Dynamic dipole polarizabilities of the Li atom and the Be\textsuperscript{+} ion

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I. INTRODUCTION

The advent of cold-atom physics has lead to increased importance being given to the precise determination of atomic polarizabilities and related quantities. One very important source of systematic error in the new generation of atomic frequency standards is the blackbody radiation (BBR) shift [1–3]. The differential Stark shifts caused by the ambient electromagnetic field leads to a temperature-dependent shift in the transition frequency of the two states involved in the clock transition. The dynamic polarizability is also useful in the determination of the magic wavelength in optical lattices [4–7]. Another area where polarization phenomena is important is in the determination of global potential surfaces for diatomic molecules [8].

When consideration is given to all the atoms and ions commonly used in cold-atom physics, the Li atom and the Be\textsuperscript{+} ion have the advantage that they have only three electrons. This makes them accessible to calculations using correlated basis sets with the consequence that many properties of these systems can be computed to a high degree of precision. The results of these first-principles calculations can serve as atomic-based standards for quantities that are not amenable to precision measurement. For example, cold-atom interferometry has been used to measure the ground-state polarizabilities of Li and Na atoms [9,10]. However, the polarizability ratio $\alpha_d(X)/\alpha_d(Li)$ can be measured to a higher degree of precision than individual polarizabilities [11]. Thus, measurements of this ratio, in conjunction with a high-precision \textit{ab initio} calculation, could lead to a new level of accuracy in polarizability measurements for the atomic species most commonly used in cold-atom physics.

Calculations and measurements of Stark shifts are particularly important in atomic-clock research since the BBR shift is predominantly determined by the Stark shift of the two levels involved in the clock transition. The best experimental measurements of the Stark shift have been carried out for the alkali-metal atoms, and accuracies better than 0.1% have been reported [12,13]. Experimental work at this level of accuracy relies on a very precise determination of the electric field strength in the interaction region [13–15]. High-precision Hylleraas calculations of the type presented herein provide an invaluable test of the experimental reliability since they provide an independent means for the calibration of electric fields [16].

The dynamic Stark shift in oscillating electromagnetic fields is also of interest. The so-called magic wavelength (i.e., the precise wavelength at which the Stark shifts for upper and lower levels of the clock transition are the same) is an important parameter for optical lattices. The present calculation is used to estimate the magic wavelength for the Li 2\textsuperscript{2}S $\rightarrow$ 2\textsuperscript{2}P transition. The present calculations of the ac Stark shift potentially provides an atomic-based standard of electromagnetic (EM) field intensity for finite-frequency radiation.

There have been many calculations of the static polarizabilities of the ground and excited states of Li atoms and Be\textsuperscript{+} ions [17–23]. The most precise calculations on Li and Be\textsuperscript{+} are the Hylleraas calculations by Tang and collaborators [17,23]. The Hylleraas calculations were nonrelativistic and also included finite-mass effects for Li. Large-scale calculations using fully correlated Hylleraas basis sets can attain a degree of precision not possible for calculations based on orbital basis sets [19,24,25]. There have been many calculations of the dynamic polarizability for Li [20,26–33], but fewer for Be\textsuperscript{+} [28,32]. The present calculation is by far the most precise calculation of the dynamic polarizability that is based upon a solution of the nonrelativistic Schrödinger equation. And the present dynamic polarizabilities are obtained at real frequencies, which is different from the work of Derevianko et al. [27] who calculated the electric-dipole polarizabilities at imaginary frequencies. One particularly noteworthy treatment is the relativistic single-double all-order many-body perturbation-theory calculation (MBPT-SD) by Safronova et al. [33]. This calculation is fully relativistic and treats correlation effects to a high level of accuracy, although it does not achieve the same level of precision as the present Hylleraas calculation.

The present work computes the dynamic dipole polarizabilities of the Li atom and the Be\textsuperscript{+} ion in the 2\textsuperscript{2}S and 2\textsuperscript{2}P levels using a large variational calculation with a Hylleraas.
basis set. This methodology allows for the determination of the computational uncertainty related to the convergence of the basis set. Analytic representations of the dynamic polarizabilities are made so they can subsequently be computed at any frequency. Finally, the difference between the calculated and experimental binding energies is used to estimate the size of the relativistic correction to the polarizability. The final polarizabilities should be regarded as the recommended polarizabilities for comparison with experiment. All quantities given in this work are reported in atomic units except where indicated otherwise.

II. STRUCTURE CALCULATIONS

A. Hamiltonian and Hylleraas coordinates

The Li atom and Be\(^{+}\) ion are four-body Coulomb systems. After separating the center-of-mass coordinates, the nonrelativistic Hamiltonian can be written in the form [36]

\[
H_0 = -\sum_{i=1}^{3} \frac{1}{2\mu_i} \nabla_i^2 - \sum_{i>j=1}^{3} \frac{1}{m_{ij}} \nabla_i \cdot \nabla_j - \sum_{i} Z \frac{1}{r_i} - \sum_{i<j=1}^{3} \frac{1}{r_{ij}},
\]

where \(r_{ij} = |r_i - r_j|\) is the distance between electrons \(i\) and \(j\), \(\mu = m_pm_e/(m_o + m_e)\) is the reduced mass between the electron and the nucleus, and \(Z\) is the nuclear charge. In our calculation, the wave functions are expanded in terms of the explicitly correlated basis set in Hylleraas coordinates:

\[
\phi(r_1, r_2, r_3) = \sum_{\ell_1\ell_2\ell_3} Y^{\ell_1\ell_2\ell_3}_{\ell_1\ell_2\ell_3}(\hat{r}_1, \hat{r}_2, \hat{r}_3) \chi(1, 2, 3),
\]

where \(Y^{\ell_1\ell_2\ell_3}_{\ell_1\ell_2\ell_3}(\hat{r}_1, \hat{r}_2, \hat{r}_3)\) is the vector-coupled product of spherical harmonics to form an eigenstate of total angular momentum \(\ell\) and component \(L\) of

\[
\sum_{m_{\ell_1}} Y_{\ell_1 m_1}(\hat{r}_1) Y_{\ell_2 m_2}(\hat{r}_2) Y_{\ell_3 m_3}(\hat{r}_3),
\]

and \(\chi(1, 2, 3)\) is the three-electron spin-\(\frac{1}{2}\) wave function. The variational wave function is a linear combination of antisymmetrized basis functions \(\phi\). With some truncations to avoid potential numerical linear dependence, all terms in Eq. (2) are included such that

\[
j_1 + j_2 + j_3 + j_{12} + j_{23} + j_{31} \leq \Omega,
\]

where \(\Omega\) is an integer. The computational details in evaluating the necessary matrix elements of the Hamiltonian may be found in [25]. The nonlinear parameters \(\alpha\), \(\beta\), and \(\gamma\) in Eq. (2) are optimized using Newton’s method.

The convergence for the energies and other expectation values is studied by increasing \(\Omega\) progressively. The basis sets are essentially the same as two earlier Hylleraas calculations of the static polarizabilities [17,23]. The maximum \(\Omega\) used in the present calculations is 12. The uncertainty in the final value of any quantity is usually estimated to be equal to the size of the extrapolation from the largest explicit calculation.

Figure 1 is a schematic diagram showing the nonrelativistic energy levels of the most important states of the Li atom. The energy-level diagram for the low-lying states of Be\(^{+}\) is similar.

The energies of the ground states for \(^{\infty}\)Li and \(^{7}\)Li are \(-7.478060\,323\,91(5)\) and \(-7.477\,451\,930\,65(5)\) a.u., respectively. The respective energies for the \(^{\infty}\)Be\(^{+}\) and \(^{9}\)Be\(^{+}\) ground states are \(-14.324\,763\,176\,93(3)\) and \(-14.323\,863\,494\,2(3)\) a.u. Table I gives the binding energies of the Li-atom and Be\(^{+}\)-ion systems with respect to the two-electron Li\(^{+}\) and Be\(^{2+}\) cores. The Hylleraas basis was optimized to compute the \(2^{2}\)S- and \(2^{2}\)P-state polarizabilities, so some of the \(n = 4\) state energies have significant deviations from the experimental \(n = 4\) state energies. The states with significant energy differences can be regarded as pseudostates. The uncertainties listed in Table I represent the uncertainties in energy with respect to an infinite-basis calculation. The actual computational uncertainty is very small and there is no computational error in any of the calculated digits listed in Table I.

With one exception, all the finite-mass binding energies are less tightly bound than experiment. The differences from experiment are most likely due to relativistic effects. The exception where experiment is less tightly bound than the finite-mass calculation is the \(4^{2}F\) state of Li. This exception was not investigated since the properties of this state do not enter into any of the polarizability calculations.

B. Polarizability definitions

The dynamic polarizability provides a measure of the reaction of an atom to an external electromagnetic field. The dynamic polarizability at real frequencies can be expressed in terms of a sum over all intermediate states, including the continuum. The dynamic dipole polarizability is expressed in terms of the dynamic scalar and tensor dipole polarizabilities, \(\alpha_{d}(\omega)\) and \(\alpha_{t}(\omega)\), which can be expressed in terms of the reduced matrix elements of the dipole transition operator:

\[
\alpha_{d}(\omega) = \sum_{L_{\omega}} \alpha_{d}(L_{\omega},\omega),
\]
TABLE I. Comparisons of the binding energies in atomic units (a.u.) of Li and Be⁺ in their low-lying states. The experimental valence binding energies are taken from the National Institute of Standards database [34]. The J-weighted average is used for states with \( L \geq 1 \). The ground-state energies for the \(^{\infty}\)Li⁺ and \(^{\infty}\)Be⁺ ions are \(-7.279\,913\,412\,669\,305\,9\) and \(-13.655\,566\,238\,423\,586\,7\) a.u., respectively [35]. The ground-state energies for \(^{7}\)Li⁺ and \(^{8}\)Be⁺ are \(-7.279\,321\,519\,815\,674\,4\) and \(-13.654\,790\,268\,282\,791\,7\) a.u., respectively [35]. Underlining is used to indicate digits that have not converged with respect to basis-set enlargement.

| State   | \(^{\infty}\)Li Theory | \(^{7}\)Li Theory | \(^{6}\)Li Theory |
|---------|------------------------|-------------------|-------------------|
| \(^2^S\)  | \(-0.198\,146\,911\,24\) | \(-0.198\,130\,410\,84\) | \(-0.198\,142\) |
| \(^2^P\)  | \(-0.130\,243\,119\,63\) | \(-0.130\,236\,238\,76\) | \(-0.130\,236\) |
| \(^3^S\)  | \(-0.074\,183\,813\,50\) | \(-0.074\,177\,770\,25\) | \(-0.074\,182\) |
| \(^3^P\)  | \(-0.057\,237\,698\,23\) | \(-0.057\,234\,245\,77\) | \(-0.057\,236\) |
| \(^3^D\)  | \(-0.055\,610\,129\,74\) | \(-0.055\,605\,785\,43\) | \(-0.055\,606\) |
| \(^4^S\)  | \(-0.037\,528\,709\,57\) | \(-0.037\,524\,450\,73\) | \(-0.038\,615\) |
| \(^4^P\)  | \(-0.031\,390\,736\,13\) | \(-0.031\,388\,143\,90\) | \(-0.031\,975\) |
| \(^4^D\)  | \(-0.031\,275\,844\,34\) | \(-0.031\,273\,439\,38\) | \(-0.031\,274\) |
| \(^4^F\)  | \(-0.031\,253\,555\,31\) | \(-0.031\,251\,112\,02\) | \(-0.031\,243\) |

FIG. 2. (Color online) Dynamic dipole polarizability \(\alpha_1(\omega)\) of a ground-state Li atom. The singularities in the polarizability at the \(2^2S\) \(\rightarrow\) \(n^2P\) frequencies are marked.

and for \(L = 1\),

\[
\alpha_1(\omega) = \alpha_1(S,\omega) + \alpha_1(P,\omega) + \alpha_1(D,\omega),
\]

\[
\alpha_1^T(\omega) = -\alpha_1(S,\omega) + \frac{1}{2}\alpha_1(P,\omega) - \frac{1}{10}\alpha_1(D,\omega).
\]

In Eqs. (11) and (12), \(\alpha_1(P,\omega)\) is the contribution from the even-parity configuration \((pp')P\). The scalar and tensor polarizabilities can be easily related to the polarizabilities of the magnetic sublevels, \(\alpha_{1M}(\omega)\):

\[
\alpha_{1,0}(\omega) = \alpha_1(\omega) - 2\alpha_1^T(\omega),
\]

\[
\alpha_{1,\pm}(\omega) = \alpha_1(\omega) + \alpha_1^T(\omega).
\]

III. DYNAMIC POLARIZABILITY FOR \(^{\infty}\)LI ATOMS AND \(^{\infty}\)Be⁺ IONS

A. Ground-state dynamic polarizabilities

Figure 2 shows the dynamic dipole polarizability of the Li ground state as a function of photon energy. The chief errors in the dynamic polarizability are related to the convergence of the \(n^2P\) excited-state energies. The largest calculation used a basis with dimensions \((N_s, N_p) = (6412, 5761)\). The difference between the \(\alpha_1(\omega)\) and polarizability computed with a basis \((N_s, N_p) = (4172, 3543)\) would be barely discernible in Fig. 2. The convergence of \(\alpha_1(\omega)\) is best at photon energies far from the discrete excitation energies of the \(n^2P\) excitations. The polarizability is very susceptible to small changes in the physical energies at photon energies close to the \(n^2P\) excitation energies.

The uncertainties in the dynamic dipole polarizabilities of the Li ground state as well as the polarizabilities themselves are listed in Table II. All of the values listed are accurate to about ±1 in the fifth digit for \(\omega \leq 0.113\) a.u. Some of the alternate calculations of the \(\alpha_1(\omega)\) polarizabilities [20, 26, 28, 29, 33] are listed in Table II. Dynamic polarizabilities from some less accurate calculations [30–32] have not been tabulated.

One feature of Table II is the excellent agreement with the MBPT-SD calculation of Safronova et al. [33]. The MBPT-SD
Relativistic effects would tend to decrease the calculation also gives no consideration of finite-mass effects. The MBPT-SD calculation is less exact than the present calculation. The MBPT-SD theoretical uncertainty is agreement when the MBPT-SD theoretical uncertainty is calculation and the present Hylleraas calculation are in perfect agreement when the MBPT-SD theoretical uncertainty is relativistic correction.

The static polarizabilities for Be$^+$ ground states are depicted in Figs. 2 and 3. There are obvious similarities in shapes of the two $\alpha_1(\omega)$ curves but with the Li polarizability being about 5–10 times larger in magnitude at comparable values of $\omega/\omega_p$. One difference between the two curves is that Be$^+$ has zeros in $\alpha_1(\omega)$ at a discernible frequency difference before the 3$^2P$ and 4$^2P$ excitations while the $\alpha_1(\omega)$ negative-to-positive crossovers for Li occur much closer to the transition frequencies.

B. Excited-state dynamic polarizabilities

The scalar and tensor dipole polarizabilities for the excited 2$^2P$ state of the Li atom are listed in Table IV. As far as we know, the present calculations are the only dynamic polarizabilities presented for this state. The structure of the dynamic polarizability is complicated since both downward and upward transitions leads to singularities. This is seen most clearly in Fig. 4, which plots the polarizabilities for photon energies up to 0.10 a.u. The tensor polarizability is generally small except in the vicinity of the 2$^2S$, 3$^2S$, and
3^2D transitions. The tensor polarizability can become large when a single transition tends to dominate Eq. (12). The scalar and tensor polarizabilities tend to be opposite in sign. The main contribution to the polarizabilities comes from transitions to

\[ \alpha (\omega) \]

\[ \omega \]

\[ \alpha_{\text{CI-Hylleraas}} \]

\[ \alpha_{\text{Rec. Be}^+} \]

\[ [32] \]

\[ \omega \text{(a.u.)} \]

\[ \text{Be}^+ \]

\[ {}^9\text{Be}^+ \]

\[ {}^9\text{Be}^+ \]

\| \]

\[ \begin{array}{cccc}
0.00 & 24.496 (1) & 24.506 (1) & 24.489 (4) & 24.3 \\
0.01 & 24.608 (1) & 24.618 (7) & 24.601 (4) & 24.4 \\
0.02 & 24.951 (8) & 24.962 (9) & 24.943 (4) & 24.7 \\
0.04 & 26.429 (1) & 26.440 (4) & 26.419 (4) & 26.2 \\
0.06 & 29.339 (9) & 29.352 (8) & 29.325 (5) & 29.1 \\
0.08 & 34.735 (8) & 34.755 (9) & 34.715 (6) & 34.3 \\
0.10 & 45.650 (9) & 45.683 (6) & 45.609 (7) & 44.9 \\
0.12 & 74.785 (7) & 74.872 (4) & 74.656 (12) & \\
0.15 & –367.870 (8) & –365.803 (9) & –371.860 (60) & \\
0.18 & –43.203 (8) & –43.174 (5) & –43.273 (7) & \\
0.20 & –25.319 (5) & –25.309 (9) & –25.348 (4) & \\
0.30 & –5.796 (7) & –5.795 (1) & –5.801 (2) & \\
0.40 & –0.291 (2) & –0.287 (3) & –0.296 (2) & \\
0.50 & –2.149 (7) & –2.161 (7) & –2.164 (8) & \\
\end{array} \]

\[ \begin{array}{cccc}
\text{TABLE III. Dynamic dipole polarizabilities } \alpha_1(\omega) \text{ (in a.u.) for the Be}^+ \text{ ground state. The results of the fourth column incorporate relativistic effects. The numbers in parentheses are the uncertainties in the last digits arising from incomplete convergence of the basis set. The recommended (Rec.) polarizabilities in the fourth column reflect uncertainties other than purely computational.} \end{array} \]

\[ \begin{array}{cccc}
\text{TABLE IV. The dynamic dipole polarizabilities of the } 2^3P \text{ state of Li and Be}^+. \text{ Both the scalar and tensor polarizabilities are tabulated. The numbers in parentheses are the uncertainties in the last digits arising from incomplete convergence of the basis set. Values without uncertainties have no numerical uncertainties in any of the quoted digits. The recommended (Rec.) polarizabilities in the sixth and seventh columns have estimated corrections from relativistic effects. The recommended polarizabilities reflect uncertainties other than purely computational.} \end{array} \]

\[ \begin{array}{cccc}
\text{FIG. 3. (Color online) The dynamic dipole polarizability } \alpha_1(\omega) \text{ for the ground state of Be}^+. \text{ The singularities in the polarizability at the } 2^2S \rightarrow n^2P \text{ frequencies are marked.} \end{array} \]

\[ \begin{array}{cccc}
\text{the } S \text{ and } D \text{ states. The coefficients in the sum rules, Eqs. (11) and (12), for these terms are opposite in sign.} \end{array} \]

\[ \begin{array}{cccc}
\text{The dynamic polarizabilities for the } \text{Be}^+ 2^2P \text{ state are also tabulated in Table IV and depicted in Fig. 5 for photon frequencies below 0.40 a.u. There are three resonances in this frequency range. The scalar and tensor dynamic polarizabilities are similar in shape but with the opposite sign. As far as we know, there has been no previous calculation of the } 2^2P \text{ state dynamic polarizability.} \end{array} \]

\[ \begin{array}{cccc}
0.00 & 24.496 (1) & 24.506 (1) & 24.489 (4) \\
0.01 & 24.608 (1) & 24.618 (7) & 24.601 (4) \\
0.02 & 24.951 (8) & 24.962 (9) & 24.943 (4) \\
0.04 & 26.429 (1) & 26.440 (4) & 26.419 (4) \\
0.06 & 29.339 (9) & 29.352 (8) & 29.325 (5) \\
0.08 & 34.735 (8) & 34.755 (9) & 34.715 (6) \\
0.10 & 45.650 (9) & 45.683 (6) & 45.609 (7) \\
0.12 & 74.785 (7) & 74.872 (4) & 74.656 (12) \\
0.15 & –367.870 (8) & –365.803 (9) & –371.860 (60) \\
0.18 & –43.203 (8) & –43.174 (5) & –43.273 (7) \\
0.20 & –25.319 (5) & –25.309 (9) & –25.348 (4) \\
0.30 & –5.796 (7) & –5.795 (1) & –5.801 (2) \\
0.40 & –0.291 (2) & –0.287 (3) & –0.296 (2) \\
0.50 & –2.149 (7) & –2.161 (7) & –2.164 (8) \\
\end{array} \]
FIG. 4. (Color online) The dynamic polarizabilities $\alpha_1(\omega)$ and $\alpha_T(\omega)$ (in a.u.) of the Li $^2P$ state for photon frequencies below 0.10 a.u. The scalar polarizability is given by the solid line while the tensor polarizability is given by the chain curve.

C. Static $^2S \rightarrow ^2P$ Stark shift

The static Stark shift $\delta G$ for the change in the $^2S \rightarrow ^2P$ energy interval in an electric field of strength $F$ is written as

$$\delta G_{^2S^2P, M} = -\frac{1}{2} F^2(\alpha_{^2S} - \alpha_{^2P, M}) - \frac{1}{24} F^4(\gamma_{^2S} - \gamma_{^2P, M}) + \ldots,$$

where $\gamma$ is the hyperpolarizability. The Stark shift depends on the magnetic quantum number $M$ of the $^2P$ state. The relative size of $\Delta \alpha$ and $\Delta \gamma$ determines the extent to which the Stark shift is influenced by the hyperpolarizability at high field strengths. The relative importance of $\Delta \alpha$ and $\Delta \gamma$ is given by the ratio

$$X = \frac{F^2(\gamma_{^2S} - \gamma_{^2P, M})}{12(\alpha_{^2S} - \alpha_{^2P, M})} = \frac{F^2 \Delta \gamma}{12 \Delta \alpha}.$$

Using the static polarizability and static hyperpolarizability for the Li atom results in $\Delta \alpha = 37.1$ and $\Delta \gamma = 9.99 \times 10^6$ giving $X = 0.0001$ at $F = 6.67 \times 10^{-3}$ a.u. (344 kV/cm) and $X = 0.001$ at $F = 2.11 \times 10^{-2}$ a.u. (1087 kV/cm). These estimates of the critical field strength where the quadratic Stark shift is valid depend slightly on the magnetic quantum number, and exact values can be determined by using $M$-dependent polarizabilities. Stark shifts of higher order than the hyperpolarizability can be comfortably ignored at the 0.01% level, provided the field strength is less than 1100 kV/cm. The static Stark shift for Be$^+$ is not interesting since it is difficult to measure as a Be$^+$ ion immersed in a finite electric field is accelerated away from the finite-field region.

D. Dynamic $^2S \rightarrow ^2P$ Stark shift

The Li Stark shifts, $\alpha(2s) - \alpha(2pM)$, are plotted as a function of frequency in Fig. 6. It is seen that there are magic wavelengths for $M = 0$ just below the $^2P \rightarrow ^3S$ threshold and between the $^2S \rightarrow ^2P$ and $^2P \rightarrow ^3D$ thresholds. The actual energies for which the polarizability difference is zero are given in Table V. The Stark shifts get very large for frequencies between 0.058 and 0.070 a.u.

The Be$^+$ Stark shifts, $\alpha(2s) - \alpha(2pM)$, are plotted as a function of frequency in Fig. 7. The Stark shifts are much smaller in magnitude than the Li atom shifts. One difference from Li is that the Be$^+$ shift has no zero for energies below the $^2S \rightarrow ^2P$ threshold. The first zero in the Stark shift (excepting those related to a singularity) is at 0.263 a.u.
TABLE V. The photon energies for which there is no Stark shift for the $2^2S \rightarrow 2^2P$ transition. Underlined digits indicate uncertain digits arising from lack of basis set convergence. Digits in brackets indicate possible uncertainties associated with relativistic corrections in the recommended (Rec.) values.

| System   | $M = 0$          | $M = 1$          |
|----------|------------------|------------------|
| $\infty$Li | 0.046 317 680 06 | 0.084 763 957 2  |
|          | 0.081 021 795 5  |                  |
|          | 0.093 664 330 5  |                  |
| $^7$Li   | 0.046 335 687 8  | 0.084 766 087 0  |
|          | 0.081 024 478 9  |                  |
|          | 0.093 661 899 1  |                  |
| Rec. $^7$Li | 0.046 297(4) | 0.084 756(2) |
|          | 0.081 014(2) |                  |
|          | 0.093 661 3(2) |                  |
| $^9$Be$^+$ | 0.262 920 267 8 | 0.378 457 000 4  |
|          | 0.370 371 502 7 |                  |
|          | 0.390 752 146 3 |                  |
| $^9$Be$^+$ | 0.262 917 360 3 | 0.378 451 843 7  |
|          | 0.370 279 952 2 |                  |
|          | 0.390 455 356 8 |                  |
| Rec. $^9$Be$^+$ | 0.262 895 6(7) | 0.378 443(2) |
|          | 0.370 274(1) |                  |
|          | 0.390 454 6(2) |                  |

E. Analytic representation

The utility of the present calculations can be increased by constructing a closed-form expression for the dynamic polarizability. This is done by retaining the first 3 terms in Eq. (7) explicitly and then expanding the energy denominator in the remainder. The expressions explicitly include oscillator strengths up to the $n = 4$ principal quantum numbers. The closed form expression is

$$\alpha(\omega) = \left( \sum_{n=2}^{4} \frac{f_{2s-2p}}{\Delta E_{2snp} - \omega^2} \right) + S(-2) + \omega^2 S(-4) + \omega^4 S(-6) + \cdots + \omega^{14} S(-16) + C(\omega),$$

where

$$S(-m) = \sum_{n=5}^{\infty} \frac{f_{2s-2p}}{\Delta E_{2snp} - \omega^2} m^m,$$

and

$$C(\omega) = \frac{\eta_1 \alpha_{16} S(-16)}{1 - \eta_1 \omega^2}.$$  

Here, $f_{2s-2p}$ are the dipole oscillator strengths for the $2^2S \rightarrow n^2P$ transitions with transition energies $\Delta E_{2snp} \approx E_{np} - E_{2s}$. The oscillator strength is defined as

$$f_{npL \rightarrow nL'} = \frac{8\pi}{(2\ell + 1)(2\ell' + 1)} \Delta E_{nL\ell nL'} |\langle n_0 L || T_\ell || nL' \rangle|^2.$$  

The $S(-n)$ are the Cauchy moments of the remainder of the oscillator-strength distribution and are independent of $\omega$. The term $C(\omega)$ is an approximate term to represent the summation from the term $S(-18)$ to $S(\infty)$. The ratio $\eta_1 = S(-n - 2)/S(-n)$ is assumed to be constant and its value is set to $S(-16)/S(-14)$. Numerical values of the various constants in Eq. (16) can be found in Table VI. Inclusion of the remainder term has greatly increased the precision of the analytic fit to the exact dynamic polarizability.

The analytic representation for the Li $2^2S$ state is accurate to 0.01 a.u. for $\omega \leq 0.1612$ a.u. and to an accuracy of 0.1 a.u. for $\omega \leq 0.1728$ a.u. The dynamic polarizability for the Be$^+$ $2^2S$ state maintains its accuracy over a larger $\omega$ range. It is accurate to 0.001 a.u. for $\omega \leq 0.543$ a.u., to 0.01 a.u. for $\omega \leq 0.586$ a.u., and to 0.1 a.u. for $\omega \leq 0.6$ a.u.

The presence of zeros in the dynamic polarizability near the singularities means that the relative error in the analytic representation can get very large in a frequency range very close to the zeros. Neglecting these localized regions with anomalously high relative uncertainties, the relative difference between the analytic representation and actual dynamic polarizability for the Li $2^2S$ state was less than 0.001% for $\omega \leq 0.1399$ a.u., 0.01% for $\omega \leq 0.1551$ a.u., and 0.1% for $\omega \leq 0.1651$ a.u. The relative difference for the Be$^+$ $2^2S$ state obtained by the variational Hylleraas method was less than 0.001% for $\omega \leq 0.4737$ a.u., 0.01% for $\omega \leq 0.5067$ a.u., and 0.1% for $\omega \leq 0.5257$ a.u. The inclusion of the remainder term $C(\omega)$ improved the accuracy of the analytic representation by one or two orders of magnitude within the frequency range listed above.

The dynamic dipole polarizabilities of the $2^2P$ states of Li and Be$^+$ have both scalar $\alpha(\omega)$ and tensor $\alpha_T(\omega)$ parts. The scalar part can be written as

$$\alpha(\omega) = \left( \sum_{n=2}^{4} \frac{f_{2p-ns}}{\Delta E_{2pns} - \omega^2} \right) + \left( \sum_{n=3}^{4} \frac{f_{2p-nd}}{\Delta E_{2pnd} - \omega^2} \right) + S(-2) + \omega^2 S(-4) + \omega^4 S(-6) + \cdots + \omega^{14} S(-16) + C(\omega),$$

where

$$S(-m) = \sum_{n=5}^{\infty} \frac{f_{2p-ns}}{\Delta E_{2pns} - \omega^2} m^m + \sum_{n=5}^{\infty} \frac{f_{2p-nd}}{\Delta E_{2pnd} - \omega^2} m^m.$$
The 2p → n′P excitation involves a core excitation and the intermediate state is an unnatural parity 2Pc state. The tensor part is

\[
\alpha_{1T}(\omega) = -\sum_{n=2}^{4} \frac{f_{2p-nS}}{\Delta E_{2P_{ns}}} - \omega^2 - \frac{1}{10} \sum_{n=3}^{4} \frac{f_{2p-nD}}{\Delta E_{2P_{nd}}} - \omega^2 + S^T(-2) + \omega^2 S^T(-4) + \omega^4 S^T(-6) + \cdots + \omega^{14} S^T(-16) + C^T(\omega),
\]

(22)

where

\[
S^T(m) = -\sum_{n=5} \frac{f_{2p-nS}}{\Delta E_{2P_{ns}}} + \omega^2 \sum_{n=5} \frac{f_{2p-nD}}{\Delta E_{2P_{nd}}} + \omega^2 \sum_{n=5} \frac{f_{2p-nP}}{\Delta E_{2P_{nP}}}, \quad C^T(\omega) = \frac{\eta_1^T \omega^{16} S^T(-16)}{1 - \eta_1^T \omega^2}.
\]

(23)

(24)

where \( f_{2p-n_{mL}} \) means the oscillator strength from the 2p-state to the \( mL \)-state transition. The coefficients \( S^T(-2), S^T(-4), S^T(-6), \ldots \) correspond to the \( \omega^0, \omega^2, \omega^4, \ldots \) terms of the tensor part. The remainder term \( C^T(\omega) \) is an approximate expression to take into account the \( S^T(-18) \rightarrow S^T(\infty) \) summations. The factor \( \eta_1^T \) is set to be \( \eta_1^T = S(-16)/S(-14) \). All parameters in the analytic representation are given in Table VII.

The first two terms of Eqs. (20) and (22) include five resonances which make the major contribution to the polarizability, with the second term involving excitations to \( D \) states being the most important. This is clearly seen in the Li \( \alpha_1(\omega) \) of 185.542(S) a.u. at \( \omega = 0.04 \) a.u. The contribution of the first summation of Eq. (20) was \(-8.8717\) a.u., while the second summation contributed 175.8241 a.u. The value given by Eq. (20) was 185.5378 a.u., which agrees with the exact value at the level of 0.0004%.

The analytic representation for the scalar polarizability \( \alpha_1(\omega) \) of the Li 2^3P state is accurate to 0.01 a.u. for \( \omega \leq 0.0855 \) a.u. and to 0.1 a.u. for \( \omega \leq 0.0937 \) a.u. The analytic representation for the tensor polarizability \( \alpha_{1T}(\omega) \) is accurate to 0.01 a.u. for \( \omega \leq 0.0926 \) a.u. and to 0.10 a.u. for \( \omega \leq 0.1 \) a.u.

The relative error in the analytic representation of \( \alpha_1(\omega) \) for the 2^3P state of the Li atom is less than 0.001% for \( \omega \leq 0.082 \) a.u., 0.01% for \( \omega \leq 0.0871 \) a.u., and 0.1% for \( \omega \leq 0.0906 \) a.u. The relative error of the analytic representation for \( \alpha_{1T}(\omega) \) is less than 0.001% for \( \omega \leq 0.0815 \) a.u., 0.01% for \( \omega \leq 0.0932 \) a.u., and 0.1% for \( \omega \leq 0.0995 \) a.u. The dynamic polarizability of the Be^+ 2P state maintains its accuracy over a larger range of \( \omega \). It is accurate to 0.001 a.u. for \( \omega \leq 0.3513 \) a.u., to 0.01 a.u. for \( \omega \leq 0.3837 \) a.u., and 0.1 a.u. for \( \omega \leq 0.4111 \) a.u. The absolute error for \( \alpha_{1T}(\omega) \) is 0.001 a.u. for \( \omega \leq 0.3788 \) a.u., 0.01 a.u. for \( \omega \leq 0.4077 \) a.u., and 0.1 a.u. for \( \omega \leq 0.4291 \) a.u.

The relative error between the analytic representation and Hylleraas values of \( \alpha_1(\omega) \) for the Be^+ 2P state is less than 0.001% for \( \omega \leq 0.332 \) a.u., 0.01% for \( \omega \leq 0.3536 \) a.u., and 0.1% for \( \omega \leq 0.3708 \) a.u. The relative error for \( \alpha_{1T}(\omega) \) of the Be^+ 2P state is less than 0.001% for \( \omega \leq 0.3265 \) a.u., 0.01% for \( \omega \leq 0.3434 \) a.u., and 0.1% for \( \omega \leq 0.3534 \) a.u.

IV. FINITE-MASS CORRECTIONS

The effect of the finite mass was to decrease the Li atom and Be^+ ion binding energies listed in the Table I. Therefore, it is not surprisingly that the \( \omega = 0 \) polarizabilities of the Li and Be^+ ground states are increased in Tables II and III. The overall changes of the \( \omega = 0 \) polarizabilities are 0.03% and 0.04% for Li and Be^+ respectively. The finite-mass polarizabilities are larger than the infinite-mass values at \( \omega = 0 \). These differences can be taken as indicative of the overall change in the polarizabilities at finite frequencies below the first excitation threshold. The differences are naturally larger near thresholds.

The finite-mass effect for the Li 2^3P state increased its polarizability by 0.001% (Table IV) while decreasing the
TABLE VII. The parameters defining the frequency-dependent polarizabilities of the $2^2P$ state of Li and Be$^+$. The numbers in the square brackets denote powers of 10. The recommended (Rec.) results of the fourth and the seventh columns incorporate relativistic effects.

| Parameter | $^{\infty}$Li | $^7$Li | Rec., $^7$Li | $^{9}$Be$^+$ | $^{9}$Be$^+$ | Rec., $^{9}$Be$^+$ |
|-----------|----------------|--------|-------------|-------------|-------------|----------------|
| $f_{^2P\rightarrow^2S}$ | $-0.248$ | $-0.248$ | $-0.249$ | $-0.166$ | $-0.166$ | $-0.166$ |
| $A_E^{2P\rightarrow^2S}$ | $-0.067$ | $-0.067$ | $-0.145$ | $-0.145$ | $-0.145$ | $-0.145$ |
| $\delta E^{2P\rightarrow^2S}$ | $0.110$ | $0.110$ | $0.064$ | $0.064$ | $0.064$ | $0.064$ |
| $\Delta E^{2P \rightarrow 3P}$ | $0.056$ | $0.056$ | $0.256$ | $0.256$ | $0.256$ | $0.256$ |
| $\Delta E^{2P \rightarrow 4S}$ | $0.014$ | $0.014$ | $0.012$ | $0.012$ | $0.012$ | $0.012$ |
| $\Delta E^{2P \rightarrow 4D}$ | $0.638$ | $0.638$ | $0.631$ | $0.632$ | $0.632$ | $0.632$ |
| $\Delta E^{2P \rightarrow 4F}$ | $0.074$ | $0.074$ | $0.301$ | $0.301$ | $0.301$ | $0.301$ |
| $\Delta E^{2P \rightarrow 4G}$ | $0.122$ | $0.122$ | $0.122$ | $0.122$ | $0.122$ | $0.122$ |
| $\Delta E^{2P \rightarrow 4H}$ | $0.098$ | $0.098$ | $0.398$ | $0.398$ | $0.398$ | $0.398$ |
| $\Delta E^{2P \rightarrow 4I}$ | $1.684$ | $1.684$ | $1.075$ | $1.075$ | $1.075$ | $1.075$ |
| $\eta_1$ | $77.128$ | $77.135$ | $4.760$ | $4.760$ | $4.760$ | $4.760$ |
| $\eta_2$ | $-2.730$ | $-2.731$ | $-0.156$ | $-0.156$ | $-0.156$ | $-0.156$ |
| $\eta_3$ | $-154.670$ | $-154.702$ | $-0.544$ | $-0.544$ | $-0.544$ | $-0.544$ |
| $\eta_4$ | $-9.881$ | $-9.884$ | $-2.109$ | $-2.110$ | $-2.110$ | $-2.110$ |
| $\eta_5$ | $-6.716$ | $-6.718$ | $-8.715$ | $-8.718$ | $-8.718$ | $-8.718$ |
| $\eta_6$ | $-9.735$ | $-9.737$ | $-37.508$ | $-37.520$ | $-37.520$ | $-37.520$ |
| $\eta_7$ | $-3.422$ | $-3.424$ | $-166.164$ | $-166.226$ | $-166.226$ | $-166.226$ |
| $\eta_8$ | $-2.519$ | $-2.520$ | $-752.681$ | $-753.003$ | $-753.003$ | $-753.003$ |
| $\eta_9$ | $-1.880$ | $-1.881$ | $-3471.37$ | $-3472.06$ | $-3472.06$ | $-3472.06$ |
| $\eta_{10}$ | $74.665$ | $74.671$ | $4.612$ | $4.612$ | $4.612$ | $4.612$ |

Correcting for the relativistic energy is simply a matter of replacing the theoretical energies in the sum rules by the experimental values. The spin-orbit weighted averages were used for states with $\ell \geq 1$. The corrections to the transition matrix elements are made by recourse to calculations using a semiempirical model potential that supplements the potential field of a frozen Hartree-Fock (HF) core with a tunable polarization potential [21,23,37]. Polarizabilities for Li and Be$^+$ computed with this approach reproduce the Hylleraas calculation at the 0.1%-accuracy level [17,21,23].

The method used to estimate the relativistic effect upon matrix elements relies on comparing two very similar

V. OTHER EFFECTS AND UNCERTAINTIES

A. Estimate of relativistic effects

The major omission from the present calculation is the inclusion of relativistic effects. The larger part of the energy difference between the present finite-mass calculations and the experimental binding energies in Table I is due to the omission of relativistic effects. Relativistic effects will alter the polarizability calculation in two ways. First, the energy differences will be changed. Generally, the binding energies of all states can be expected to be slightly larger. Secondly, there will be some changes in the reduced matrix elements. The wave functions for the $n^2S$ and $n^2P$ states can be expected to be slightly more compact since they are more tightly bound.
calculations. One calculation has its polarization potentials tuned to reproduce the finite-mass energies of Table I. The other calculation is tuned to give the experimental energies. The matrix elements for the low-lying transitions that dominate the dynamic polarizabilities are then compared. The differences between the “finite-mass” calculation and the “experimental” calculations are then determined. These changes in the matrix elements are then applied as corrections to the set of Hylleraas matrix elements. The only matrix elements that are changed are those involving transitions inside the $^2 \Sigma$ and $^3 \Sigma$ level space. Transitions to these states dominate the $^2 \Sigma$ and $^2 \Pi$ polarizabilities. The actual change in the Li $^2 \Sigma \rightarrow ^2 \Pi$ matrix element was a reduction of 0.0054%. The reduction in the Be$^+$ $^2 \Sigma \rightarrow ^2 \Pi$ matrix element was 0.011%.

Using the new set of corrected matrix elements gives a ground state polarizability of 164.114 a.u. (Table I). This represents a reduction of the polarizability by 0.047 a.u. A coupled-cluster calculation of the Li ground state estimated that relativistic effects reduced its polarizability by 0.06 a.u. [38]. The static polarizability of the $^2 \Pi$ state of $^7$Li; namely 126.947 a.u., was increased to 126.970 a.u. (Table IV). This gives a Stark shift of $-37.144$ a.u., which is in agreement with the experiment of Hunter et al. [13] which gave $-37.14(2)$ for the $^7$Li $^2 \Sigma^+ - ^2 \Pi_3$ Stark shift. Another calculation was made to check the $^2 \Pi_1/2 - ^2 \Pi_3/2$ polarizability difference. The MBPT-SD calculation gave a difference of 0.015 a.u. [22]. Doing two calculations tuned to give a $^2 \Pi_1/2 - ^2 \Pi_3/2$ Stark shift and that of 1.77 $\times$ 10$^{-6}$ a.u. (the energy splitting in the MBPT-SD calculation [22]) gave a polarizability difference of 0.008 a.u.. The energy splitting in the MBPT-SD calculation [22] was increased to 0.0145 a.u. The energy splitting in the MBPT-SD calculation [22] gave a polarizability difference of 0.0145 a.u. A further test was made by examination of the line strengths of the $^3 \Sigma^+ - ^3 \Pi$ matrix elements, the polarizabilities were recomputed, and the differences assigned as the uncertainty in the recommended values. This difference is actually larger than the estimated relativistic change in the matrix element. Therefore, the recommended static polarizability of the Li ground state is 164.11(3) a.u. Uncertainties in the 2(3)$^P$–2(3)$^P$ matrix elements are smaller (relativistic effects have a smaller impact on these matrix elements) and have not been included in the uncertainty analysis. The final value for the static scalar polarizability of the $^2 \Pi$ state was 126.970(4) a.u., while the tensor polarizability was 1.61(2) a.u.

The same uncertainty analysis was applied to the Be$^+$ ion polarizabilities. The recommended value for the ground state is 24.489(4) a.u. The static $^2 \Pi$ scalar polarizability was set as 2.0285(10) a.u. while the tensor polarizability was set to 5.8528(10) a.u.

Uncertainties in the recommended dynamic polarizabilities in Tables II–V were computed by making corrections to the matrix elements, recomputing, and then observing the change. These uncertainties are best interpreted as indicative, as opposed to rigorous estimates.

VI. SUMMARY

Definitive nonrelativistic values for the dynamic dipole polarizabilities of Li and Be$^+$ in their low-lying $^2 \Sigma$ and $^2 \Pi$ states have been established using the variational method with Hylleraas basis sets. Calculation for both finite and infinite nuclear-mass systems have been performed. Analytic
representations for the dynamic polarizabilities of the Li atom and the Be$^+$ ion have also been developed. These results can serve as a standard against which any other calculation can be judged.

Subsidiary calculations have been used to estimate the impact of relativistic effects that are not explicitly included in the Hylleraas calculation. It is recommended that the value of 164.11(3) a.u. be adopted as the static polarizability of $^7$Li. The uncertainty of 0.03 a.u. is based on the difference between the present $C_3$ and that of Le Roy et al. [8]. This accuracy level is also supported by the $^7$Li $2\overline{S}−2\overline{P}_{1/2}$ Stark shift of −37.14 a.u., which is in perfect agreement with the value of −37.14(2) given by the high precision experiment of Hunter et al. [13]. The recommended static polarizability for Be$^+$ is 24.489(4) a.u.

The dynamic polarizabilities that have been obtained can be used as an atom-based standard for electromagnetic field intensity. These polarizabilities can be regarded as an initial attempt to develop atom-based standards for polarizability and Stark-shift measurements. The primary virtue of the method with which the relativistic corrections were evaluated was simplicity of computation. For present purposes, the estimate of the relativistic corrections only has to be accurate to 10%–20% for the recommended polarizabilities to be valid. The comparisons that have been done with fully relativistic calculations suggest that the estimates of the relativistic corrections are indeed accurate at this level. However, a more rigorous estimate using the Briet-Pauli Hamiltonian and perturbation theory would be desirable [41–43].

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