PHYSICAL REVIEW A **87**, 032518 (2013)

Tune-out wavelengths for potassium

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(Received 25 February 2013; published 26 March 2013)

The five longest tune-out wavelengths for the potassium atom are determined using a relativistic structure model which treats the atom as consisting of a single valence electron moving outside a closed shell core. The importance of various terms in the dynamic polarizability in the vicinity of the $4p_J$, $5p_J$, and $6p_J$ transitions are discussed.

DOI: 10.1103/PhysRevA.87.032518 PACS number(s): 31.15.ac, 32.10.Dk, 31.15.ap

I. INTRODUCTION

The dynamic polarizability of an atom gives a measure of the energy shift of the atom when it is exposed to an electromagnetic field [1,2]. For an atom in any given state, one can write

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

where $\alpha_d(\omega)$ is the polarizability of the quantum state at frequency ω, and F is a measure of the strength of the ac electromagnetic field. The limiting value of the dynamic polarizability in the $\omega \to 0$ limit is the static dipole polarizability.

The dynamic polarizability will go to zero for certain frequencies of the applied electromagnetic field. The wavelengths at which the polarizability goes to zero are called the tune-out wavelengths [3,4]. Atoms trapped in an optical lattice can be released by changing the wavelength of the trapping laser to that of the tune-out wavelength for that atom. Very recently, tune-out wavelengths have been measured for the rubidium and the potassium atoms [5,6]. The advantage of a tune-out wavelength measurement is that it is effectively a null experiment; it measures the frequency at which the polarizability is equal to zero. Therefore it does not rely on a precise determination of the strength of an electric field or the intensity of a laser field.

In the present manuscript a calculation of the five longest tune-out wavelengths for the potassium atom is presented. The method applied is a fully relativistic version of a nonrelativistic semiempirical fixed core approach that has been successfully applied to the description of many one- and two-electron atoms [7–10]. An extensive discussion is made about those parts of the oscillator strength sum rule that have the largest influence in the determination of the tune-out wavelengths.

II. FORMULATION

The calculation methodology is as follows. The first step involves a Dirac-Fock (DF) calculation of the K^+ ground state. The single particle orbitals are written as linear combinations of analytic basis functions. The functions chosen are the S-spinors introduced by Grant and Quiney [11,12]. S-spinors can be regarded as relativistic generalizations of the familiar Slater-type orbital.

The effective interaction of the valence electrons with the core is then written

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

where m is the electron mass, c is the speed of light, $\boldsymbol{p}$ is the momentum operator, $\boldsymbol{\alpha}$ and β are 4×4 matrices of the Dirac operators [12]. The core operator is

$$V_{\mathrm{core}}(\mathbf{r}) = -\frac{Z}{r} + V_{\mathrm{dir}}(\mathbf{r}) + V_{\mathrm{exc}}(\mathbf{r}) + V_{\mathrm{p}}(\mathbf{r}). \tag{3}$$

The direct and exchange interactions of the valence electron with the DF core were calculated exactly. The ℓ-dependent polarization potential V_{p} was semiempirical in nature with the functional form,

$$V_{\mathrm{p}}(r) = -\sum_{\ell j}\frac{\alpha_{\mathrm{core}}g_{\ell j}^2(r)}{2r^4}|\ell j\rangle\langle\ell j|. \tag{4}$$

The factor α_{core} is the static dipole polarizability of the core and $g_{\ell j}^2(r) = 1-\exp(-r^6/\rho_{\ell j}^6)$ is a cutoff function designed to make the polarization potential finite at the origin. The cutoff parameters $\rho_{\ell j}$ were tuned to reproduce the binding energies of the ns ground state, and the np and nd excited states and are listed in Table I.

The effective Hamiltonian for the valence electron was diagonalized in a large L-spinor basis [11]. L-spinors can be regarded as a relativistic generalization of the Laguerre-type orbitals that are often used when solving the Schrödinger equation [7]. This basis can be enlarged towards completeness without any linear dependence problems occurring. There is effectively no error due to the incompleteness of the basis set in the present calculation. The present relativistic configuration interaction plus core polarization calculations typically used 50 positive energy and 50 negative energy L-spinors for each (ℓ,j) symmetry. This approach is named the relativistic configuration interaction plus core polarization approach (RCICP). The nonrelativistic approach from which the method is derived is called the configuration interaction plus core polarization (CICP) method [7]. For the purpose of comparison, we present results of calculations using the all-order single-double implementation of relativistic many-body perturbation theory [13,14] (MBPT-SD). The area of commonality between the RCICP and MBPT-SD approaches is that both calculations have minimal numerical uncertainties.

TABLE I. The cutoff parameters $\rho_{\ell j}$ of the core polarization potential.

ℓ	J	$\rho_{\ell j}$ (units of a_0)
s	1/2	2.1360
p	1/2	2.0324
	3/2	2.0289
d	3/2	2.3610
	5/2	2.3633

The two methods use different approximations to treat the interaction with the core and core-valence correlations, but the subsequent calculations within their respective theoretical frameworks have effectively no significant errors due to basis set incompleteness.

III. RESULTS

A. Energies

Table II gives the energies of some of the low-lying states of potassium. One of the interesting aspects of the table concerns the spin-orbit splitting of the $5p_J$ and $6p_J$ states. The polarization potential parameters $\rho_{1,1/2}$ and $\rho_{1,3/2}$ were tuned to give the correct spin-orbit splitting of the $4p_J$ states. Making this choice resulted in the spin-orbit splittings for the $5p_J$ and $6p_J$ states also being very close to experiment. Similarly, tuning the $\rho_{2,3/2}$ and $\rho_{3,5/2}$ parameters to give the correct $3d_J$ spin-orbit splitting also resulted in the spin-orbit splittings for the $4d_J$ and $5d_J$ levels also in agreement with experiment.

B. Dipole matrix elements

Table III gives the reduced matrix elements for a number of the low-lying transitions of the potassium atom. These matrix elements were computed with a modified transition operator [8,16,17], e.g.,

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

The cutoff parameter used in Eq. (5) was 2.176 a_0, the average of the s, p, and d cutoff parameters (note, the weighting of the s was doubled to give it the same weighting as the two p and d orbitals). These matrix elements are compared to the MBPT-SD matrix elements [13,18]. Some reduced matrix elements derived from experiment are also given [13]. It should be noted that there are some small differences between the most recent MBPT-SD reduced matrix elements [13] and earlier work using this method [19].

TABLE II. Theoretical and experimental energy levels (in Hartree) for some of the low-lying states of K. The energies are given relative to the energy of the K$^+$ core. The experimental data were taken from the National Institute of Science and Technology (NIST) tabulation [15].

	J	Present	Experiment
$4s$	1/2	−0.1595191	−0.1595165
$4p$	1/2	−0.1003515	−0.1003516
	3/2	−0.1000886	−0.1000886
$5s$	1/2	−0.0636441	−0.0637124
$3d$	5/2	−0.0613971	−0.0613972
	3/2	−0.0613867	−0.0613867
$5p$	1/2	−0.0469469	−0.0469687
	3/2	−0.0468616	−0.0468832
$4d$	5/2	−0.0346107	−0.0346862
	3/2	−0.0346058	−0.0346813
$6s$	1/2	−0.0344071	−0.0344418
$6p$	1/2	−0.0273728	−0.0273861
	3/2	−0.0273345	−0.0273476

The agreement between the RCICP and MBPT-SD calculations for the larger matrix elements is very good. The two calculations agree to better that 1% for the $4s$-$4p$, $4p$-$5s$, $5p$-$6s$, and $3d$-$4p$ transition manifolds. The same level of agreement is achieved for the nonrelativistic CICP matrix elements. The CICP matrix elements are taken from earlier calculations of dispersion coefficients for the atomic pair involving potassium [7,20–22]. The agreement between the CICP, RCICP, and MBPT-SD matrix is not so good for transitions with much smaller matrix elements such as $4s \to 6p_J$.

The ratio of the line strengths for the $4s \to 4p_J$ transition would be exactly 2.0 in a nonrelativistic model. Experiment and theory both indicate that the difference of the $4s$-$4p$ transition ratio from 2.0 is very small. The current calculation and the MBPT-SD calculation indicate that the matrix element ratio is slightly smaller than 2.0. However, the ratio differs substantially from 2.0 for the $4s \to 5p_J$ and $4s \to 6p_J$ transitions. The main cause for the deviation of the ratio from 2.0 is the slightly different wave function for the spin-orbit doublet arising from the slightly different energies [27]. We have done nonrelativistic calculations and have been able to reproduce the ratios given in Table III by simply tuning the polarization potential to separately give the experimental binding energies of each spin-orbit doublet.

C. Polarizabilities and tune-out wavelengths

The computations of the static polarizabilities utilized the RCICP matrix elements but with the excitation energies for the $4p_J$, $5p_J$, and $6p_J$ set to be those of experiment. The dynamic polarizability is defined as

$$\alpha(\omega) = \sum_n \frac{f_{0n}}{(\epsilon_{0n}^2 - \omega^2)}, \tag{6}$$

where f_{0n} is the oscillator strength for the dipole transition. For low frequencies, the dynamic polarizability can be expanded:

$$\alpha(\omega) = \alpha(0) + S(-4)\omega^2 + \cdots, \tag{7}$$

where $\alpha(0)$ is the static dipole polarizability calculated at $\omega = 0$ and $S(-4)$ is calculated using the oscillator strength sum rule,

$$S(-4) = \sum_n \frac{f_{0n}}{\epsilon_{0n}^4}. \tag{8}$$

Polarizabilities for the potassium ground state from different sources are listed in Table IV. The present RCICP calculation

TABLE III. Comparison of reduced dipole matrix elements (a.u.) for the principal transitions of potassium with experimental values and other calculations.

Transition	RCICP	MBPT-SD [13,18,19,23]	CICP	Expt.
$4s$-$4p_{1/2}$	4.1030	4.098	4.1017	4.102(5) [24] 4.106(4) [25]
$4s$-$4p_{3/2}$	5.8016	5.794	5.8006	5.800(8) [24] 5.807(7) [25]
$4s$-$5p_{1/2}$	0.2634	0.271(5)	0.2696	
$4s$-$5p_{3/2}$	0.3886	0.398(8)	0.3812	
$4s$-$6p_{1/2}$	0.0756	0.084	0.0791	
$4s$-$6p_{3/2}$	0.1162	0.128	0.1118	
$4p_{1/2}$-$5s$	3.8879	3.885(8)	3.9058	
$4p_{3/2}$-$5s$	5.5384	5.54(1)	5.5236	
$5s$-$5p_{1/2}$	9.4967	9.49(3)	9.4918	
$5s$-$5p_{3/2}$	13.410	13.40(4)	13.423	
$5p_{1/2}$-$6s$	8.7766	8.79(2)	8.8088	
$5p_{3/2}$-$6s$	12.490	12.50(2)	12.458	
$4p_{1/2}$-$3d_{3/2}$	7.9662	7.97(3)	7.9812	7.979(35) [13]
$4p_{3/2}$-$3d_{3/2}$	3.5731	3.57(1)	3.5693	3.578(16) [13]
$4p_{3/2}$-$3d_{5/2}$	10.719	10.72(3)	10.708	10.734(47) [13]
$4p_{1/2}$-$4d_{3/2}$	0.1403	0.112(14)	0.1246	
$4p_{3/2}$-$4d_{3/2}$	0.0529	0.040(6)	0.0557	
$4p_{3/2}$-$4d_{5/2}$	0.1553	0.115(15)	0.1672	
$3d_{3/2}$-$5p_{1/2}$	7.1687	7.16(10)	7.1476	
$3d_{3/2}$-$5p_{3/2}$	3.1934	3.19(5)	3.1965	
$3d_{5/2}$-$5p_{3/2}$	9.5743	9.57(10)	9.5895	
$5p_{1/2}$-$4d_{3/2}$	17.040	17.04(6)	17.076	
$5p_{3/2}$-$4d_{3/2}$	7.6432	7.64(3)	7.6367	
$5p_{3/2}$-$4d_{5/2}$	22.932	22.93(8)	22.910	
$\frac{\vert\langle 4p_{3/2}\Vert D\Vert 4s\rangle\vert^2}{\vert\langle 4p_{1/2}\Vert D\Vert 4s\rangle\vert^2}$	1.99935	1.9987 [5]	2.0	2.0005(40) [5] 1.999(4) [24] 2.002(3) [25] 2.01 [26]
$\frac{\vert\langle 5p_{3/2}\Vert D\Vert 4s\rangle\vert^2}{\vert\langle 5p_{1/2}\Vert D\Vert 4s\rangle\vert^2}$	2.17787	2.17964	2.0	2.15 [26]
$\frac{\vert\langle 6p_{3/2}\Vert D\Vert 4s\rangle\vert^2}{\vert\langle 6p_{1/2}\Vert D\Vert 4s\rangle\vert^2}$	2.35799	2.31894	2.0	2.28 [26]

gave essentially the same polarizability, 290.1 a_0^3 as its nonrelativistic CICP predecessor. The nonrelativistic CICP model had its valence energies tuned to experimental energies [in this case, the $(2J+1)$ weighted energy of any spin-orbit doublet], just like the present calculation. The $4s$-$4p_J$ radial matrix elements are dominated by a long-range form of the wave function, and that is practically the same for the CICP and the relativistic RCICP calculations. The present RCICP calculation agrees with experiment [28,29] within the experimental uncertainties.

TABLE IV. Static dipole polarizabilities (in a.u.) for potassium. A short description of the details behind some of the polarizabilities can be found in Ref. [2].

	α_1	$10^3\alpha_2$
Theory: Present RCICP	290.1	5.000
Theory: CICP [7]	290.0	5.005
Theory: MBPT-SD [19]	289.3	5.018
Theory: RCCSD [30]	301.28	5.018
Expt.: $E \times H$ [31]	293(6)	
Expt.: Interferometer [28]	290.8(1.4)	
Hybrid: Sum rule [29]	290.2(8)	

The relativistic coupled cluster calculation (RCCSD) [30] gives a dipole polarizability that is about 3% larger than experiment.

The core polarizability is given by a pseudo-oscillator strength distribution [7,32,33]. The distribution is tabulated in Table V. The distribution is derived from the single-particle energies of the Hartree-Fock core. Each separate (n,ℓ) level is identified with one transition with a pseudo-oscillator strength equal to the number of electrons in the shell. The excitation

TABLE V. Pseudospectral oscillator strength distribution for the potassium core. Energies are given in a.u..

n	ε_n	f_n
1	133.6890020	2.0
2	14.6459330	2.0
3	11.6752580	6.0
4	1.90477720	2.0
5	1.11041710	6.0

TABLE VI. Breakdown of contributions to the potassium ground-state polarizability at different wavelengths.

λ (nm) ω (a.u.)	∞ 0	768.97075 0.059252386	405.9173 0.11224787	404.7217 0.11257945	344.9099 0.13210218	344.7861 0.13214964
$4s$-$4p_{1/2}$	94.8454	−32032.4796	−36.4876	−36.1911	−23.7987	−23.7774
$4s$-$4p_{3/2}$	188.7902	32025.7787	−73.5278	−72.9282	−47.9006	−47.8575
$4s$-$5p_{1/2}$	0.2054	0.2842	38.5906	−364.9459	−0.5438	−0.5424
$4s$-$5p_{3/2}$	0.4469	0.6180	65.4323	468.0690	−1.1901	−1.1870
$4s$-$6p_{1/2}$	0.0144	0.0181	0.0519	0.0527	33.7885	−49.5664
$4s$-$6p_{3/2}$	0.0340	0.0426	0.1221	0.1240	33.7302	117.0156
Remainder valence	0.2426	0.2528	0.2957	0.2963	0.3712	0.3717
α_{core}	5.4708	5.4852	5.5229	5.5232	5.5433	5.5434
Total	290.050	0	0	0	0	0

energy is set by adding a constant to the Koopman energies and tuning the constant until the core polarizability from the oscillator strength sum rule is equal to the known core polarizability. In the present case, the K$^+$ core polarizability was set to 5.47 a.u. [34,35].

The tune-out wavelengths all tend to be close to the wavelengths for excitation of the np_J excited states. There are two scenarios that lead to tune-out wavelengths. In the first, the tune-out wavelength occurs in the middle of an np_J spin-orbit doublet. The wavelength will be shorter than the transition wavelength to the $np_{1/2}$ state and longer than the wavelength to the $np_{3/2}$ state. When this occurs, the dynamic polarizabilities of the $np_{1/2}$ and $np_{3/2}$ states will have the opposite sign and this will lead to a zero in the total dynamic polarizability occurring for all spin-orbit doublets. The second scenario leading to a tune-out wavelength occurs when the wavelength is shorter than that for excitation of the $4p_J$ states. When this occurs, the contribution to the dynamic polarizability from the $4p_J$ states becomes negative. This leads to a series of tune-out wavelengths occurring just below the excitation energies of the $5p_{1/2}, 6p_{1/2}, 7p_{1/2}, \ldots$states.

Simplified expressions can be used to describe the dynamic polarizabilities in the vicinity of the tune-out wavelengths. The first tune-out wavelength occurs when the wavelength lies between the $4p_{1/2}$ and $4p_{3/2}$ resonant wavelengths. The dynamic polarizability here can be written,

$$\alpha_1(\omega) = \frac{f_{4p_{1/2}}}{\left(\Delta E^2_{4\text{p}_{1/2}} - \omega^2\right)} + \frac{f_{4p_{3/2}}}{\left(\Delta E^2_{4\text{p}_{3/2}} - \omega^2\right)} + \alpha_{\text{rem}}(\omega), \tag{9}$$

where $\alpha_{\text{rem}}(\omega)$ is the remainder part of dynamic dipole polarizability. The energy difference $\Delta E_{4\text{p}_{3/2}}$ can be parametrized as $\Delta E_{4\text{p}_{3/2}} = \Delta E_{4\text{p}_{1/2}}(1+\delta)$. Parametrizing the line strength S (the square of the reduced matrix element) as

$$S(4s \to 4p_{3/2}) = S(4s \to 4p_{1/2})(2+R) \tag{10}$$

leads to

$$\alpha_1(\omega) = \frac{f_{4p_{1/2}}}{\left(\Delta E^2_{4\text{p}_{1/2}} - \omega^2\right)} + \frac{f_{4p_{1/2}}(2+R)(1+\delta)}{\left[\left(\Delta E_{4\text{p}_{1/2}}\right)^2(1+\delta)^2 - \omega^2\right]} + \alpha_{\text{rem}}(\omega). \tag{11}$$

The dipole oscillator strength $f_{4p_{1/2}}$ is obtained by multiplying the reduced matrix element with the experimental $4s \to 4p_{1/2}$ energy difference. The value of R is simply the ratio of computed line strength coming from the RCICP calculations. It can be seen from Table VI that the remainder polarizability, $\alpha_{\text{rem}}(\omega)$ only makes a small contribution to the total polarizability. The remainder polarizability varies relatively slowly with wavelength in the vicinity of the tune-out wavelength.

Table VII illustrates the variation in the tune-out wavelength with respect to variations in R and $\alpha_{\text{rem}}(\omega)$. The contributions to the polarizability from the $4p_{1/2}$ and $4p_{3/2}$ transitions are 5000 times larger than those from every other transition. A change in $\alpha_{\text{rem}}(\omega)$ of 1.0 a.u leads to the tune-out wavelength changing by 0.00002 nm. The tune-out wavelength is much more sensitive to variations in R. A change in R to -0.005 leads to the tune-out wavelength changing by 0.0016 nm. A value of $R = -0.005$ is 3 times larger than the MBPT-SD value and is seven times larger than the RCICP value of R.

A different parametrization should be used in the vicinity of the excited states with $n > 4$.

$$\alpha_1(\omega) = \alpha_{4p}(\omega) + \alpha_{\text{rem}}(\omega) + \frac{f_{np_{1/2}}}{\left(\Delta E^2_{\text{np}_{1/2}} - \omega^2\right)} + \frac{f_{np_{1/2}}(2+R)(1+\delta)}{\left[\left(\Delta E_{\text{np}_{1/2}}\right)^2(1+\delta)^2 - \omega^2\right]}. \tag{12}$$

Here the polarizability arising from the $4s \to 4p_J$ transitions is retained as a separate term since it is much larger than the remainder.

The tune-out wavelengths in the vicinity of the $5p_J$ levels illustrate clearly how the $\alpha_{\text{rem}}(\omega)$ and R are of different importance depending on whether the tune-out energy is located between the $5p_{1/2}$ and $5p_{3/2}$ levels or before the $5p_{1/2}$ level.

Table VI shows that the tune-out wavelength at energies below the $5p_{1/2}$ excitation threshold is caused by the cancellation of the $5p_J$ and core contributions with those coming from the $4p_J$ levels. This tune-out wavelength is effectively determined by ratio of the $4p$ and $5p$ oscillator strengths. The contribution of the core is small in absolute terms, and a 5% uncertainty in the core polarizability will have a small effect on the tune-out wavelength. The tune-out wavelength is predominantly determined by the relative size of the $4s \to 4p_J$ and $4s \to 5p_J$ matrix elements. This can be seen from Table VII. Increasing the $4s \to 5p_J$ matrix elements by 3% (roughly the difference with the MBPT-SD matrix elements) leads to the tune-out wavelength increasing by 0.077 nm. Changing the value of R by 0.02 leads to the tune-out wavelength changing by 0.007 nm. It should be noted

TABLE VII. Values of the tune-out wavelength for the K atom. The experimental transition wavelengths are taken from [36,37]. The first entry lists the tune-out wavelength as computed with RCICP matrix elements. The other entries exhibit the changes to the tune-out wavelengths when changes are made to matrix elements underlying the oscillator strength sums.

Resonance	ω (a.u.)	λ (nm)
$\Delta E_{4s-4p_{1/2}}$	0.059164859	770.10836
$\Delta E_{4p_{3/2}}$	0.059427807	766.70089
$R = -0.0006476$, $\alpha_{\mathrm{rem}}(\omega) = 6.701$	0.059252386	**768.97077**
$\alpha_{\mathrm{rem}}(\omega) = 5.701$	0.059252387	768.97075
$R = -0.005$	0.059252513	768.96912
MBPT-SD [4]	0.0592524(2)	768.971(3)
Expt. [5]	0.0592523(1)	768.9712(15)
$\Delta E_{4s-5p_{1/2}}$	0.11254778	404.8356
$\Delta E_{4s-5p_{3/2}}$	0.11263324	404.5285
$R = 0.17787$, $\alpha_{\mathrm{rem}}(\omega) = -104.023$	0.11224787	**405.9173**
$R = 0.15787$	0.1122499	405.9100
$\lvert\langle 5p_J \Vert D \Vert 4s\rangle\rvert \times 1.03$	0.1122120	405.9943
MBPT-SD [4]	0.11223(1)	405.98(4)
$R = 0.17787$, $\alpha_{\mathrm{rem}}(\omega) = -103.300$	0.11257946	**404.7217**
$R = 0.15787$,	0.11257967	404.7210
$\lvert\langle 5p_J \Vert D \Vert 4s\rangle\rvert \times 1.03$	0.11257898	404.7228
MBPT-SD [4]	0.11258(1)	404.72(4)
$\Delta E_{4s-6p_{1/2}}$	0.13213040	344.8363
$\Delta E_{4s-6p_{3/2}}$	0.13216885	344.7359
$R = 0.35799$, $\alpha_{\mathrm{rem}}(\omega) = -67.5188$	0.13210218	**344.9099**
$R = 0.30799$,	0.13210256	344.9089
$\lvert\langle 6p_J \Vert D \Vert 4s\rangle\rvert \times 1.10$	0.13209360	344.9323
MBPT-SD [4]	0.1320933(4)	344.933(1)
$R = 0.35799$, $\alpha_{\mathrm{rem}}(\omega) = -67.4492$	0.13214964	**344.7861**
$R = 0.30799$,	0.13214992	344.7853
$\lvert\langle 6p_J \Vert D \Vert 4s\rangle\rvert \times 1.10$	0.13214825	344.7897

that our definition of R does imply an overall increase in the total oscillator strength to the $5p_J$ states.

The tune-out wavelength at the energies between the $5p_{1/2}$ and $5p_{3/2}$ levels does have some dependence on α_{rem} since it now incorporates the contribution from the $4s \rightarrow 4p_J$ transitions. A 5% change in the matrix element leads to a change in the tune-out wavelength of 0.0024 nm; this is 60 times smaller than the effect on the tune-out wavelength at 405.9173 nm. The sensitivity to a change in the value of R by 0.02 was only 0.0007 nm. In relative terms, the tune-out wavelength is more sensitive to the value of R than $\lvert\langle 5p_J \Vert D \Vert 4s\rangle\rvert$ in the $5p_{1/2}$ to $5p_{3/2}$ energy gap, than it is in the energy region before $5p_{1/2}$ excitation.

Table VII also gives the tune-out wavelengths in the vicinity of the $6p_J$ levels. Once again the tune-out wavelengths are very sensitive to the absolute size of the $\lvert\langle 6p_J \Vert D \Vert 4s\rangle\rvert$ transition matrix element. A 10% change in the matrix element (the difference between the RCICP and MBPT-SD calculations) leads to a change of 0.0234 nm in the tune-out wavelength just below the $6p_{1/2}$ threshold. The considerations that determine the values of the tune-out wavelengths in the vicinity of the $5p_J$ states also apply to the tune-out wavelengths in the vicinity of the $6p_J$ states.

Finally, it is noted that the tune-out wavelengths were also evaluated using the MBPT-SD matrix elements in Table III but with other aspects of the calculation taken from the RCICP calculation. The resulting tune-out wavelengths were identical to the MBPT-SD tune-out wavelengths in Table VII to all quoted digits.

D. Uncertainties

Part of this manuscript is focused on the prediction of the tune-out wavelengths, but another and possibly more important part concerns the extraction of useful atomic structure information from an experimental value of the tune-out wavelength. Knowledge of the np_J tune-out wavelengths permits the determination of the np_J oscillator strengths to a high degree of precision.

The most important atomic parameters that contribute to the long wavelength dynamic polarizability are listed in Table VIII. These parameters are derived from the RCICP calculations and uncertainties are estimated by examination of the difference with experiment or MBPT-SD calculations.

The determination of the $4p_{1/2} : 4p_{3/2}$ line strength ratio is only weakly dependent on the value of the non-$4p$ terms in the dynamic polarizability since these terms are small.

Knowledge of the np_J tune-out wavelengths permits the determination of the np_J oscillator strengths for $n > 4$ to a high degree of precision. The polarizability becomes zero when the contributions to the polarizability from the np_J levels and the remainder cancel exactly. The biggest terms in the remainder are α_{4p_J} and α_{core} which together constitute 99% of the remainder. Moreover, both of these terms are known with a reasonable degree of precision.

TABLE VIII. Tabulation of atomic parameters, with estimated uncertainties that can be used as reduced dipole matrix elements (a.u.) for the principal transitions of potassium with experimental values and other calculations.

Parameter	RCICP
$4s$-$4p_{1/2}$	4.1030(7)
$4s$-$4p_{3/2}$	5.8016(10)
$4s$-$5p_{1/2}$	0.2634(8)
$4s$-$5p_{3/2}$	0.3886(100)
$4s$-$6p_{1/2}$	0.0756(100)
$4s$-$6p_{3/2}$	0.1162(14)
α_{core}	5.4708(1000)
$S_{\text{core}}(-4)$	4.10(80)
$\alpha_{\text{core-valence}}$ [23]	−0.13
$\alpha_{\text{RemainderValence}}$	0.243(111)
$S_{\text{RemainderValence}}(-4)$	2.67(134)

The uncertainties in the experimental $4s \rightarrow 4p_J$ line strengths do not exceed 0.3% and the RCICP transition matrix element lies between two experimental estimates [24,25]. There is 2% variation between the RCICP and MBPT-SD estimates of the $4s \rightarrow 5p_J$ matrix elements and a 10% variation between $4s \rightarrow 6p_J$ matrix elements. Taken together, $4s \rightarrow 5p_J$ and $4s \rightarrow 6p_J$ would contribute less than 0.01 a.u. to the uncertainty of the total polarizability at $\omega = 0$ a.u.

The uncertainty in the core polarizability of 5.47 a.u. itself is stated to be about 2% [34]. This polarizability was based on the binding energies of the $4f$, $6f$, and $9f$ levels of potassium using spectral data from 1955 [38]. There is scope for an improvement in the precision of the core polarizability and this could be easily accomplished by spectroscopic experiments that measured the energies of the ng levels. The construction of pseudo-oscillator strength distribution for the K$^+$ core permits the energy variation of α_{core} to be incorporated into the calculation. The uncertainty of 20% was estimated by using the same procedure to construct the pseudo-oscillator strength distribution to argon and making reference to a highly accurate pseudo-oscillator strength distribution [33].

The core-valence term $\alpha_{\text{core-valence}}$ is a term that compensates for Pauli-principle violating excitations from the core to the valence $4s$ orbital. This value is sourced from an MBPT-SD calculation [23] since it is not incorporated in the RCICP calculation. No uncertainty has been assigned to this contribution to the polarizability.

The valence remainder term contains contributions from highly excited discrete transitions as well as contributions from the continuum. The present value is 0.243 a.u. at $\omega = 0$. This is more than twice the size of a MBPT-SD estimate of 0.07 a.u. [23]. However, much of the MBPT-SD valence remainder is computed in the DF approximation. We have performed calculations in the DF approximation, and the DF oscillator strengths embedded in the continuum beyond the cooper minimum at 0.010 a.u. [39] are typically a factor of 3 and 4 smaller than the RCICP oscillator strengths at those energies Nevertheless, the uncertainty in this term has been conservatively assessed at 50%. Comparisons of the RCICP and MBPT-SD oscillator strength distributions in the continuum, and further comparisons with experimental photoionization cross sections would be helpful in refining the estimate and uncertainty of this rather small term.

The parameter set and error budget in Table VIII can be utilized to help convert tune-out wavelengths into oscillator strengths. There is room for improvement in the parameter set. Measurements of the tune-out wavelengths near the $5p_J$ excitation will result in better estimates of the $5p_J$ matrix elements. Parameters obtained from theory do not have to be exclusively obtained from a single calculation, for example, some information from Table VIII might be best obtained from a MBPT-SD calculation while others, e.g., the valence remainder might be best estimated from the RCICP calculation or some RCICP/MBPT-SD hybrid.

IV. CONCLUSION

The five lowest tune-out wavelengths for the potassium atom are computed by a relativistic structure model. A detailed analysis is performed regarding the contribution that the different terms make to the polarizability. The results illustrate the dependence of the tune-out wavelengths on a relatively small number of atomic parameters.

The lowest energy tune-out wavelength is primarily determined by the ratio of the line strengths for the $4s \rightarrow 4p_J$ transitions. The present calculation, and the MBPT-SD calculation are in agreement with existing experimental data [5]. The precision of the experiment would need to improve by an order of magnitude to provide a stringent test of the $4p_J$ state line strength ratio. However, Holmgren *et al.* [5] suggest that it might be possible to improve the precision by up to 3 orders of magnitude.

The tune-out wavelengths near the $5p_J$ excited states are most sensitive to the ratio of the $4s \rightarrow 4p_J$ and $4s \rightarrow 5p_J$ matrix elements. The remainder term incorporating all transitions except for the $4s \rightarrow 5p_J$ is dominated by the $4s \rightarrow 4p_J$ and core polarizabilities which comprise 99.5% of the remainder polarizability. The tune-out wavelengths here provide a means to determine the $5s \rightarrow 5p_J$ oscillator strengths to high precision. Measurement of the tune-out wavelength to a precision of 0.01 nm would lead to oscillator strengths with a precision better than 1%.

Holmgren *et al.* [5] suggested that measurements of the tune-out wavelengths near the $5p_{1/2}$ excited states could be used to determine the core polarizability. We do not agree with this statement. The remainder terms near the $5p_J$ excitation are dominated by $\alpha_{4p}(\omega)$ and $\alpha_{\text{core}}(\omega)$. The uncertainty in $\alpha_{4p}(\omega)$ at 405 nm would be about 0.3 a.u. and this uncertainty limits the precision with which the core polarizability could be measured. The preferred approach is to treat the $\alpha_{4p}(\omega)$ and $\alpha_{\text{core}}(\omega)$ polarizabilities as known quantities with relatively small uncertainties and use measurements of the tune-out wavelength to extract precision values of the $5p_J$ oscillator strengths.

ACKNOWLEDGMENTS

This research was supported by the Australian Research Council Discovery Project No. DP-1092620. We thank Dr. M. S. Safronova for helpful communications regarding her matrix elements.

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