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Long-range interactions of the Sr$^+$ ion

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A number of properties of the low-lying states of the Sr$^+$ ion are evaluated by diagonalizing a semiempirical Hamiltonian in a large dimension single electron basis. These properties include the oscillator strengths connecting the low-lying states, the quadrupole moments, and the polarizabilities. In addition, the long-range dispersion coefficients for the states of this ion interacting with a number of atoms are given. The polarizabilities and dispersion coefficients can be used to estimate frequency shifts of the Sr$^+$ $5s \rightarrow 4d$ clock transition due to background fields, including the blackbody radiation shift, and shifts due to collisions with a buffer gas.

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I. INTRODUCTION

This paper gives a systematic presentation of many properties of the Sr$^+$ ion, largely motivated by the importance of this ion in a number of application areas, mainly in astrophysics and cold ion physics. First, the abundance of the Sr-Y-Zr sequence of elements can reveal information about the post-main-sequence evolution of cool giant stars [1]. The lifetimes and other data of Sr$^+$ are useful in determining strontium elemental abundances [2,3]. Second, the long lifetime of the $5s \rightarrow 4d$ transition of the ^{88}Sr$^+$ ion makes it a promising candidate for a trapped ion frequency standard [4–8]. Various atomic properties are useful in evaluating the uncertainty budget, for example, blackbody radiation shift is predominantly determined by the difference between the polarizabilities of the 4d and 5s levels. In addition, there have been a number of investigations of pressure broadening of the Sr$^+$ transitions in a variety of buffer gases [2,9–11]. Knowledge of the long-range part of the ion-atom interaction is useful in determining the pressure broadening and shift [12,13]. Finally, the Sr$^+$Ar and Sr$^+$Kr molecules have been synthesized and the present information can improve the characterizations of the potential surface [14,15].

In the present work, a one-electron model of the Sr$^+$ ion is constructed with a semiempirical core potential to describe the interaction of the valence electron with the rest of the atom. The polarizabilities and dispersion coefficients are evaluated using sum rules [16,17]. All quantities are reported in atomic units, with the exception of lifetimes and decay rates which are stated in SI units.

II. THEORETICAL DEVELOPMENT

A. Overview of dispersion constant calculations

The long-range interaction between one electrically charged atom and one electrically neutral atom has two components [18–20] when terms up to second order in perturbation theory are included. There is the polarization interaction, which can be written

$$V(R) = -\frac{\alpha_d}{2R^4} - \frac{\alpha_q}{2R^6} - \cdots , \tag{1}$$

where α_d and α_q are the dipole and quadrupole polarizabilities of the neutral atom. The distance between the two nuclei is R. This part of the long-range interaction does not lead to a frequency shift between the different states of the ion.

There is also the dispersion interaction. For two spherically symmetric atoms in their ground states, this interaction can be written [21,22] as

$$V(R) = -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} - \cdots . \tag{2}$$

The C_n parameters are the dispersion coefficients. The dispersion interaction leads to a frequency shift between the different ion states when the ion is immersed in a buffer gas.

The approach used to generate the dispersion coefficients [16,17] is based on the work of Dalgarno who derived expressions in terms of oscillator strength sum rules [21,22]. This reduced the calculation of the C_n parameters for two spherically symmetric atoms to sums over the products of the absorption oscillator strengths (originating in the ground state) divided by an energy denominator. The sums should include contributions from all discrete and continuum excitations. In practice a pseudostate representation is used which gives a discrete representation of the continuum [17,23,24]. Finite dimension sums over a pseudostate basis give a rapidly convergent expansion of the continuum of intermediate states provided all the pseudostates are retained [25–27]. The sum over the oscillator strengths needs to be rewritten in terms of a sum over the reduced matrix elements of the electric multipole operator in cases where one (or both) of the atoms is in a state with $L > 0$ [17].

The major part of any calculation involves the generation of the lists of reduced transition matrix elements for the two atomic states. In the present approach this is done by diagonalizing a semiempirical model potential in a large single electron basis. This gives a discretization of the positive energy continuum, as well as the spectrum of low-lying physical states. It is then straightforward to process the lists of matrix elements and generate the dispersion coefficients [17].

B. Wave functions and transition operators for Sr$^+$

The wave functions and transition operators were computed by diagonalizing the semiempirical Hamiltonian [24,28–31] in a large mixed Laguerre-type orbital (LTO) and Slater-type orbital (STO) basis set [24].

The initial step was to perform a Hartree-Fock (HF) calculation to define the core. In this case, calculations of the Sr $5s^2$ ground states were done in a STO basis [32]. The core wave functions were then frozen, giving the working Hamiltonian for the valence electron,

$$H = -\frac{1}{2}\nabla^2 + V_{\mathrm{dir}}(\mathbf{r}) + V_{\mathrm{exc}}(\mathbf{r}) + V_p(\mathbf{r}). \tag{3}$$

The direct and exchange interactions of the valence electron with the HF core were calculated exactly. The ℓ-dependent polarization potential, V_p, was semiempirical in nature with the functional form

$$V_p(r) = -\sum_{\ell m} \frac{\alpha_d g_\ell^2(r)}{2r^4} |\ell m\rangle\langle \ell m|. \tag{4}$$

The coefficient, α_d is the static dipole polarizability of the core and $g_\ell^2(r) = 1 - \exp(-r^6/\rho_\ell^6)$ is a cutoff function designed to make the polarization potential finite at the origin. The cutoff parameters, ρ_ℓ were tuned to reproduce the binding energies of the *ns* ground state and the *np*, *nd*, and *nf* excited states. The dipole polarizability for Sr^{2+} was chosen as $\alpha_d = 5.813 a_0^3$ [24,33]. The cutoff parameters for $\ell = 0 \rightarrow 3$ were 1.746, 2.0184, 2.7146, and 2.402 a_0, respectively. The energies of the states with $\ell \geq 1$ were assigned to the statistical average of their respective spin-orbit doublets. The Hamiltonian was diagonalized in a very large orbital basis with about 50 Laguerre-type orbitals for each ℓ value. Although the wave functions are constructed as linear combinations of LTOs, all matrix element evaluations were done using Gaussian quadratures and are accurate to close to machine precision. The cutoff parameters were different for each $\ell \leq 3$. The parameters for $\ell > 3$ were set to ρ_3. The oscillator strengths (and other multipole expectation values) were computed with operators that included polarization corrections [24,29,34–36]. The quadrupole core polarizability was chosen as $17.15 a_0^5$ [24,33] while the octupole polarizability was set to zero. The cutoff parameter for the polarization corrections to transition operator was fixed at $2.16 a_0$ (the average of ρ_0, ρ_1, and ρ_2).

The model potential is realistic since the direct and exchange interactions with the core were computed without approximation from the HF wave function, and only the core polarization potential is described with a model potential. Comparisons with more sophisticated *ab initio* methods have revealed that the present semiempirical approach often gives oscillator strengths, polarizabilities, and dispersion coefficients that lie within a couple of percent of the best calculations [24,37–39]. There is one complication. The $4d$ orbital of Sr$^+$ is compact and does penetrate into the core like the $3d$ orbital of Ca$^+$ [40,41]. Defining the polarization potential by tuning to the $4d$ energy leads to the rest of the *nd* series being slightly under bound, and then there is the issue of the accuracy of the $4d$ state itself. Consequently, quantities which explicitly involve the Sr$^+$ *nd* set of states can be expected to have larger uncertainties than the other states.

TABLE I. Theoretical and experimental energy levels (in hartree) of some of the low-lying states of the Sr$^+$ ion. The energies are given relative to the energy of the Sr^{2+} core. The experimental energies (taken from [43]) for the doublet states are averages with the usual $(2J+1)$ weighting factors.

State	Theory	Experiment
$5s$	−0.4055220	−0.405350
$4d$	−0.3382475	−0.338262
$5p$	−0.2948544	−0.294861
$6s$	−0.1874692	−0.187846
$5d$	−0.1612374	−0.162323
$6p$	−0.1501503	−0.150369
$4f$	−0.1274513	−0.127451

C. Wave functions and transition operators or other atoms

The transition arrays for hydrogen and the rare gases are exactly the same as those in previous investigations of the dispersion interactions involving the low-lying states of the alkali-metal atoms and magnesium with these atoms [38,42]. The arrays for hydrogen and helium should be regarded as being capable of giving essentially exact polarizabilities and dispersion coefficients.

III. RESULTS

A. Energy levels

The binding energies of the low-lying states of the Sr$^+$ are tabulated and compared with experiment in Table I. The agreement between the present energies and the experimental energies is generally of order 10^{-4} hartree with the exception of the $5d$ level where there is a discrepancy of 1.1×10^{-3} hartree. The value of ρ_2 was tuned to the $4d$ energy which penetrates into the core [28,36,40,41]. Tuning the cutoff parameter to the $4d$ level leads to the binding energy of the $5d$ and higher levels being underestimated [28,40].

B. Oscillator strengths

The absorption oscillator strength for a multipole transition from $n_a \rightarrow n_b$, with an energy difference of $\Delta E_{n_b n_a} = E_{n_b} - E_{n_a}$, is defined as

$$f_{n_a n_b}^{(k)} = \frac{2|\langle \psi_{n_a}; L_a \| r^k \mathbf{C}^k(\hat{\mathbf{r}}) \| \psi_{n_b}; L_b\rangle|^2 \Delta E_{n_b n_a}}{(2k+1)(2L_a+1)}. \tag{5}$$

In this expression, L_a is the orbital angular momentum of the initial state while k is the polarity of the transition. Table II

TABLE II. Absorption oscillator strengths for various transitions of Sr$^+$. All of the oscillator strengths are for dipole transitions with three exceptions. Theoretical oscillator strengths from other groups are identified by an acronym denoting the type of calculation and a citation. The numbers in the square brackets in the column labeled "Present" denote powers of 10.

Transition	Present	Other
$f^{(1)}_{5s\to5p}$	1.0262	1.10 CA, Ref. [44]; 1.027 MCHF, Ref. [1]; 0.997 MBPT, Ref. [45]
$f^{(1)}_{5s\to6p}$	0.402[−4]	0.0066 CA, Ref. [44]
$f^{(1)}_{4d\to5p}$	0.08233	0.0936 CA, Ref. [44]; 0.0715 MCHF, Ref. [1]; 0.072 MBPT, Ref. [45]
$f^{(1)}_{4d\to6p}$	0.845[−4]	0.0031 CA, Ref. [44]
$f^{(1)}_{4d\to4f}$	0.3038	0.325 CA, Ref. [44]; 0.246 MCHF, Ref. [1]
$f^{(1)}_{5p\to6s}$	0.2075	0.178 CA, Ref. [44]
$f^{(1)}_{5p\to5d}$	0.8339	0.793 CA, Ref. [44]
$f^{(1)}_{5d\to4f}$	0.8519	0.8532 CA, Ref. [44]
$f^{(2)}_{5s\to4d}$	4.140	
$f^{(2)}_{5s\to5d}$	20.09	

lists the present oscillator strengths for a number of Sr$^+$ transitions. Values from three other calculations are listed [1,44,45] for the dipole transitions. The Coulomb approximation (CA) values are mainly included because they are a part of a set that covers all the transitions. More sophisticated calculations are the multiconfiguration Hartree-Fock (MCHF) calculation of Brage *et al.* [1] and the many-body perturbation theory (MBPT) calculation by Guet and Johnston [45]. There is a 3% variation among the calculations of the $f_{5s\to5p}$ oscillator strength. The MCHF and MBPT calculations were both relativistic and the values given in Table II are the sums of the f values of the spin-orbit doublet.

Although the lifetime for the $5p$ level has been measured on numerous occasions [46,47], it is not possible to directly determine the $5s\to5p$ oscillator strength from this information since the $5p$ level can decay into both the $4d$ and $5s$ levels. Accordingly, we have converted the present oscillator strengths listed in Table II into a $5p$ lifetime of 7.00×10^{-9} s for comparison with experiment. The most recent beam-foil experiment gave $7.39(7)\times10^{-9}$ s and $6.63(7)\times10^{-9}$ s [47] for the lifetime of the $5p_{1/2}$ and $5p_{3/2}$ states, respectively. Previously, another beam-foil experiment gave $7.47(7)\times10^{-9}$ s and $6.69(7)\times10^{-9}$ s [48] for the lifetimes of the $5p_{1/2}$ and $5p_{3/2}$ states. Taking a statistically weighted average of the experimental values would result in average lifetimes that are within a couple of percent of the present lifetime. This level of accuracy is the best that can be expected from an underlying theoretical model that does not allow for spin-orbit splitting.

The branching ratio for the decay to the $5s$ and $4d$ levels have also been determined [46]. For the decay from the $5p_{3/2}$ level the branching ratio was 14.8 ± 2.5 while the ratio for the $5p_{1/2}$ state was 13.4 ± 2 [46]. The present calculation gives a branching ratio of 16.2. Other calculations give branching ratios that range between 16.0 to 18.8 [1,45]. A more precise experimental determination of this branching ratio would allow better discrimination between the different models of the Sr$^+$ structure.

There is a surprisingly large difference between the MCHF and present value of $f_{4d\to4f}$ with the present calculation yielding 0.3038 and the MCHF calculation yielding 0.246. This problem can be resolved by reference to the experimental lifetimes from a beam foil experiment [47]. The lifetime of the $4f$ level has been measured as 3.09(6) ns and 2.97(5) ns for the $4f_{5/2}$ and $4f_{7/2}$ states, respectively [47]. The current calculations give a $4f$ lifetime of 3.00 ns. Although the $4f$ level can also decay to the $5d$ level, the total decay rate is dominated by the $4d\to4f$ transition and the $4d:5d$ branching ratio is 13.3. The experimental $4f$ lifetime thus suggests that the present $f_{4d\to4f}$ should be preferred to the MCHF value.

C. Lifetimes of the 4*d* levels

The transition rate for the $5s\to4d$ transition has been the subject of many recent investigations [49–52], and the oscillator strength for this transition is also given in Table II. The decay rate of an LS coupled state decaying by a quadrupole transition is related to the reduced matrix element by the identity [53]

$$A_{E2}=\frac{1.120\times10^{18}}{(2L_b+1)\lambda^5}|\langle\psi_{n_a};L_a\|r^k\mathbf{C}^k(\hat{\mathbf{r}})\|\psi_{n_b};L_b\rangle|^2, \tag{6}$$

where λ is given in Å. The present calculation using the theoretical energy difference gives a lifetime of 0.4135 s. The lifetime is sensitive to small changes in the transition energy as it depends on the fifth power of the transition energy. If the lifetime is computed with the actual energy differences of the spin-orbit doublet, we obtain $\tau_{3/2}=0.443$ s and $\tau_{5/2}=0.404$ s. It should be noted that magnetic dipole decays from the $4d_{3/2}$ and $4d_{5/2}$ states are possible, but they have small decay rates and a very small effect on the lifetimes [45,49].

There is some scatter between even some recent estimates of the $4d_{3/2}$ lifetimes. The three recent lifetime measurements gave 0.434(4) s [50], 0.434(4) s [54], and 0.455(29) s [54] while an older experiment gave 0.395(38) s [55]. The relativistic MBPT calculation of Guet and Johnson gave $\tau_{3/2}=0.454$ s^{-1} [45], while a relativistic coupled cluster method with single and double excitations (CCSD) gave $\tau_{3/2}=0.426$ s [49].

The nature of the scatter among the different estimates of $\tau_{5/2}$ is bimodal in nature. There is one set of estimates that predict a lifetime of about 0.40 s, while another set of estimates predict a lifetime of about 0.36 s. For example, the most recent experiments gave $\tau_{5/2}=0.408(22)$ s [54] and $\tau_{5/2}=0.3908(16)$ s [52]. However some older experiments have given $\tau_{5/2}=0.345(33)$ s [55], $\tau_{5/2}=0.347(33)$ s [56], and $\tau_{5/2}=0.372(25)$ s [57]. The relativistic MBPT calculation gave $\tau_{5/2}=0.405$ s [45] while the CCSD calculation gave $\tau_{5/2}=0.357$ s [49].

TABLE III. The dipole, quadrupole, and tensor polarizabilities (for dipole excitations) for the low-lying states of Sr$^+$. A description of the other calculations can be found in the text of Ref. [2]. The quadrupole moments are computed for $L=M$ which are the same as the $J=M_J=L+1/2$ state. The numbers in the square brackets denote powers of 10.

	α_1 (a.u.)		$\alpha_{1,2LL}$ (a.u.)	α_2 (a.u.)	α_3 (a.u.)	Q_{LL}
State	Present	Other	Present	Present	Present	Present
$5s$	89.88	93.3 $f^{(1)}$ sums, Ref. [2]	0	1346	1.543[4]	0
$4d$	61.77	57.0 $f^{(1)}$ sums, Ref. [2]	−47.20	49.54	1.528[4]	−2.840
$5p$	−23.13	−32.6 $f^{(1)}$ sums, Ref. [2]	10.58	1.798[3]	6.973[4]	−5.246
$6s$	1.089[3]		0	8.860[4]	3.845[6]	0
$5d$	2.099[3]		−1.543[3]	9.475[3]	8.215[6]	−20.49
$6p$	−2.056[3]		363.5	1.157[5]	2.517[6]	−21.00

There is a significant difference in the results of the CCSD [49] calculations and the MBPT calculations [45]. The ratio of the two lifetimes for the MBPT calculation is 1.111 while the ratio of the two lifetimes for the CCSD calculation is 1.193. Assuming that the reduced matrix elements connecting the $4d$ and $5s$ states are the same (when angular momentum factors are taken into account), Eq. (6) suggests the lifetimes should scale as the fifth power of the energy difference and this gives a ratio of 1.100. Examining Table 1 of Sahoo *et al.* [49] reveals that the lifetime ratio of the $3d$ levels for Ca$^+$ is 1.068 while a value of 1.023 is expected from energy factors alone. Two relativistic MBPT calculations gave 1.027 [58] and 1.028 [45]. Further, the ρ_2 parameter in the present calculation was changed to give the $4d$ state a binding energy equal to the $4d_{5/2}$ experimental energy. The resulting change in the radial distribution of the $4d$ orbital caused the $4d_{5/2}$ lifetime to decrease by only 0.37%. The results of the present and MBPT calculations suggest that the CCSD calculations of Sahoo *et al.* are tending to systematically overestimate the differences between the $nd_{5/2}$ and $nd_{3/2}$ lifetimes for Ca$^+$ and Sr$^+$. A similar conclusion was previously reached by Kreuter *et al.* [58] after an extensive analysis.

D. Quadrupole moments

Of the quadrupole moments given in Table III, the one of most interest is that of the $4d$ state. This is due to the possible use of the Sr$^+$ $4d \rightarrow 5s$ transition as an optical frequency standard [8,59].

The quadrupole moment of this state has been determined in two recent large-scale calculations [59,60]. The relativistic configuration interaction (RCI) calculations of Itano *et al.* [59] gave quadrupole moments of $Q_{3/2}=2.11$ a.u. and $Q_{5/2}=3.02$ a.u. for the $4d_{3/2}$ and $4d_{5/2}$ states, respectively. The relativistic coupled-cluster (RCC) approach gave quadrupole moments of $Q_{3/2}=2.12$ a.u. and $Q_{5/2}=2.94$ a.u. [60]. A recent experiment has determined the quadrupole moment, $Q_{5/2}$, to be 2.6(3) a.u. [61].

The present estimate of the quadrupole moment for the $4d$ level is 2.840 a.u., which is 3–5 % smaller than the two calculations, but closer to the recent experiment. This is reminiscent of the situation for Ca$^+$ where a semiempirical model potential method [16] gave a quadrupole moment smaller than the two *ab initio* calculations [59,60] (and in better agreement with experiment). Examination of the convergence pattern of the RCI and RCC calculation reveals that substantial cancellations exist between some quite large terms and relatively small imperfections of the calculation of any of these terms could translate to errors in the final quadrupole moment. The present calculation may not be definitive, but there is less scope for error (within the framework of the frozen core approximation) and it should be preferred to the RCC and RCI estimates of the quadrupole moments.

E. Polarizabilities

The polarizabilities of the lowest six levels of Sr$^+$ are listed in Table III and compared with the results of other calculations. The dipole polarizability for the ground state, $89.88a_0^3$ is about 3% smaller than the estimate of $93.3a_0^3$ derived from oscillator strength sums using experimental data [2] (note, the core polarizability of $5.8a_0^3$ was added to the values listed in [2]). The uncertainty in the present polarizability for the ground state should be about 2–3 % and this mainly results from the uncertainty in the $5s \rightarrow 5p$ oscillator strength.

The polarizability for the $4d$ state is smaller than that of the ground state because there are no strong dipole transitions from the $4d$ state to the other low-lying levels. The negative polarizability for the $5p$ state is caused by the transitions to the states of lower energy. The respective size of the polarizabilities of the $5s$, $4d$, and $5p$ levels are similar to the respective sizes of the polarizabilities for the $4s$, $3d$, and $4p$ levels for Ca$^+$ [16].

F. Blackbody shift

The difference between the polarizabilities of the $5s$ and $4d$ states contributes to the blackbody shift through the approximate result [62]

$$\Delta\nu = -\frac{1}{2}(831.9\ \ \mathrm{V/m})^2\left(\frac{T(\mathrm{K})}{300}\right)^4[\alpha_d(4d)-\alpha_d(5s)]. \quad (7)$$

The polarizabilities in Eq. (7) are assumed to be in SI units which can be obtained by multiplying the values in Table III

TABLE IV. The dispersion coefficients (in a.u.) between the Sr^{+}(5s) and Sr^{+}(6s) states and the rare-gas atoms and atomic hydrogen. The Barklem *et al.* estimates [2] used oscillator strength sums to evaluate the dispersion constants. The numbers in the square brackets denote powers of 10.

System	C_6	C_8	C_{10}
Sr^{+}(5s)-H	62.70	2.697[3]	1.288[5]
$f^{(1)}$ sums, Ref.[2]	51.9		
Sr^{+}(5s)-He	24.37	912.5	4.105[4]
Sr^{+}(5s)-Ne	48.55	1.918[3]	9.005[4]
Sr^{+}(5s)-Ar	177.8	8.108[3]	4.171[5]
Sr^{+}(5s)-Kr	260.0	1.264[4]	6.869[5]
Sr^{+}(5s)-Xe	400.7	2.165[4]	1.291[6]
Sr^{+}(6s)-H	329.1	4.904[4]	8.227[6]
Sr^{+}(6s)-He	105.4	1.551[4]	2.643[6]
Sr^{+}(6s)-Ne	205.0	3.058[4]	5.280[6]
Sr^{+}(6s)-Ar	829.0	1.279[5]	2.228[7]
Sr^{+}(6s)-Kr	1248	1.955[5]	3.434[7]
Sr^{+}(6s)-Xe	2004	3.225[5]	5.761[7]

by 2.488 32 × 10^{-8} [62]. Using the present polarizabilities gives $\Delta\nu$=0.242 Hz at 300 K. One recent estimate of the frequency shift by Madej *et al.* gave 0.30 ± 0.11 Hz [8]. Their estimate of the frequency shift is larger than the present value because Madej *et al.* underestimated the polarizability of the 4d states since they did not include the contribution from the continuum. Their value of $54a_0^3$ (a core polarizability of $5.8a_0^3$ was added to the number reported in [8]) is about 10% smaller than the present polarizability of $61.77a_0^3$.

The possible influence of the spin-orbit splitting on the blackbody shift is estimated by replacing the spin-orbit averaged energy of the ^2D doublet with the actual energy with the $^2D_{5/2}$ level at −0.003 377 5 hartree [43]. When this was done, the 4d polarizability increased to $62.92a_0^3$ since the energy difference between the 4$d_{5/2}$ and the 5p levels is slightly smaller. The net effect of the slightly largely polarizability is a 4% reduction in the blackbody shift to 0.233 Hz at 300 K.

G. Dispersion coefficients with buffer atoms

The dispersion coefficients of a number of low-lying states interacting with hydrogen and the rare gases are listed in Tables IV–VI. The dispersion coefficients involving the Sr^{+} ground state are listed in Table IV. Dispersion coefficients involving the 4d and 5p excited states are given in Tables V and VI, respectively. There is relatively little data available for comparison [2].

The C_6 estimate of Barklem *et al.* [2] for the Sr^{+}(5s)-H configuration uses the Sr^{+} oscillator strengths which are taken from other sources. As such, there is no contribution from the Sr^{2+} core. The hydrogen oscillator strength distribution is based on an Unsold-type approximation [2,63] where the entire distribution is represented by a single term with an appropriately chosen excitation energy. The present estimate of C_6=62.70 a.u. is about 20% larger than the Barklem *et al.* estimate of C_6=51.9 a.u. The core contribution, which was omitted by Barklem *et al.*, was about 20%.

TABLE V. The dispersion coefficients (in a.u.) between the 4d states of Sr^{+} and the rare-gas atoms and atomic hydrogen. The Barklem *et al.* estimates [2] used oscillator strength sums to evaluate the dispersion constants and is assumed to represent an average over possible magnetic quantum numbers. The numbers in the square brackets denote powers of 10.

System		C_6	C_8	C_{10}
Sr^{+}(4d)-H	Σ	45.09	3.852[3]	2.650[5]
Sr^{+}(4d)-H	Π	41.26	1.515[3]	3.175[4]
Sr^{+}(4d)-H	Δ	29.76	261.1	4969
$f^{(1)}$ sums, Ref. [2]		13.8		
Sr^{+}(4d)-He	Σ	18.45	1295	8.781[4]
Sr^{+}(4d)-He	Π	17.14	526.2	7334
Sr^{+}(4d)-He	Δ	13.21	65.98	419.5
Sr^{+}(4d)-Ne	Σ	37.11	2628	1.832[5]
Sr^{+}(4d)-He	Π	34.56	1130	2.057[4]
Sr^{+}(4d)-He	Δ	26.91	209.5	2183
Sr^{+}(4d)-Ar	Σ	131.7	1.077[4]	7.904[5]
Sr^{+}(4d)-Ar	Π	121.6	4728	1.249[5]
Sr^{+}(4d)-Ar	Δ	91.37	1143	2.395[4]
Sr^{+}(4d)-Kr	Σ	191.2	1.647[4]	1.247[6]
Sr^{+}(4d)-Kr	Π	176.2	7388	2.302[5]
Sr^{+}(4d)-Kr	Δ	131.2	2026	5.215[4]
Sr^{+}(4d)-Xe	Σ	292.1	2.728[4]	2.188[6]
Sr^{+}(4d)-Xe	Π	268.4	1.272[4]	5.000[5]
Sr^{+}(4d)-Xe	Δ	197.2	4127	1.357[5]

The dispersion coefficients for the 4d states are larger than the value of Barklem *et al.* [2] which can be interpreted as an average over the different molecular symmetries. This is due to the omission of the $4d \rightarrow \epsilon\ell$ continuum in the intermediate sum of Barklem *et al.* [2]. Barklem *et al.* postulate a maximum value of 32.8 a.u. can arise from the subsequent inclusion of the valence state continuum.

The dispersion coefficients of the 4d level are generally smaller than the dispersion coefficients of the 5s level. This is similar to the situation in Ca^{+} where the dispersion coefficients for the 3d level were generally smaller than those for the 4s ground state. This occurs because there are no strong transitions between the 4d level and the other low-lying levels of Sr^{+} (refer to dipole oscillator strengths in Table II). The lack of any strong transitions to the low-lying states also manifested itself in the smaller polarizabilities of the 4d state.

Although the dipole polarizability of the 5p state is smaller than the polarizability of the 5s state, the dispersion coefficients involving the 5p state are larger than those involving the ground state. This is explained by the energy distribution of the 5p oscillator strength set. The transitions to the 4d and 5s states with negative oscillator strengths involve smaller transition energies than any of the upward

TABLE VI. The dispersion coefficients (in a.u.) between the $\mathrm{Sr}^+(5p)$ state and the rare-gas atoms and atomic hydrogen. The Barklem *et al.* estimates [2] used oscillator strength sums to evaluate the dispersion constants and is assumed to represent an average over possible magnetic quantum numbers. The numbers in the square brackets denote powers of 10.

System		C_6	C_8	C_{10}
$\mathrm{Sr}^+(5p)$-H	Σ	161.1	1.736[4]	1.332[6]
$\mathrm{Sr}^+(5p)$-H	Π	91.38	1157	3.695[4]
$f^{(1)}$ sums, Ref. [2]		104.3		
$\mathrm{Sr}^+(5p)$-He	Σ	52.24	5.716[3]	4.352[5]
$\mathrm{Sr}^+(5p)$-He	Π	32.07	343.2	8.507[3]
$\mathrm{Sr}^+(5p)$-Ne	Σ	102.3	1.138[4]	9.016[5]
$\mathrm{Sr}^+(5p)$-Ne	Π	63.35	856.2	2.308[4]
$\mathrm{Sr}^+(5p)$-Ar	Σ	406.7	4.691[4]	3.902[6]
$\mathrm{Sr}^+(5p)$-Ar	Π	242.3	4302	1.457[5]
$\mathrm{Sr}^+(5p)$-Kr	Σ	611.8	7.152[4]	6.143[6]
$\mathrm{Sr}^+(5p)$-Kr	Π	360.1	7309	2.799[5]
$\mathrm{Sr}^+(5p)$-Xe	Σ	983.2	1.179[5]	1.072[7]
$\mathrm{Sr}^+(5p)$-Xe	Π	568.6	1.430[4]	6.401[5]

transitions. So the impact of the downward transitions is maximized in the polarizability calculation with its $1/\Delta E^2$ energy denominator. However, the downward transitions have less impact in the C_6 calculation which uses different energy weighting factors.

IV. CONCLUSIONS

A survey of atomic parameters of the Sr^+ ion states relevant to the description of long-range interactions have been computed with a semiempirical method. The derived parameters have application in a number of different areas of physics. The main limitation of the present method is the absence of spin-orbit splitting and the results given here should be regarded as averages.

One aspect of the present calculation that may be regarded as unusual is that in a number of instances the present results are in better agreement with experiment than the results of apparently more sophisticated *ab initio* calculations. Two specific examples are the $4d \to 4f$ oscillator strength and the $4d$ quadrupole moment. It must be kept in mind that the polarization potentials are tuned to the experimental energies. Therefore, the radial dependence of the single electron wave functions are guaranteed to be correct at large distances. Many of the matrix elements relevant to the observables reported here are strongly weighted by the large-r form of the wave function. So tuning the model energy levels to experiment does go a long way to ensuring many other of the interesting observables will be predicted accurately. It would clearly be interesting to apply the present semiempirical approach within a relativistic framework.

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