	790.0325203	790.0326434	790.0326845
780.2331259	780.2330860	780.2468572	780.2468488	780.2468458
780.2328185	780.2328473	780.2463937	780.2464233	780.2464334
423.0217422	423.0217345	423.0258015	423.0258118	423.0258153
421.6702358	421.6702489	421.6742534	421.6742354	421.6742294
421.0731328	421.0731283	421.0771545	421.0771603	421.0771623
420.2965477	420.2965439	420.3005609	420.3005601	420.3005598
420.2965184	420.2965212	420.3005169	420.3005197	420.3005206

TABLE XIV. Tune-out wavelengths λ_{zero} (in nm) of the different magnetic sublevels of the $5s_{1/2}, F = 2$ and $5s_{1/2}, F = 3$ states of ^{85}Rb. Tune-out wavelengths are given to seven digits after the decimal point.

$F = 2$			$F = 3$			
$M_F = -2,2$	$M_F = -1,1$	$M_F = 0$	$M_F = -3,3$	$M_F = -2,2$	$M_F = -1,1$	$M_F = 0$
794.9753668	794.9754056	794.9754185	794.9815835	794.9815382	794.9815110	794.9815020
790.0235316	790.0236506	790.0234980	790.0298900	790.0299180	790.0299347	790.0299403
780.2379826	780.2379764	780.2379743	780.2440913	780.2440888	780.2440870	780.2440865
780.2378566	780.2378612	780.2378629	780.2438904	780.2438990	780.2439042	780.2439060
423.0232785	423.0232769	423.0232764	423.0250000	423.0250014	423.0250024	423.0250028
421.6716741	421.6716777	421.6716789	421.6734579	421.6734538	421.6734513	421.6734505
421.0746085	421.0746070	421.0746065	421.0763902	421.0763917	421.0763927	421.0763930
420.2979853	420.2979847	420.2979845	420.2997688	420.2997685	420.2997683	420.2997683
420.2979732	420.2979737	420.2979738	420.2997495	420.2997503	420.2997508	420.2997510

and properties of ^{85}Rb should be interpreted with the contents of the previous section in mind. The differences between the tune-out wavelengths of the hyperfine states of ^{85}Rb are smaller than those of ^{87}Rb. This is understandable since ^{85}Rb has smaller hyperfine-structure constants than ^{87}Rb. Similarly, the differences between the tune-out wavelengths of the hyperfine magnetic sublevels of ^{85}Rb are also smaller than those of ^{87}Rb.

D. Some comments on accuracy

The uncertainties of the dipole reduced matrix elements of the $5s$-$5p_J$ transitions are mainly caused by the correlation effects of frozen-core model. These uncertainties are smaller than 0.5%; thus, we set 0.5% as the uncertainties of the dipole reduced matrix elements. The uncertainties of the dipole reduced matrix elements for the transitions of more highly excited states are derived from the first-order parametric functions of their energies. By considering the uncertainties of dipole reduced matrix elements, the uncertainties of three tune-out wavelengths of the ground state of Rb are obtained.

Compared with the present calculations and available experimental results [8,9], the absolute precision of tune-out wavelengths should be about 0.0005 nm. The method used to determine the tune-out wavelengths of hyperfine states was unorthodox, being essentially a second-order calculation using energy and matrix element shifts applied prior to the evaluation of the oscillator strength sum rules. There are three main factors that influence the accuracy of the present tune-out wavelengths. Table XV shows the estimated errors of the first primary tune-out wavelengths of the $5s_{1/2}, F = 1,2$ states of ^{87}Rb and $5s_{1/2}, F = 2,3$ states of ^{85}Rb.

The first factor is the uncertainties of $5s$-$5p_J$ matrix elements. An uncertainty analysis has been done for the tune-out wavelengths. First, the matrix elements of $5s$-$5p_{1/2}$ and $5s$-$5p_{3/2}$ transitions are changed by 0.05% according to the errors between the present RCICP calculations and Ref. [9]. The matrix elements are adjusted accordingly, and tune-out wavelengths are recomputed. In this case, the ratio of line strengths $5s$-$5p_J$ is not changed. The shifts in the first primary tune-out wavelengths near 790.0 nm of ^{87,85}Rb are about 5 fm. This is too small to explain the differences between the present calculations and experimental results [8,9]. The shifts in the other primary tune-out wavelengths near 423.0 nm which lie in the $5s$-$5p_{3/2}$ and $5s$-$6p_{1/2}$ transitions of ^{87,85}Rb are 2034 fm. The shifts in the primary tune-out wavelengths near 421.0 nm which lie in the $5s$-$6p_{1/2}$ and $5s$-$6p_{3/2}$ transitions of ^{87,85}Rb are about 257 fm. The shifts in the tune-out wavelengths which lie in the np_J hyperfine splittings are smaller than 10^{-11} nm. Then, the ratio of line strengths $5s$-$5p_J$ is changed by 0.00003. The shifts in the first primary tune-out wavelengths of ^{87,85}Rb near 790.0 nm are 13 fm. These shifts are still much smaller than the differences between the present calculations and latest experiments [8,9]. The shifts in the other primary tune-out wavelengths of ^{87,85}Rb near 423.0 nm are about 6 fm. The shifts in the primary tune-out wavelengths of ^{87,85}Rb near 421.0 nm are about 0.7 fm.

We also have checked the sensitivity of the tune-out wavelengths to the small changes in the energy-adjusted matrix elements. The tune-out wavelengths are recalculated without the modifications of matrix elements due to the energy adjustment. The tune-out wavelengths are insensitive to these small changes; they are totally different from the hyperfine stark shifts, which are critically reliant on the use of energy-adjusted matrix elements. For example, the energy-adjusted reduced matrix elements make the 0.5-fm shifts to the first primary tune-out wavelengths of the $F = 1,2$ ground states of ^{87}Rb. The shifts in the first primary tune-out wavelengths of the $F = 2,3$ ground states of ^{85}Rb are about 0.2 fm. These shifts are two or three orders smaller than latest experimental error bars [8,9].

The second factor is the uncertainties in the contributions to the polarizabilities from the highly excited, continuum, and

TABLE XV. The estimated errors (in fm) of the first primary tune-out wavelengths of the $5s_{1/2}, F = 1,2$ states of ^{87}Rb and $5s_{1/2}, F = 2,3$ states of ^{85}Rb. $\delta\lambda_1$ is the error that is caused by the 0.05% uncertainties of $5s$-$5p_{1/2}$ and $5s$-$5p_{3/2}$ matrix elements. $\delta\lambda_2$ is the error that is caused by the 0.00003 uncertainty of the ratio of $5s$-$5p_J$ line strengths. $\delta\lambda_3$ is the error that is caused by 5% uncertainties of the matrix elements from the high-excited, continuum, and core-excited states. $\sum\delta\lambda_i$ is the sum of $\delta\lambda_1$,$\delta\lambda_2$, and $\delta\lambda_3$.

	F	λ_{zero}(nm)	$\delta\lambda_1$	$\delta\lambda_2$	$\delta\lambda_3$	$\sum\delta\lambda_i$
^{87}Rb	1	790.0181865	5	13	175	193
	2	790.0326024	5	13	175	193
^{85}Rb	2	790.0235148	5	13	200	218
	3	790.0299179	5	13	200	218

core-excited states. The contribution from excited states above the $5p$ state is 11.14 a.u. in the present RCICP calculations of tune-out wavelengths, which is a 4.1% difference from the value given by Leonard *et al.* [9]. So we changed the matrix elements of highly excited states by 5%, and the tune-out wavelengths were recomputed. The first primary tune-out wavelengths will shift 175 fm for ^{87}Rb and 200 fm for ^{85}Rb. These shifts are close to the difference between the present calculation and the latest experiment [9].

The third factor is the uncertainties in transition energies of hyperfine states. In the present calculations, the experimental resonance transition energies [47] for the hyperfine transitions are used, in which the uncertainties are smaller than 10^{-7} nm. The effect of hyperfine structure for the level higher than $6p$ is negligible. So this factor can be ignored in the present analysis.

V. CONCLUSIONS

The static and dynamic polarizabilities of the ground state of Rb were calculated by using the RCICP method. Combining the most exact $5s$-$5p_J$ matrix elements [9], the three longest tune-out wavelengths of the $5s_{1/2}$ state were determined. After considering the hyperfine splittings of energy levels, the static and dynamic polarizabilities and the tune-out wavelengths of the hyperfine ground states of ^{87,85}Rb were further determined. The present hyperfine stark shifts are in good agreement with the available theoretical and experimental results. Considering the contributions of tensor polarizabilities, the tune-out wavelengths for the different magnetic sublevels M_F of the hyperfine states F were obtained. It was found that the differences of the tune-out wavelengths for the different magnetic sublevels do not exceed 10^{-4} nm.

The first primary tune-out wavelengths of the $5s_{1/2}, F = 1,2$ states of ^{87}Rb are 790.018187(193) and 790.032602(193) nm, respectively. The first primary tune-out wavelengths of the $5s_{1/2}, F = 2,3$ states of ^{85}Rb are 790.023515(218) and 790.029918(218) nm, respectively. The present results were compared with recent experiments [8,9]. The differences between the present calculations and recent experiments are still larger than the experimental error bars [8,9]. But the present RCICP first primary tune-out wavelength of the $5s_{1/2}, F = 2$ state of ^{87}Rb is longer than that observed in the recent experiment [9]. Meanwhile, the present RCICP first primary tune-out wavelength of the $5s_{1/2}, F = 1, M_F = 0$ state of ^{87}Rb is shorter than that observed in the latest experiment [8]. It seems that the main uncertainty of the polarizabilities from the highly excited, continuum, and core-excited states cannot explain this difference completely because the uncertainty of the remaining polarizabilities can lead only to wavelengths that are consistently longer or consistently shorter than but not to some that are longer and some that are shorter than the first primary tune-out wavelengths in recent experiments [8,9]. Hence, further study will be essential.

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[1] M. S. Safronova, U. I. Safronova, and S. G. Porsev, Phys. Rev. A **87**, 032513 (2013).
[2] M. S. Safronova, S. G. Porsev, U. I. Safronova, M. G. Kozlov, and C. W. Clark, Phys. Rev. A **87**, 012509 (2013).
[3] S. G. Porsev and A. Derevianko, Phys. Rev. A **74**, 020502 (2006).
[4] T. Middelmann, S. Falke, C. Lisdat, and U. Sterr, Phys. Rev. Lett. **109**, 263004 (2012).
[5] Y. Cheng, J. Jiang, and J. Mitroy, Phys. Rev. A **88**, 022511 (2013).
[6] L. J. LeBlanc and J. H. Thywissen, Phys. Rev. A **75**, 053612 (2007).
[7] W. F. Holmgren, R. Trubko, I. Hromada, and A. D. Cronin, Phys. Rev. Lett. **109**, 243004 (2012).
[8] F. Schmidt, D. Mayer, M. Hohmann, T. Lausch, F. Kindermann, and A. Widera, Phys. Rev. A **93**, 022507 (2016).
[9] R. H. Leonard, A. J. Fallon, C. A. Sackett, and M. S. Safronova, Phys. Rev. A **92**, 052501 (2015).
[10] J. Catani, G. Barontini, G. Lamporesi, F. Rabatti, G. Thalhammer, F. Minardi, S. Stringari, and M. Inguscio, Phys. Rev. Lett. **103**, 140401 (2009).
[11] B. M. Henson, R. I. Khakimov, R. G. Dall, K. G. H. Baldwin, L.-Y. Tang, and A. G. Truscott, Phys. Rev. Lett. **115**, 043004 (2015).
[12] B. Arora, M. S. Safronova, and C. W. Clark, Phys. Rev. A **84**, 043401 (2011).
[13] G. Lamporesi, J. Catani, G. Barontini, Y. Nishida, M. Inguscio, and F. Minardi, Phys. Rev. Lett. **104**, 153202 (2010).
[14] C. D. Herold, V. D. Vaidya, X. Li, S. L. Rolston, J. V. Porto, and M. S. Safronova, Phys. Rev. Lett. **109**, 243003 (2012).
[15] J. Jiang, L.-Y. Tang, and J. Mitroy, Phys. Rev. A **87**, 032518 (2013).
[16] J. Jiang and J. Mitroy, Phys. Rev. A **88**, 032505 (2013).
[17] I. P. Grant and H. M. Quiney, Phys. Rev. A **62**, 022508 (2000).
[18] I. P. Grant, *Relativistic Quantum Theory of Atoms and Molecules: Theory and Computation* (Springer, New York, 2007).
[19] W. Johnson, D. Kolb, and K.-N. Huang, At. Data Nucl. Data Tables **28**, 333 (1983).
[20] S. G. Porsev and A. Derevianko, J. Chem. Phys. **119**, 844 (2003).
[21] A. Kramida, Yu. Ralchenko, J. Reader, and the NIST ASD Team, NIST Atomic Spectra Database, version 5.3, http://physics.nist.gov/asd.
[22] M. S. Safronova and U. I. Safronova, Phys. Rev. A **83**, 052508 (2011).
[23] M. S. Safronova, C. J. Williams, and C. W. Clark, Phys. Rev. A **69**, 022509 (2004).
[24] B. Arora, D. K. Nandy, and B. K. Sahoo, Phys. Rev. A **85**, 012506 (2012).
[25] R. Pal, M. S. Safronova, W. R. Johnson, A. Derevianko, and S. G. Porsev, Phys. Rev. A **75**, 042515 (2007).

[26] D. J. Whiting, J. Keaveney, C. S. Adams, and I. G. Hughes, Phys. Rev. A **93**, 043854 (2016).
[27] U. Volz and H. Schmoranzer, Phys. Scr. **T65**, 48 (1996).
[28] J. E. Simsarian, L. A. Orozco, G. D. Sprouse, and W. Z. Zhao, Phys. Rev. A **57**, 2448 (1998).
[29] R. F. Gutterres, C. Amiot, A. Fioretti, C. Gabbanini, M. Mazzoni, and O. Dulieu, Phys. Rev. A **66**, 024502 (2002).
[30] J. Mitroy, M. S. Safronova, and C. W. Clark, J. Phys. B **43**, 202001 (2010).
[31] T. Lee, T. P. Das, and R. M. Sternheimer, Phys. Rev. A **11**, 1784 (1975).
[32] J. L. Snider, Phys. Lett. **21**, 172 (1966).
[33] J. Migdalek and Y.-K. Kim, J. Phys. B **31**, 1947 (1998).
[34] Y.-B. Tang, C.-B. Li, and H.-X. Qiao, Chin. Phys. B **23**, 063101 (2014).
[35] J. Mitroy and M. W. J. Bromley, Phys. Rev. A **68**, 052714 (2003).
[36] I. S. Lim, P. Schwerdtfeger, B. Metz, and H. Stoll, J. Chem. Phys. **122**, 104103 (2005).
[37] K. Kaur, J. Kaur, B. Arora, and B. K. Sahoo, Phys. Rev. B **90**, 245405 (2014).
[38] J. Kaur, D. K. Nandy, B. Arora, and B. K. Sahoo, Phys. Rev. A **91**, 012705 (2015).
[39] M. S. Safronova, W. R. Johnson, and A. Derevianko, Phys. Rev. A **60**, 4476 (1999).
[40] A. Derevianko, W. R. Johnson, M. S. Safronova, and J. F. Babb, Phys. Rev. Lett. **82**, 3589 (1999).
[41] R. W. Molof, H. L. Schwartz, T. M. Miller, and B. Bederson, Phys. Rev. A **10**, 1131 (1974).
[42] W. F. Holmgren, M. C. Revelle, V. P. A. Lonij, and A. D. Cronin, Phys. Rev. A **81**, 053607 (2010).
[43] M. D. Gregoire, I. Hromada, W. F. Holmgren, R. Trubko, and A. D. Cronin, Phys. Rev. A **92**, 052513 (2015).
[44] E. Arimondo, M. Inguscio, and P. Violino, Rev. Mod. Phys. **49**, 31 (1977).
[45] L. J. Armstrong, *Theory of the Hyperfine Structure of Free Atoms* (Wiley-Interscience, New York, 1971).
[46] U. D. Rapol, A. Krishna, and V. Natarajan, Eur. Phys. J. D **23**, 185 (2003).
[47] D. A. Steck, Rubidium 87 D line Data, version 2.1.4, http://steck.us/alkalidata.
[48] E. J. Angstmann, V. A. Dzuba, and V. V. Flambaum, Phys. Rev. A **74**, 023405 (2006).
[49] M. S. Safronova, D. Jiang, and U. I. Safronova, Phys. Rev. A **82**, 022510 (2010).
[50] J. R. Mowat, Phys. Rev. A **5**, 1059 (1972).
[51] Y. Dallal and R. Ozeri, Phys. Rev. Lett. **115**, 183001 (2015).