

# Tune-out wavelengths of alkali-metal atoms and their applications

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Using first-principles calculations, we identify “tune-out” optical wavelengths,  $\lambda_{\text{zero}}$ , for which the ground-state frequency-dependent polarizabilities of alkali-metal atoms vanish. Our approach uses high-precision, relativistic all-order method in which all single, double, and partial triple excitations of the Dirac-Fock wave functions are included to all orders of perturbation theory. We discuss the use of tune-out wavelengths for sympathetic cooling in two-species mixtures of alkali metals with group II and other elements of interest. Special cases in which these wavelengths coincide with strong resonance transitions in a target system are identified.

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## I. INTRODUCTION

The realization of mixtures of trapped ultracold atomic gases [1–5] has opened new paths toward the formation of ultracold diatomic molecules [6–10], quantum-state control of chemical reactions [11], prospects for quantum computing with polar molecules [12–14], tests of fundamental symmetries [15–17] and studies of fundamental aspects of correlated many-body systems [18], and dilute quantum degenerate systems [19–23]. Cotrapped diamagnetic-paramagnetic mixtures have also made possible experimental realization of interspecies Feshbach resonances [24–26], two-species Bose-Einstein condensates and mixed Bose-Fermi and Fermi-Fermi degenerate gases [18,27–29].

In an optical lattice, atoms can be trapped in the intensity maxima or minima of the light field by the optical dipole force [30]. This force arises from the dispersive interaction of the induced atomic dipole moment with the intensity gradient of the light field and is proportional to the ac polarizability of the atom. When its ac polarizability vanishes, as can happen at certain wavelengths, an atom experiences no dipole force and thus is unaffected by the presence of an optical lattice. Our present work provides accurate predictions of the  $\lambda_{\text{zero}}$  which lead to zero Stark shifts for alkali-metal atoms. These wavelengths have been introduced as “tune-out wavelengths” by LeBlanc and Thywissen [31].

We suggest some possible uses for such wavelengths, all of which take advantage of the fact (demonstrated below), that tune-out wavelengths are highly dependent upon atomic species and state. For a given atomic species and state A, let  $L_A$  designate an optical lattice or trap made with light at one of the tune-out wavelengths of A. We start with a model configuration consisting of the gas A embedded in  $L_A$  and confined by another trap, T. Some process is performed on the gas, after which T is turned off. Members of A will depart and  $L_A$  may confine whatever is left. For example, one might photoassociate some A atoms into dimers during the initial period and thereby be left with a nearly pure population of dimers trapped in  $L_A$  at the end. LeBlanc and Thywissen [31] have pointed out the advantage of tune-out wavelengths for traps containing two species. If another species B is added to the model configuration, it will ordinarily be affected by  $L_A$ ,

so B can be moved by shifting  $L_A$  while A remains unaffected. Schemes of this type have been used for entropy transfer and controlled collisions between  $^{87}\text{Rb}$  and  $^{41}\text{K}$  [32–34]. For bichromatic optical lattice schemes, such as those discussed by Brickman Soderberg, *et al.* [35,36], it could be useful to incorporate  $L_B$  into the model configuration, so as to be able to move A and B completely independently. In another application, a Sr lattice at a  $^3P_0$  tune-out wavelength was suggested for realization of quantum information processing [37].

In the next section, we briefly discuss the calculation of frequency-dependent polarizabilities of alkali-metal atoms. In Sec. III, we present the tune-out wavelengths for the alkali metals from Li to Cs and discuss some of their applications.

## II. FREQUENCY-DEPENDENT POLARIZABILITIES

The background to our approach to calculation of atomic polarizabilities is treated in a recent review article [38]. Here we summarize points salient to the present work. The frequency-dependent scalar polarizability  $\alpha_0(\omega)$  of an alkali-metal atom in its ground state  $v$  may be separated into a contribution from the core electrons,  $\alpha_{\text{core}}$ , a core modification due to the valence electron,  $\alpha_{vc}$ , and a contribution from the valence electron,  $\alpha_0^v(\omega)$ . Since core electrons have excitation energies in the far-ultraviolet region of the spectrum, the core polarizability depends weakly on  $\omega$  for the optical frequencies treated here. Therefore, we approximate the core polarizability by its dc value as calculated in the random-phase approximation (RPA) [39], an approach that has been quite successful in previous applications. The core polarizability is corrected for Pauli blocking of core-valence excitations by introducing an extra term  $\alpha_{vc}$ . For consistency, this is also calculated in RPA. Therefore, the ground-state polarizability may be separated as

$$\alpha_0(\omega) = \alpha_{\text{core}} + \alpha_{vc} + \alpha_0^v(\omega). \quad (1)$$

The valence contribution to the static ac polarizability is calculated using the sum-over-states approach [40]:

$$\alpha_0^v(\omega) = \frac{2}{3(2j_v + 1)} \sum_k \frac{\langle k \| D \| v \rangle^2 (E_k - E_v)}{(E_k - E_v)^2 - \omega^2}, \quad (2)$$

where  $\langle k \| D \| v \rangle$  is the reduced electric-dipole ( $E1$ ) matrix element. In this equation,  $\omega$  is assumed to be at least several linewidths off resonance with the corresponding transitions. We use the shorter designation  $\alpha_0$  for frequency-dependent scalar polarizability below. Unless stated otherwise, we use the conventional system of atomic units, a.u., in which  $e$ ,  $m_e$ ,  $4\pi\epsilon_0$ , and the reduced Planck constant  $\hbar$  have the numerical value 1. Polarizability in a.u. has the dimension of volume, and its numerical values presented here are expressed in units of  $a_0^3$ , where  $a_0 \approx 0.052918$  nm is the Bohr radius. The atomic units for  $\alpha$  can be converted to SI units via  $\alpha/h$  [ $\text{Hz}/(\text{V}/\text{m})^2$ ] =  $2.48832 \times 10^{-8} \alpha$  [a.u.], where the conversion coefficient is  $4\pi\epsilon_0 a_0^3/h$  and the Planck constant  $h$  is factored out.

The calculation of the ground-state frequency-dependent polarizabilities in alkali-metal atoms has been previously discussed in [41,42], and we give only brief summary of the approach. The sum over intermediate  $k$  states in Eq. (2) converges rapidly. Therefore, we separate the valence state polarizability into two parts:  $\alpha_{\text{main}}$ , containing the contributions from the few lowest  $np$  states, and the remainder,  $\alpha_{\text{tail}}$ . We note that our calculations are carried out with the finite basis set constructed using  $B$  splines [43] making the sum finite. In the calculation of  $\alpha_{\text{main}}$ , we use the experimental values compiled in Ref. [44] along with their uncertainties for the first  $ns$ - $np$  matrix elements, for example the  $4s$ - $4p_j$  matrix elements in K. For all other terms, we use the relativistic all-order values [44,45] of the matrix elements and the experimental values of the energies [46–48]. In the relativistic all-order method, all single-double (SD) or single-double and partial valence triple (SDpT) excitations of the Dirac-Fock (DF) wave function are included to all orders of perturbation theory [40,44,49]. We conduct additional semiempirical scaling of our all-order values (SD<sub>sc</sub>) where we expect scaled values to be more accurate or for more accurate evaluation of the uncertainties. Our scaling procedure and evaluation of the uncertainties of the all-order results have been recently discussed in Ref. [50]. Briefly, the uncertainties of the all-order matrix elements are given by the spread of their SD, SDpT, SD<sub>sc</sub>, and SDpT<sub>sc</sub> values. These are also used to calculate the uncertainties in the state-by-state contributions to the frequency-dependent polarizability. The tail contributions  $\alpha_{\text{tail}}$  are calculated in the DF approximation using complete basis set functions that are linear combinations of  $B$  splines [51]. In the cases treated here, the tail contribution is of the order of 1% of the net valence contribution  $\alpha_0^v$ .

We define the tune-out wavelength  $\lambda_{\text{zero}}$  as the wavelength where the ac polarizability of the ground state vanishes. In practice, we calculated  $\alpha_0(\omega)$  for a range of values in the vicinity of relevant resonances and identified values of  $\omega$  where the polarizability turned to zero with sufficient numerical accuracy.

We illustrate the cancellation of all contributions to  $5s$  Rb polarizability at  $\lambda_{\text{zero}} = 423.0448$  nm in Table I. Since this wavelength is between  $5s$ - $5p_{3/2}$  and  $5s$ - $6p_{1/2}$  resonances, the contributions of the  $5p_j$  and  $6p_j$  terms strongly dominate. However, the contribution from the core is significant (11% of the largest valence term). This table shows that  $\lambda_{\text{zero}}$  is located where the valence contribution to the polarizability cancels the adjusted core contribution, a feature that is common to all the cases treated here. The zero-crossing point is in the close

TABLE I.  $5s$ - $np$  contributions to the frequency-dependent polarizability of the ground state of Rb at  $\lambda_{\text{zero}} = 423.0448$  nm =  $1/(23638.16 \text{ cm}^{-1})$ . Absolute values of electric-dipole matrix elements are expressed in a.u. ( $ea_0$ ), and the corresponding energy differences are expressed in conventional wave-number units ( $\text{cm}^{-1}$ ).

Contribution	$ \langle 5s \  D \  np_{1/2} \rangle $	$E_{np_j} - E_{5s}$	$\alpha_0$
$5p_{1/2}$	4.231	12 579.0	-41.130
$6p_{1/2}$	0.325	23 715.1	50.235
$7p_{1/2}$	0.115	27 835.0	0.124
$8p_{1/2}$	0.059	29 835.0	0.023
$np_{1/2}$ tail			0.085
$5p_{3/2}$	5.978	12 816.5	-84.938
$6p_{3/2}$	0.528	23 792.6	66.140
$7p_{3/2}$	0.202	27 870.1	0.383
$8p_{3/2}$	0.111	29 853.8	0.081
$np_{3/2}$ tail			0.285
$\alpha_{\text{core}}$			9.076
$\alpha_{vc}$			-0.367
$\alpha_0^v$			-8.712
Total $\alpha_0(\omega)$			0.00

vicinity of the  $5s$ - $6p_{1/2}$  resonance owing to the relative size of the  $5s$ - $5p_j$  and  $5s$ - $6p_j$  reduced electric-dipole matrix elements given in the second column of Table I. The  $5s$ - $6p$  matrix elements are more than an order of magnitude smaller than the  $5s$ - $5p$  matrix elements. Since polarizability contributions are proportional to the square of the matrix element, the denominators of the  $6p_j$  terms have to become very small to cancel out the  $5p$  contributions.

This tune-out wavelength is illustrated in Fig. 1 where we plot the ground-state polarizability of the Rb atom in a.u. in the vicinity of the  $5s$ - $6p_j$  resonances. Another zero-crossing point shown in the figure is located between  $5s$ - $6p_{1/2}$  and  $5s$ - $6p_{3/2}$  resonances, as expected. The next tune-out wavelength will be located close to the  $5s$ - $7p_{1/2}$  resonance since the values of the matrix elements continue to decrease with  $n$ .

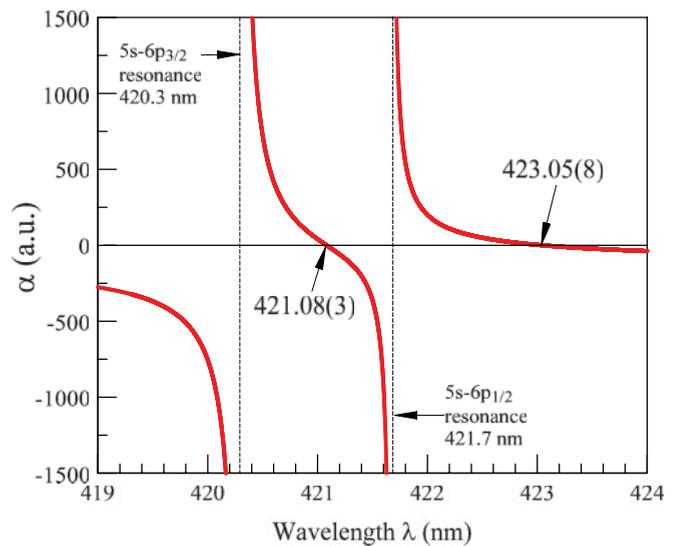


FIG. 1. (Color online) Frequency-dependent polarizability of the Rb ground state. The first two tune-out wavelengths are marked with arrows.

### III. RESULTS AND APPLICATIONS

In Table II, we list the vacuum  $\lambda_{\text{zero}}$  wavelengths for alkali-metal atoms from Li to Cs. For convenience of presentation, we also list the resonant wavelength  $\lambda_{\text{res}}$  in vacuum in the relevant range of wavelengths. We order the lists of the resonant wavelengths and  $\lambda_{\text{zero}}$  to indicate the respective placements of  $\lambda_{\text{zero}}$  and their distances from resonances. The resonant vacuum wavelength values are obtained from energy levels from National Institute of Standards and Technology (NIST) database [46] with the exception of the  $2s-2p_{1/2}$  and  $2s-2p_{3/2}$  transition wavelengths for  ${}^6\text{Li}$  and  ${}^7\text{Li}$  that are taken from recent measurements [52].

Since alkali-metal ground states have electric dipole transitions only to  $p$  states, their polarizabilities will cross zero only between two  $ns-n'p$  resonances. We set the wavelength of the  $ns-(n+2)p_{1/2}$  resonance as a lower-wavelength bound for our search. The fine structure of the  $(n+2)p$  level is sufficiently small for all alkali metals to make the zero point between  $ns-(n+2)p_{1/2}$  and  $ns-(n+2)p_{3/2}$  relatively difficult to use in practice, so we do not list it. We omit the  $\lambda_{\text{zero}}$  between  $2s-3p_j$  resonances for the same reason. The wavelengths of the next zero crossing near the  $ns-(n+3)p_{1/2}$  resonances are in the ultraviolet and not as readily accessible in most laboratories, so we have not calculated them. However, this would be a routine matter for future work. There are no  $\lambda_{\text{zero}}$  at wavelengths greater than those of the primary  $ns-np_{1/2}$  resonances. Within these constraints, we have found four  $\lambda_{\text{zero}}$  for Na, K, Rb, and Cs and three  $\lambda_{\text{zero}}$  for Li, as shown in Table I.

The stated uncertainties in the  $\lambda_{\text{zero}}$  values are taken to be the maximum difference between the central value and the crossing of the  $\alpha_0 \pm \delta\alpha_0$  with zero, where  $\delta\alpha_0$  is the uncertainty in the ground-state polarizability value at that wavelength. The uncertainties in the values of polarizabilities are obtained by adding uncertainties in the individual polarizability contributions in quadrature.

We find small but significant differences in the first tune-out wavelengths of  ${}^6\text{Li}$  and  ${}^7\text{Li}$  due to the isotope shift. These values refer to the centers of gravity of all hyperfine states and do not take into account the hyperfine structure. Therefore, this  $\lambda_{\text{zero}}$  and the corresponding  $2s-2p_j$  resonance wavelengths are listed separately. We verified that isotope shift of the  $2s-2p$  transitions in Li does not affect the next tune-out wavelength, 324.18(6) nm, so we use NIST data for the other transitions. We also investigated possible dependence of the first tune-out wavelengths on the isotope shift for  ${}^{39}\text{K}$ ,  ${}^{40}\text{K}$ ,  ${}^{41}\text{K}$ ,  ${}^{85}\text{Rb}$ , and  ${}^{87}\text{Rb}$ . The  $D_1$  ( $4s-4p_{1/2}$ ) and  $D_2$  ( $4s-4p_{3/2}$ ) line wavelengths for  ${}^{39}\text{K}$ ,  ${}^{40}\text{K}$ , and  ${}^{41}\text{K}$  have been measured using a femtosecond laser frequency comb by Falke *et al.* [53]. We carry out three calculations of the first tune-out wavelength using  $D_1$ ,  $D_2$  wavelengths for the specific isotope in our calculations. The resulting value for  ${}^{39}\text{K}$  and  ${}^{40}\text{K}$ , 768.971(3) nm, is the same as the value quoted in Table II. The  ${}^{41}\text{K}$  value is 768.970(3) nm, with the difference being well below our quoted uncertainty. The calculations of the first tune-out wavelength in Rb using  $D_1$  and  $D_2$  frequencies for  ${}^{85}\text{Rb}$  and  ${}^{87}\text{Rb}$  listed in [54,55] gave results identical to result from Table II, 790.034(7) nm that was obtained using NIST data. We note that our values for the first tune-out wavelengths are in good agreement with the LeBlanc and Thywissen [31] calculations with the exception of their value for  ${}^{40}\text{K}$ .

TABLE II. Tune-out wavelengths  $\lambda_{\text{zero}}$  for alkali-metal atoms from Li to Cs. The resonant wavelengths  $\lambda_{\text{res}}$  for relevant transitions are also listed. The wavelengths (in vacuum) are given in nm.

Atom	Resonance	$\lambda_{\text{res}}$	$\lambda_{\text{zero}}$
${}^6\text{Li}$	$2s-2p_{1/2}$	670.992 478	
${}^6\text{Li}$			670.987 445(1)
${}^6\text{Li}$	$2s-2p_{3/2}$	670.977 380	
${}^7\text{Li}$	$2s-2p_{1/2}$	670.976 658	
${}^7\text{Li}$			670.971 626(1)
${}^7\text{Li}$	$2s-2p_{3/2}$	670.961 561	
Li			324.18(6)
Li	$2s-3p_{1/2}$	323.3576	
Li	$2s-3p_{3/2}$	323.3566	
Li			274.911(7)
Li	$2s-4p_{1/2}$	274.2001	
Na	$3s-3p_{1/2}$	589.7558	
Na			589.5565(3)
Na	$3s-3p_{3/2}$	589.1583	
Na			331.905(3)
Na	$3s-4p_{1/2}$	330.3929	
Na			330.3723
Na	$3s-4p_{3/2}$	330.3319	
Na			285.5817(8)
Na	$3s-5p_{1/2}$	285.3850	
K	$4s-4p_{1/2}$	770.1083	
K			768.971(3)
K	$4s-4p_{3/2}$	766.7009	
K			405.98(4)
K	$4s-5p_{1/2}$	404.8356	
K			404.72(4)
K	$4s-5p_{3/2}$	404.5285	
K			344.933(1)
K	$4s-6p_{1/2}$	344.8363	
Rb	$5s-5p_{1/2}$	794.9789	
Rb			790.034(7)
Rb	$5s-5p_{3/2}$	780.2415	
Rb			423.05(8)
Rb	$5s-6p_{1/2}$	421.6726	
Rb			421.08(3)
Rb	$5s-6p_{3/2}$	420.2989	
Rb			359.42(3)
Rb	$5s-7p_{1/2}$	359.2593	
Cs	$6s-6p_{1/2}$	894.5929	
Cs			880.25(4)
Cs	$6s-6p_{3/2}$	852.3472	
Cs			460.22(2)
Cs	$6s-7p_{1/2}$	459.4459	
Cs			457.31(3)
Cs	$6s-7p_{3/2}$	455.6557	
Cs			389.029(4)
Cs	$6s-8p_{1/2}$	388.9714	

The first tune-out wavelength in Rb has been measured to be 789.85(1) nm in [32]. Some discrepancy with our result is most likely due to approximate linear polarization of the beam in [32]. The difference is compatible with a shift in the tune-out wavelength caused by few percent spurious  $\sigma^-$  polarization component [56].

TABLE III. Wavelength (in vacuum) of selected transitions in Mg, Ca, Zn, Cd, Sr, Ba, Hg, Yb, Dy, Ho, and Er in nm. Comparison of these values with tune-out wavelengths listed in Table II yields many instances of resonant transitions that are very close to  $\lambda_{\text{zero}}$  in alkali metals.

Atom	Transition	Wavelength	Transition	Wavelength
Mg	$3s^2\ ^1S_0-3s3p\ ^1P_1$	285.3	$3s^2\ ^1S_0-3s3p\ ^3P_1$	457.2
Ca	$4s^2\ ^1S_0-4s4p\ ^1P_1$	422.8	$4s^2\ ^1S_0-4s4p\ ^3P_1$	657.5
Sr	$5s^2\ ^1S_0-5s5p\ ^1P_1$	460.9	$5s^2\ ^1S_0-5s5p\ ^3P_1$	689.5
Ba	$6s^2\ ^1S_0-6s6p\ ^1P_1$	553.7	$6s^2\ ^1S_0-6s6p\ ^3P_1$	791.4
Zn	$4s^2\ ^1S_0-4s4p\ ^1P_1$	213.9	$4s^2\ ^1S_0-4s4p\ ^3P_1$	307.7
Cd	$5s^2\ ^1S_0-5s5p\ ^1P_1$	228.9	$5s^2\ ^1S_0-5s5p\ ^3P_1$	326.2
Hg	$6s^2\ ^1S_0-6s6p\ ^1P_1$	184.9	$6s^2\ ^1S_0-6s6p\ ^3P_1$	253.7
Yb	$6s^2\ ^1S_0-6s6p\ ^1P_1$	398.9	$6s^2\ ^1S_0-6s6p\ ^3P_1$	555.8
Dy	$4f^{10}6s^2\ ^5I_8-4f^{10}6s6p(^1P_1)\ J = 9$	421.3		
Er	$4f^{12}6s^2\ ^3H_6-4f^{12}6s6p(^3P_1)\ J = 7$	582.8		
Ho	$4f^{11}6s^2\ ^4I_{15/2}-4f^{11}6s6p(^3P_1)\ J = 17/2$	598.5		
Ho	$4f^{11}6s^2\ ^4I_{15/2}-4f^{11}6s6p(^1P_1)\ J = 13/2$	416.4		

Below, we identify two main applications of tune-out wavelengths. First, these wavelengths are advantageous for cooling of group II and other more complicated atoms, by sympathetic cooling using an accompanying alkali-metal atom.

Recently, group II atoms have been the subject of various experiments and proposals in atomic clock research and quantum information. BECs of  $^{84}\text{Sr}$  have been reported recently by two groups [57,58]. The element Yb has four boson and two fermion isotopes, all of which have been cooled to the microkelvin range. Several exciting new prospects for quantum information processing with the ground-state nuclear spin have recently been identified in group II elements [37]. Also, Sr or Yb are useful for polarized mixtures of fermions, or Bose-Fermi mixtures, where isotopic mixtures can be studied.

More complex systems have become of interest in the development of frequency standards and quantum information processing schemes. For example, the rare earth holmium is a candidate for quantum information applications [59] due to its rich ground-state hyperfine structure. Erbium has been a subject of recent experimental work [60,61], stimulated by its possible use in a variety of applications, including narrow linewidth laser cooling and spectroscopy, unique collision studies, and degenerate bosonic and fermionic gases with long-range magnetic dipole coupling.

Some species, particularly fermions, are difficult to cool by themselves due to unfavorable ultracold collisional dynamics. In such cases, it may be possible to use sympathetic cooling in a mixture of the target species and one of the alkali metals, where the alkali-metal atom is cooled directly by standard techniques. This has recently been demonstrated in Yb:Rb mixtures [62]. Use of  $\lambda_{\text{zero}}$  trap wavelengths could allow one to release alkali-metal atoms after the target atoms of the other species are sufficiently cold, in a hybrid trap configuration that combines optical and magnetic traps or bichromatic optical traps. If the final trap configuration utilizes a  $\lambda_{\text{zero}}$  wavelength, strong trapping of the target atom is possible while alkali-metal atoms will be released by turning off its separate trapping potential. Since placement of the resonances varies significantly among the alkali-metal atoms, a wide range of  $\lambda_{\text{zero}}$  is available, as shown in Table II.

We list the resonant wavelengths for variety of atomic systems in Table III. For consistency with the other tables, we list vacuum wavelengths obtained from the NIST energy levels database [48]. Both strong and intercombination lines that can be used for trapping of these species are listed. Comparing Tables II and III yields many instances of resonant transitions that are very close to  $\lambda_{\text{zero}}$ . Here are a few of the very close cases: Mg 285.3 - Na 285.6, Sr 460.9 - Cs 460.2, Dy 421.3 - Rb 421.1, and Ho 598.5 - Na 589.6.

Tune-out-wavelength laser light may be also useful in three-species cooling schemes such as reported in Ref. [63] by allowing easy release of one of the species from the trap. The work [63] demonstrated that the efficiency of sympathetic cooling of the  $^6\text{Li}$  gas by  $^{87}\text{Rb}$  was increased by the presence of  $^{40}\text{K}$  through catalytic cooling.

Measurements of the tune-out wavelengths may be used as high-precision benchmark tests of theory and to determine the excited-state matrix elements that are difficult to measure by other methods. Matrix elements of  $ns-n'p$  transitions of alkali-metal atoms, where  $ns$  is the ground state, are difficult to calculate accurately owing to large correlation corrections and small values of the final numbers. Experimental measurements of the  $\lambda_{\text{zero}}$  predicted in this work will serve as an excellent benchmark test of the all-order calculations. Moreover, it will be possible to combine these measurements with theoretical calculations to infer the values of these small matrix elements. Only one high-precision measurement of such matrix elements ( $6s-7p_j$  transitions in Cs) has been carried out to date [64].

#### IV. CONCLUSION

In summary, we calculate tune-out wavelengths in alkali-metal atoms from Li to Cs and estimate their uncertainties. Applications of these tune-out wavelengths to sympathetic cooling of group II and other more complicated atoms with alkali metals are discussed. Special cases where these wavelengths coincide with strong resonance transition in group II atoms, Yb, Dy, Ho, and Er are identified. Measurements of the tune-out wavelengths for benchmark tests of theory and experiment are proposed.

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