

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

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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 $^{87,85}\text{Rb}$ have been calculated by using 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) nm and 790.032602(193) nm severally, 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 [*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) nm 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 Stark effect can be written as

$$\Delta E \approx -\frac{1}{2}\alpha_d(\omega)F^2 + \dots, \quad (1)$$

where $\alpha_d(\omega)$ is the dynamic dipole polarizability of 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 the certain value, the dynamic polarizability goes to zero and the corresponding wavelength is called tune-out wavelength.

With the recent development of atomic manipulation and measurement in experimental optical traps, studies on polarizabilities of atoms and ions have been of great interest. The knowledge of static polarizabilities can be used to evaluate Stark effect [1] and the blackbody radiation(BBR) shift [2] which are very important to determine the uncertainty of 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 trapping laser is equal to the tune-out wavelength of this 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 has been measured with an accuracy about 30 fm [9] by using a condensate interferometer. This accuracy is better than the precision of other previous 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 also has been measured with sub pm accuracy by Schmidt *et al.* [8]. These experiments give some very good opportunities for testing of 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 $^{87,85}\text{Rb}$ have been calculated by using relativistic configuration interaction plus core polarization(RCICP) approach. Firstly, the wavefunctions, energies, and transition matrix elements of 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 $^{87,85}\text{Rb}$ are also determined. In Sec. II., a brief description of the theoretical method is presented. In Sec. III. and Sec. 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 unit used in the present calculations is atomic unit(a.u.), in which, mass of electron m_e and \hbar have the numerical

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

ℓ	J	$\rho_{\ell,j}$ (units : 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

value 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 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-spinors basis functions, which were introduced by Grant and Quiney [17, 18]. S-spinors can be treated as relativistic generalizations of the Slater-type orbitals.

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

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

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

$$V_{core}(\mathbf{r}) = -\frac{Z}{r} + V_{dir}(\mathbf{r}) + V_{exc}(\mathbf{r}) + V_p(\mathbf{r}). \quad (3)$$

The direct interaction $V_{dir}(\mathbf{r})$ and exchange interaction $V_{exc}(\mathbf{r})$ 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

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

Here, the factors $\alpha_{core}^{(k)}$ are the static k -th 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.

TABLE II: Theoretical and experimental energy levels (in Hartree) 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 Science 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

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 Science 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 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 0.0000020 and 0.0000135 Hartree.

B. Dipole matrix elements

Table III gives the reduced electric dipole(E1) matrix elements for a number of low-lying excited states transitions of Rb. The matrix elements are calculated with a

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)		
$5d_{5/2} - 6p_{3/2}$	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		
$\frac{ (5p_{3/2} D 5s_{1/2}) ^2}{ (5p_{1/2} D 5s_{1/2}) ^2}$	1.994(40)	1.992(65)	1.997(62)	1.99145	1.995(3) ^a 1.99221(3) [9]

^aThese values are the average of several experiments [26–28] and given by Leonard *et al.* [9]

modified transition operator [29–31],

$$\mathbf{r} = \mathbf{r} - [1 - \exp(-\frac{r^6}{\rho^6})]^{1/2} \frac{\alpha_d \mathbf{r}}{r^3}, \quad (5)$$

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 the 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 single-double and the important valence triple excitation method(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 a good agreement with the average values of experiments [26–28] 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 present RCICP results and other theoretical results.

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 wavefunctions for the spin-orbit doublet arising from the small differences of energies [32]. The present RCICP ratio 1.994(40) is in excellent agreement with average experimental value 1.995(3), larger than the latest experimental ratio 1.99221(3) which has been determined by the measurement of tune-out wavelength and the experimental matrix element of $5s - 5p_{1/2}$ 4.233 [9]. So far none of theoretical results are within the latest experimental error bar, but the RMBPT all-order result is the closest to this latest experimental ratio.

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 [33]	317.62	6.4810	2.3783
CICP [34]	315.7	6.480	2.378
RCCSD [35]	316.17		
RCCSD [36, 37]	318.47/318.3(6)	6.491(18)	
MBPT-SD [38]	317.39		
RMBPT all-order [22, 39]	316.4/322(4)	6.525(37)	2.374(16)
RMBPT [20]		6.520(80)	2.37
Expt.E×H [40]	319(6.1)		
Expt. [41]	318.79(1.42)		
Expt. [42]	320.1(6)		

C. Polarizabilities of the ground state

The static scalar polarizability is written as

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

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

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

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 present RCICP results agree with the DFCEP results [33] very well. The DFCEP method is the same as the present RCICP method except that DFCEP uses the B-spline basis. The RCICP dipole polarizability is larger than that calculated by the nonrelativistic configuration interaction plus core polarization(CICP) [34], RCCSD of Lim *et al.* [35], and the RMBPT all-order method [39], but smaller than the RCCSD result of Kaur *et al.* [36, 37], the earlier MBPT-SD result [38], and the experimental values [40, 41]. 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 [41] very well. So the differences of static dipole polarizabilities between experiments and the present results are mainly from the differences of $5s - 5p_J$ matrix elements. The latest experimental value [42], 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, the relativistic many-body perturbation theory(RMBPT), RCCSD, and RMBPT all-order. The differences of the present RCICP calculations and other available results[20, 22, 34, 36, 37] are not more than 0.6%.

TABLE V: Pseudospectral oscillator strength distribution for the Rb^+ . Transition energies ε_n are given in a.u..

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]	789.85(1) [10]
		790.034(7) [12]	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]
$5s - 6p_{3/2}$			

D. Tune-out wavelengths of the ground state

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

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

The core polarizability is given by a pseudospectral oscillator strength distribution [34]. The distribution is derived from the single particle energies of Hartree-Fock core and 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 that the tune-out wavelengths occur. The first case is that the tune-out wavelength exists between $np_{1/2}$ and $np_{3/2}$ spin-orbit doublet, such as 790.02765 nm lies in the $5s - 5p_J$ splitting and 421.07565 nm 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] of the longest tune-out wavelength of the $5s$ state available. 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 with the available values [9, 12, 13] and the present RCICP calculation. The reason of this difference should be from the light is not the linearly polarized in this experiment [10]. The present tune-out wavelength near 421 nm agrees with the RMBPT result [12] and experimental result [14] perfectly. The second case is that 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 423.02428 nm lies between the $5p_{3/2}$ and $6p_{1/2}$. This tune-out wavelength also has a good agreement with the experimental result [14] and MBPT result [12].

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 [43, 44] by

$$E = E_{NLJ} + W_F, \quad (9)$$

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

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

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

$$R = F(F+1) - I(I+1) - J(J+1). \quad (11)$$

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 $5s_{1/2}$, $5p_J$ and $6p_J$ states of $^{87,85}\text{Rb}$ are listed in Table VII. The hyperfine structure constants A and B are originated from other documents [22, 38, 43, 45]. The energy shifts of the $5s_{1/2}$ state are about one or two order 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 writ-

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 documents.

	J	A (MHz)	B (MHz)	F	W_F (a.u.)
$^{87}\text{Rb}, I = 3/2$					
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]
$^{85}\text{Rb}, I = 5/2$					
5s	1/2	1011.910813 [38]		2	-2.6914[-7]
				3	1.9224[-7]
5p	1/2	120.7 [38]		2	-3.2108[-8]
				3	2.2934[-8]
5p	3/2	25.038 [45]	26.011 [45]	1	-1.7218[-8]
				2	-1.2756[-8]
				3	-3.1143[-9]
				4	1.5248[-8]
6p	1/2	39.11 [38]		2	-1.0402[-8]
				3	7.4301[-9]
6p	3/2	8.25 [38]	8.40 [43]	1	-5.6891[-9]
				2	-4.2027[-9]
				3	-1.0156[-9]
				4	5.0211[-9]

ten as

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

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 $g \rightarrow i$ is defined as

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

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

$$A_{ij}(E_i, E_j) \approx A_{ij}(E_{0,i}, E_{0,j}) + \frac{\partial A_{ij}}{\partial E_i}(E_i - E_{0,i}) + \frac{\partial A_{ij}}{\partial E_j}(E_j - E_{0,j}), \quad (14)$$

where $E_{0,i}$ and $E_{0,j}$ are the binding energies without any hyperfine splitting. The partial derivatives are evaluated

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	$\frac{\partial A}{\partial E_{5s}}$	$\frac{\partial A}{\partial E_i}$
$5s_{1/2} - 5p_{1/2}$	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

TABLE IX: The scalar $\alpha^{(1)}$ and tensor $\alpha_T^{(1)}$ dipole polarizabilities of the hyperfine ground states of $^{87,85}\text{Rb}$. 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]

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 [46]. The uncertainties of these resonance transition energies reach to 3.8×10^{-8} eV.

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

$$\alpha_T^{(1)}(\omega) = 6 \left(\frac{5F_g(2F_g - 1)(2F_g + 1)}{6(F_g + 1)(2F_g + 3)} \right)^{1/2} \times \sum_i (-1)^{F_g + F_i} \left\{ \begin{matrix} F_g & 1 & F_i \\ 1 & F_g & 2 \end{matrix} \right\} \frac{f_{gi}^{(1)}}{\varepsilon_{gi}^2 - \omega^2}. \quad (15)$$

The dipole polarizabilities of the hyperfine levels can be calculated by the following equation [29],

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

Table IX gives the static scalar and tensor dipole polarizabilities of the hyperfine ground states of $^{87,85}\text{Rb}$. There are no other theoretical or experimental results that can be directly compared with these values in Table IX. However, the hyperfine stark shift, which is the

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

Method	$\Delta\alpha^{(1)}$ (a.u.)
$^{87}\text{Rb}: \alpha^{(1)}(F=2) - \alpha^{(1)}(F=1)$	
Present RCICP	0.995[-2]
RCI + MBPT [47]	0.997(8)[-2]
RLCCSDT [48]	0.997(3)[-2]
Perturbation theory [30]	0.972[-2]
Expt. [49]	0.99(24)[-2]
Expt. [50]	0.9967(32)[-2]
$^{85}\text{Rb}: \alpha^{(1)}(F=3) - \alpha^{(1)}(F=2)$	
Present RCICP	4.486[-3]
Perturbation theory [30]	4.311[-3]
Expt. [49]	4.389(96)[-3]
$^{87}\text{Rb}: \alpha_T^{(1)}(F=2) - \alpha_T^{(1)}(F=1)$	
Present RCICP	-1.0409[-4]
Expt. [50]	-0.8841(1045)[-4]
$^{85}\text{Rb}: \alpha_T^{(1)}(F=3) - \alpha_T^{(1)}(F=2)$	
Present RCICP	-6.1115[-5]

difference of 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 differences of scalar and tensor polarizabilities of the hyperfine ground states of $^{87,85}\text{Rb}$ in a.u.. There are some documents of the hyperfine Stark shifts of $^{87,85}\text{Rb}$ [30, 47–50] that are often reported as the Stark shift coefficients k , with units of $(\text{Hz}/(\text{V}/\text{m})^2)$. This is converted into a.u. by multiplying 0.4018778×10^8 [29]. The present hyperfine Stark shift of ^{87}Rb is slightly smaller than the relativistic configuration interaction plus many-body perturbation(RCI + MBPT) [47], the relativistic linearized coupled cluster single-double with partial triple contributions(RLCCSDT) [48], and larger than the perturbation theory [30]. This value is also between the experimental value [49] by Mowat *et al.* and the experimental value [50] by Dallal *et al.* The present hyperfine Stark shift of ^{85}Rb is larger than Perturbation theory [30] and experimental value [49].

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 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 -0.8841×10^{-4} a.u. [50]. The difference between experiment and the present calculation is 1.568×10^{-5} a.u., which is larger than the experimental error bar 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

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 shifts of the primary tune-out wavelengths compared to the tune-out wavelengths of $5s$ state. Tune-out wavelengths are given to six digits after the decimal point.

F=1		F=2	
λ_{zero}	$10^{-3}\Delta\lambda$	λ_{zero}	$10^{-3}\Delta\lambda$
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	-

no any 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 the hyperfine Stark shifts about half these values, namely, 5.454×10^{-3} a.u. of ^{87}Rb and 2.423×10^{-3} a.u. of ^{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 each other. 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 $5p_{3/2}$ 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 would be hard to detect due 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 nm and 790.032602 nm respectively. The present calculation, 790.032602 nm of the $5s_{1/2}, F = 2$ state, is larger than the latest experiment 790.032388(32) nm [9] and the difference is 0.000214 nm. This difference is still about seven times larger than the experimental error bar. 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 $5s$ state of Rb, and those of the $5s_{1/2}, F = 2$ state are longer than the close tune-out wavelengths of $5s$ state of Rb. The tune-out wavelengths near 780 nm, 421.67 nm, 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. Comparing with the tune-out wavelengths for the different magnetic sublevels of the same hyperfine ground state, the shifts of tune-out wavelengths due to tensor polarizabilities are less than 10^{-4} nm. Here we focus on that the difference of the first primary tune-out wavelengths for the $M_F = \pm 1$ 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 $5s_{1/2}, F = 1$ state is 790.0181259 nm. It is a little shorter than the very recent experiment 790.01858(23) nm [8], and the difference is about 0.00045 nm which is nearly two times larger than the experimental error bar. 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 nm, 790.0326434 nm 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 analysis and properties of ^{85}Rb should be interpreted with the contents of the previous section in

TABLE XII: Tune-out wavelengths λ_{zero} (in nm) of the different magnetic sublevels of $5s_{1/2}, F = 1$ 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 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 shifts of the primary tune-out wavelengths compared to the tune-out wavelengths of $5s$ state. Tune-out wavelengths are given to six digits after the decimal point.

F=2		F=3	
λ_{zero}	$10^{-3}\Delta\lambda$	λ_{zero}	$10^{-3}\Delta\lambda$
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	-

mind. The differences between the tune-out wavelengths of the hyperfine states of ^{85}Rb are smaller than those of ^{87}Rb . It is understandable since ^{85}Rb has the 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 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.

Comparing 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. Firstly, 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 of the first primary tune-out wavelengths near 790.0 nm of $^{87,85}\text{Rb}$ are about 5 fm. It is too small to explain the differences of the present calculations and experimental results [8, 9]. The shifts of the other primary tune-out wavelengths near 423.0 nm which lie in $5s - 5p_{3/2}$ and $5s - 6p_{1/2}$ transitions of $^{87,85}\text{Rb}$ are 2034 fm. The shifts of the primary tune-out wavelengths near 421.0 nm which lie in $5s - 6p_{1/2}$ and $5s - 6p_{3/2}$ transitions of $^{87,85}\text{Rb}$ are about 257 fm. The shifts of 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 of the first primary tune-out wavelengths of $^{87,85}\text{Rb}$ 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 of the other primary tune-out wavelengths of $^{87,85}\text{Rb}$ near 423.0 nm are about 6 fm. The shifts of the primary tune-out wavelengths of $^{87,85}\text{Rb}$ 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 in-

TABLE XIV: Tune-out wavelengths λ_{zero} (in nm) of the different magnetic sublevels of $5s_{1/2}, F = 2$ 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

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 errors that are caused by the 0.05 % uncertainties of $5s - 5p_{1/2}$ and $5s - 5p_{3/2}$ matrix elements. $\delta\lambda_2$ is the errors that are caused by the 0.00003 uncertainty of ratio of $5s - 5p_J$ line strengths. $\delta\lambda_3$ is the errors that are 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 the $\delta\lambda_1$, $\delta\lambda_2$, and $\delta\lambda_3$.

	F	$\lambda_{zero}(\text{nm})$	$\delta\lambda_1$	$\delta\lambda_2$	$\delta\lambda_3$	$\sum \delta\lambda_i$
^{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

sensitive to these small changes, these are totally different with 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 of 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 contributions to polarizabilities from the highly-excited, continuum, and core-excited states. The contribution from excited states above $5p$ state is 11.14 a.u. in the present RCICP calculations of tune-out wavelengths, which is 4.1% difference with 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 are recomputed. The first primary tune-out wavelengths will shift 175 fm of ^{87}Rb and 200 fm of ^{85}Rb . These shifts are close to the difference between the present calculation and the latest experiment [9].

The third factor is the uncertainties of transition energies of hyperfine states. In the present calculations, the experimental resonance transition energies [46] 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 have been calculated by using the RCICP method. Combining the most exact $5s - 5p_J$ matrix elements [9], three longest tune-out wavelengths of the $5s_{1/2}$ state are 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 $^{87,85}\text{Rb}$ are 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 are obtained. It is 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) nm and 790.032602(193) nm severally. The first primary tune-out wavelengths of the $5s_{1/2}, F = 2, 3$ states of ^{85}Rb are 790.023515(218) nm and 790.029918(218) nm respectively. The present results are compared with the recent experiments [8, 9]. The differences between the present calculations and the recent experiments are still larger than the experimental error bars [8, 9]. But the present RCICP first primary tune-out wavelength of $5s_{1/2}, F = 2$ state of ^{87}Rb is longer than that observed in the recent experiment [9]. Meanwhile, the present RCICP first primary tune-out wavelength of $5s_{1/2}, F = 1, M_F = 0$ 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 can not explain this difference completely, because the uncertainty of the remaining polarizabilities can only lead to consistently longer or consistently shorter, but not to some longer and some shorter

than the first primary tune-out wavelengths in recent experiments[8, 9]. Hence, a further study will be essential.

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