Transition wavelengths and fine structure for the doublet states of Be^+

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Seventeen bound and core-excited states of Be^+ are calculated using configuration-interaction wave functions. Relativistic and mass-polarization corrections are included. The relativistic corrections considered are correction to the kinetic energy, Darwin term, contact terms, and retardation effect. The fine structure is calculated by using spin-orbit and spin-other-orbit operators. The wavelengths computed for the transitions from the core-excited states improve the agreement between theory and experiment. The lifetimes for these states are also calculated. Our calculated transition wavelengths and fine structures for the bound states agree well in most cases with the experimental data tabulated by Bashkin and Stoner.

I. INTRODUCTION

Radiative transitions among the Be^+ doublet levels have very recently been investigated both experimentally and theoretically by Agentoft, Anderson, Froese Fischer, and Smentek-Miekzarek.[1] In that work, multiconfiguration Hartree-Fock calculations (MCHF) by Froese Fischer and Smentek-Mielczarek were used to identify the spectral lines observed by Agentoft and Anderson in a beam-foil-spectroscopy experiment. The present knowledge of these doublet levels has been preceded by a detailed understanding of the Be^+ quartet transitions (see Chung and Davis[2] and references therein).

The wavelength region that has been investigated is 90—4000 Å. Most Be^+ doublet transitions observed in this wavelength region involve core-excited states. In an earlier work,[3] the singly and doubly core-excited autoionizing states of Be^+ were calculated with the saddle-point technique. These results were used to identify the Auger lines observed by Rødbro *et al.*[4] Here we used the Rayleigh-Ritz variation method to calculate the energies and wave functions for bound states and core-excited states with the $^2P^e$, $^2D^o$, and $^2F^e$ symmetry. These core-excited states are metastable against autoionization in the *LS* coupling scheme.

To improve the nonrelativistic energy, we also evaluate the mass-polarization effect and the relativistic corrections with the first-order perturbation theory. Using these energies and wave functions, we compute the transition wavelengths, oscillator strengths, and lifetimes for these states. These results are compared with the available experimental and theoretical results in the literature. The calculated transition wavelengths and fine-structure splittings for the bound states are also compared with the tabulated experimental data of Bashkin and Stoner.[5]

II. COMPUTATION PROCEDURE AND RESULTS

The wave functions for the Be^+ doublet states are expanded in terms of configuration-interaction basis functions. In the *LS* coupling scheme, we have

$$\Psi_{LMSS_Z}=A\Sigma C_{mnk}^{l_1 l_2 L_{12} l_3}\phi_{mnk}(r_1,r_2,r_3) \times Y_{l_1 l_2 L_{12}}^{l_3 LM}(\hat{r}_1,\hat{r}_2,\hat{r}_3)\chi_{SS_Z}(1,2,3)\ . \tag{1}$$

Here A is the antisymmetrization operator and the C's are linear parameters. The explicit forms for ϕ_{mnk} and $Y_{l_1 l_2 L_{12}}^{l_3 LM}$ are given in Davis and Chung.[3] We refer the interested reader to this reference. The spin function is given by

$$\chi_{SS_Z}(1,2,3)=\sum_{m_1,m_2,m_3,\mu_Z}\langle s_3\mu m_3\mu_Z\,|\,SS_Z\rangle \times\langle s_1 s_2 m_1 m_2\,|\,\mu\mu_Z\rangle \times f_{s_1 m_1}(1)f_{s_2 m_2}(2)f_{s_3 m_3}(3)\ , \tag{2}$$

where s_1, s_2, and s_3 are $\frac{1}{2}$ and f is the corresponding single-particle spin function. There are two different spin doublets for each value of S_Z, for most core-excited states, both of these are necessary in forming the total wave function for a converged energy.

The nonrelativistic energy and wave function are obtained by the standard variation procedure. That is

$$\delta\frac{\langle\Psi\,|\,H_0\,|\,\Psi\rangle}{\langle\Psi\,|\,\Psi\rangle}=0\ , \tag{3}$$

where

$$H_0=\sum_{i=1}^{3}\left[-\frac{1}{2}\nabla_i^2-\frac{Z}{r_i}\right]+\sum_{\substack{i,j=1\\ i<j}}^{3}\frac{1}{r_{ij}}\ . \tag{4}$$

The relativistic perturbation operators considered are the mass correction to the kinetic energy, Darwin term, con-

TABLE I. Energies for the Be^+ doublet states (in a.u.) H_1 mass correction term, H_2 Darwin term, H_3 contact term, H_4 retardation effect, H_5 mass-polarization effect. For explicit form of these operators see Refs. 2 and 11. $E_{tot}=\langle H_0\rangle+\langle(H_1+H_2)\rangle+\langle H_3\rangle+\langle H_4\rangle+\langle H_5\rangle$.

State	$\langle H_0\rangle$	$\langle H_1+H_2\rangle$ (10^{-3})	$\langle H_3\rangle$ (10^{-4})	$\langle H_4\rangle$ (10^{-5})	$\langle H_5\rangle$ (10^{-5})	E_{tot}
$(1s\,1s\,2s)^2S$	−14.323 557	−2.5565	2.829	−4.90	2.738	−14.325 852
$(1s\,1s\,3s)^2S$	−13.921 072	−2.4931	2.764	−4.78	2.602	−13.923 31
$(1s\,2s\,2s)^2S$	−10.122 718	−2.1114	0.167	0.14	−0.034	−10.124 812
$[1s(2p\,2p)^1S]^2S$	−9.699 517	−1.8427	0.063	3.36	−1.869	−9.701 338
$[(1s\,2s)^3S,3s]^2S$	−9.584 848	−2.0172	0.060	0.26	−0.294	−9.586 860
$(1s\,1s\,2p)^2P^o$	−14.177 922	−2.4586	2.725	−3.32	1.005	−14.180 132
$(1s\,1s\,3p)^2P^o$	−13.883 199	−2.4697	2.758	−4.29	2.128	−13.885 415
$(1s\,1s\,4p)^2P^o$	−13.781 937	−2.4560	2.779	−4.56	2.389	−13.784 137
$[1s(2s\,2p)^3P]^2P^o$	−9.959 355	−1.9454	0.247	−2.11	2.384	−9.961 273
$[1s(2s\,2p)^1P]^2P^o$	−9.878 071	−1.9193	0.148	2.63	−2.331	−9.879 972
$[(1s\,2s)^3S,3p]^2P^o$	−9.565 455	−1.9920	0.022	−0.02	0.254	−9.567 443
$[1s(2p\,2p)^3P]^2P$	−9.799 396	−1.8125	0.083	−1.77	2.862	−9.801 189
$[(1s\,2p)^3P,3p]^2P$	−9.445 519	−1.7958	0.014	3.63	−3.370	−9.447 311
$[(1s\,2p)^1P,3p]^2P$	−9.370 039	−1.7959	0.071	−2.22	2.651	−9.372 023
$(1s\,1s\,3d)^2D$	−13.877 118	−2.4728	2.707	−4.73	2.548	−13.879 342
$(1s\,1s\,4d)^2D$	−13.779 352	−2.4700	2.734	−4.73	2.555	−13.781 571
$[1s(2p\,2p)^1D]^2D$	−9.824 858	−1.8196	0.043	3.11	−3.597	−9.826 678
$[(1s\,2s)^3S,3d]^2D$	−9.524 384	−2.0007	0.007	−0.02	0.251	−9.526 382
$[(1s\,2s)^1S,3d]^2D$	−9.432 790	−1.8552	0.256	−0.56	1.336	−9.434 612
$[(1s\,2p)^3P,3d]^2D^o$	−9.415 989	−1.7806	0.001	4.27	−4.366	−9.417 771
$[(1s\,2s)^1P,3d]^2D^o$	−9.346 491	−1.7838	0.074	−3.31	3.878	−9.348 262
$[(1s\,2p)^3P,4d]^2D^o$	−9.306 804	−1.7770	0.001	4.27	−4.163	−9.308 580
$[(1s\,2p)^3P,4f]^2F$	−9.301 988	−1.7798	0.000	4.37	−4.214	−9.303 766
$[(1s\,2p)^3P,5f]^2F$	−9.255 948	−1.7817	0.000	4.38	−4.252	−9.257 728
$[(1s\,2p)^3P,6f]^2F$	−9.231 015	−1.7810	0.000	4.38	−4.267	−9.232 795
$[1s\,1s\,4f]^2F^o$	−13.779 621	−2.4718	2.707	−4.74	2.541	−13.781 844
$[(1s\,2s)^3S,4f]^2F^o$	−9.430 895	−1.9600	0.000	0.839	−0.940	−9.432 856

tact term [with $\delta(\vec{r}_{ij})$ potential], retardation term, spin-orbit, and spin-other-orbit effect.[6] The mass-polarization effect is also included. The spin-spin interaction consists of two parts. The scalar part which contains a $\delta(r_{ij})$ potential is included in the contact term. The other part is a contracted second-order tensor. It does not contribute to a doublet system. These operators are given for two-electron systems in Bethe and Salpeter.[6] The explicit form for a three-electron system is given in earlier works;[2,7] we refer the interested reader to these references. In the case of the mass-polarization operator, the nuclear mass for $^9_4$Be is taken to be 16 531.65 times the electron mass.

Among the relativistic corrections, the mass-correction term and the Darwin term are by far the largest; these expectation values are evaluated using the first-order perturbation theory. The contributions from the other perturbation operator are much smaller. The result would be the same whether they are calculated from first-order perturbation theory or from diagonalizing the Hamiltonian with the perturbation.

For calculating the fine-structure splitting, eigenfunctions with good quantum number J are formed by

$$|JM_JLS\rangle=\sum_{M_L,M_S}|LSM_LM_s\rangle\langle LSM_LM_S\,|\,JM_J\rangle\ . \tag{5}$$

With these eigenfunctions, the expectation values of spin-orbit and spin-other-orbit operators become[8]

$$\langle H_{s.o.}\rangle=2C_{s.o.}\vec{L}\cdot\vec{S} \tag{6}$$

and

$$\langle H_{s.o.o.}\rangle=2C_{s.o.o.}\vec{L}\cdot\vec{S}\ , \tag{7}$$

where $C_{s.o.}$ and $C_{s.o.o.}$ are the reduced matrix elements.[9] The $2\vec{L}\cdot\vec{S}$ takes the values L and $-L-1$ for $J=L+\frac{1}{2}$

TABLE II. Comparison of nonrelativistic energies for Be^+ doublet states (in a.u.).

State	This work	MCHF (Ref. 1)
$(1s\,1s\,2p)^2P^o$	−14.177 922	−14.169 81
$[1s(2s\,2p)^3P]^2P^o$	−9.959 355	−9.957 84
$[1s(2p\,2p)^3P]^2P$	−9.799 396	−9.797 74
$[(1s\,2p)^3P,3p]^2P$	−9.445 519	−9.443 97
$[(1s\,2p)^1P,3p]^2P$	−9.370 039	−9.365 30
$[1s(2p\,2p)^1D]^2D$	−9.824 858	−9.823 40
$[(1s\,2p)^3P,3d]^2D^o$	−9.415 989	−9.415 72
$[(1s\,2p)^1P,3d]^2D^o$	−9.346 491	−9.345 37
$[(1s\,2p)^3P,4d]^2D^o$	−9.306 804	−9.306 63
$[(1s\,2p)^3P,4f]^2F$	−9.301 988	−9.301 78
$[(1s\,2p)^3P,5f]^2F$	−9.255 948	−9.255 71

and $L-\frac{1}{2}$, respectively.

In computing the energy and wave function, we have used anywhere from 52 to 110 linear parameters and 7 to 18 angular partial waves depending on the convergence of the particular state of interest. The calculated energies are given in Table I together with the relativistic corrections which do not contribute to the fine structure splitting. In this table, the mass-correction term and Darwin term are combined. These two effects are large and usually eighty percent of the mass-correction contribution is canceled by the Darwin term. The contact term is always positive for these systems. The retardation effect and mass-polarization effect are much smaller. They are opposite in sign for the Be^+ doublet systems considered in this work.

III. RESULTS AND DISCUSSION

To assess the accuracy of the present results for the core-excited states, we compare the nonrelativistic energies in Table I with the MCHF results of Ref. 1. This comparison is given in Table II. Our results for the metastable-autoionizing states represent upper bounds to the true nonrelativistic eigenvalue. The fact that our energies are lower (by 0.000 15 to 0.0011 a.u.) implies that these energies are probably more accurate. The comparison for the autoionizing states is not as straightforward, since the upper bound principle does not hold for these states. These autoionizing levels were obtained in Davis and Chung[3] with the saddle-point technique. They agree excellently with the high-resolution experiment of Rødbro *et al.*[4]

Bashkin and Stoner[5] have tabulated fine-structure measurements for some of the bound states. These experimental results are compared with our calculated values in Table III. The agreement is good; the largest discrepancy is for the $(1s\,1s\,3d)^2D$ state for which our result is 3.6% too large. Denne *et al.*[10] have recently measured a few of these fine structures by fast beam-level spectroscopy. They obtain 0.2433 ± 0.0002 cm^{-1} and 0.1224 ± 0.0002 cm^{-1} for the $(1s\,1s\,4d)^2D$ and $(1s\,1s\,4f)^2F$ states, respectively. There are no experimental fine-structure data available for the core-excited doublet states of Be^+. In order to stimulate further experimental interest, the results for these states are also given in Table III. Many of these fine structures are inverted. In order to show how this arises, the individual contributions from the spin-orbit and the spin-other-orbit operators are tabulated. The inverted levels are seen to arise from a larger contribution from the spin-other-orbit effect. The $2p$ electron usually gives a larger contribution to the fine-structure splitting. It is interesting to note that the $(1s\,2p\,2p)^2P$ and $(1s\,2p\,2p)^2D$ states have the regular and inverted splittings 18.7 and -22.1 cm^{-1}, respectively.

The transition energies between the doublet states are calculated by using the E_{tot} given in Table I. The corresponding wavelengths are obtained by using the conversion factor 455.6613 Å/a.u. The wavelengths for the more probable transitions are given in Table IV along with the experimental and theoretical results of Agentoft, Anderson, Froese Fischer, and Smentek-Mielczarek.[1] The comparison with this reference is for transitions among the core-excited states and between the core-excited states and the bound states. Table IV also contains some transitions between the bound states. For these transitions we only quote the experimental wavelengths tabulated by Bashkin and Stoner[5] for comparison. The oscillator strengths given in this table are obtained by using the non-

TABLE III. Fine structures for the doublet states of Be^+ (for notation see text).

State	$C_{s.o.}$ (10^{-5} a.u.)	$C_{s.o.o.}$ (10^{-5} a.u.)	$(E_{L+0.5}-E_{L-0.5})$ cm^{-1} This work	Experiment (Ref. 5)
$(1s\,1s\,2p)^2P^o$	2.571 8	−1.591	6.458	6.58
$(1s\,1s\,3p)^2P^o$	0.755 6	−0.465 1	1.912	1.92
$(1s\,1s\,4p)^2P^o$			0.786	0.78
$[1s(2p\,2p)^3P]^2P$	3.612 0	−0.778 2	18.657	
$[(1s\,2p)^3P,3p]^2P$	1.382 0	−2.127 2	−4.906	
$[(1s\,2p)^1P,3p]^2P$	1.633 6	−0.320 4	8.646	
$[1s(2s\,2p)^3P]^2P^o$	2.036 7	−0.145 9	12.449	
$[1s(2s\,2p)^1P]^2P^o$	2.109 9	−3.103 3	−6.540	
$[(1s\,2s)^3S,3p]^2P^o$	−0.194 2	−0.612 4	−5.310	
$(1s\,1s\,3d)^2D$	0.106 04	−0.053 87	0.572	0.55
$(1s\,1s\,4d)^2D$	0.044 56	−0.022 77	0.239	0.24
$[(1s\,2p)^3P,3d]^2D^o$	0.697 41	−0.706 17	−0.096	
$[(1s\,2p)^1P,3d]^2D^o$	0.251 34	−0.041 04	2.308	
$[(1s\,2p)^3P,4d]^2D^o$	0.793 99	−0.677 21	1.281	
$[1s(2p\,2p)^1D]^2D$	0.530 12	−2.541 86	−22.075	
$[(1s\,2s)^3S,3d]^2D$	−0.023 429	−0.109 50	−1.459	
$[(1s\,2s)^1S,3d]^2D$	0.580 32	−0.948 99	5.326	
$(1s\,1s\,4f)^2F^o$	0.015 85	−0.008 00	0.121	0.12
$[(1s\,2p)^3P,4f]^2F$	0.431 32	−0.338 85	1.421	
$[(1s\,2p)^3P,5f]^2F$	0.434 97	−0.335 6	1.526	
$[(1s\,2p)^3P,6f]^2F$	0.436 09	−0.334 86	1.555	
$[(1s\,2s)^3S,4f]^2F^o$	0.404 88	−0.279 31	1.929	

TABLE IV. Transition wavelengths (in Å) and oscillator strengths for the doublet states of Be^+.

Transition	Wavelength	Oscillator strength[a]	MCHF (Ref. 1)	Experiment
$(1s\,1s\,4p)^2P^o$-$(1s\,1s\,3d)^2D$	4786.1	0.307 18(−1)		4828[b]
$(1s\,1s\,4f)^2F^o$-$(1s\,1s\,3d)^2D$	4673.6	0.725 33		4673[b]
$(1s\,1s\,4d)^2D$-$(1s\,1s\,3p)^2P^o$	4387.9	0.291 71		4361[b]
$[(1s\,2p)^3P,3d]^2D^o$-$[(1s\,2s)^3S,3d]^2D$	4195.4	0.558 92(−1)		
$[(1s\,2p)^3P,4f]^2F$-$[(1s\,2p)^3P,3d]^2D^o$	3996.8	0.552 82	3999.0	3995.5 ±0.3[c]
$[(1s\,2p)^3P,3p]^2P$-$[(1s\,2s)^3S,3p]^2P^o$	3793.0	0.174 19		
$[(1s\,2p)^3P,4d]^2D^o$-$[(1s\,2p)^3P,3p]^2P$	3284.5	0.734 31		3285[c]
$(1s\,1s\,4p)^2P^o$-$(1s\,1s\,3s)^2S$	3274.0	0.225 85(−1)		3274[b]
$(1s\,1s\,2p)^2P^o$-$(1s\,1s\,2s)^2S$	3126.9	0.166 41		3131[b]
$[1s(2p\,2p)^3P]^2P$-$[1s(2s\,2p)^3P]^2P^o$	2846.4	0.217 06	2844.0	2828.8[c]
$[(1s\,2p)^3P,5f]^2F$-$[(1s\,2p)^3P,3d]^2D^o$	2847.1	0.115 58	2847.6	2845.3 ±0.3[c]
$(1s\,1s\,3s)^2S$-$(1s\,1s\,2p)^2P^o$	1774.3	0.180 42		1776[b]
$(1s\,1s\,3d)^2D$-$(1s\,1s\,2p)^2P^o$	1514.9	0.368 25		1512[b]
$[(1s\,2p)^3P,3d]^2D^o$-$[1s(2p\,2p)^3P]^2P$	1188.4	0.909 31(−1)	1192.7	1187.5 ±0.3[c]
$(1s\,1s\,4d)^2D$-$(1s\,1s\,2p)^2P^o$	1143.3	0.801 75(−1)		1143[b]
$[(1s\,2p)^3P,3d]^2D^o$-$[1s(2p\,2p)^1D]^2D$	1114.3	0.177 90	1117.6	1111.8 ±0.5[c]
$[(1s\,2p)^3P,3p]^2P$-$[1s(2s\,2p)^1P]^2P^o$	1053.2	0.961 65(−1)		
$(1s\,1s\,3p)^2P^o$-$(1s\,1s\,2s)^2S$	1034.6	0.271 61(−1)		1036.3[b]
$[(1s\,2p)^1P,3d]^2D^o$-$[1s(2p\,2p)^3P]^2P$	1006.0	0.309 84	1007.2	1006.5 ±0.5[c]
$[(1s\,2p)^1P,3d]^2D^o$-$[1s(2p\,2p)^1D]^2D$	952.44	0.350 55(−1)		
$[(1s\,2p)^3P,4d]^2D^o$-$[1s(2p\,2p)^3P]^2P$	924.99	0.610 29(−1)	927.8	923.8 ±0.5[c]
$[(1s\,2p)^3P,4d]^2D^o$-$[1s(2p\,2p)^1D]^2D$	879.49	0.122 22	881.7	877.5 ±0.5[c]
$(1s\,1s\,4p)^2P^o$-$(1s\,1s\,2s)^2S$	841.14	0.102 01(−1)		842.0[b]
$[(1s\,2p)^1P,3p]^2P$-$[1s(2s\,2p)^3P]^2P^o$	773.03	0.331 79(−1)		
$[1s(2p\,2p)^3P]^2P$-$(1s\,1s\,2p)^2P^o$	104.06	0.206 27	104.2	103.98±0.03[c]
$[(1s\,2p)^1P,3p]^2P$-$(1s\,1s\,3p)^2P^o$	100.95	0.160 02		
$[(1s\,2p)^1P,3d]^2D^o$-$(1s\,1s\,3d)^2D$	100.56	0.173 92		
$[(1s\,2p)^3P,3p]^2P$-$(1s\,1s\,2p)^2P^o$	96.28	0.256 10(−1)	96.41	96.21±0.05[c]

[a] Values in parentheses denote powers of ten; e.g., $0.307\,18(-1)=0.307\,18\times10^{-1}$.
[b] Bashkin and Stoner, Ref. 5.
[c] Agentoft *et al.*, Ref. 1.

relativistic energies and wave functions.

For the transitions among the bound states, the agreement of the present work with experiment is good except for two transitions: the $4p$ to $3d$ transition and the $4d$ to $3p$ transition. The calculated wavelength for the $4p$ to $3d$ transition is too short (theory 4786 Å, expt. 4828 Å). This indicates that the calculated energy for $4p$ is probably too high. The calculated wavelength for the $4d$ to $3p$ transition is too long (theory 4388 Å, expt. 4360 Å) indicating once again that the calculated ^2P level is too high.

For the transitions from the core-excited states, the agreement between the present work and the experimental results of Ref. 1 is good. For all the identified lines in Table IV, this work improves the agreement between theory and experiment obtained previously by the MCHF calculation.[1] In Ref. 1, the computed transition wavelengths are obtained with energies which include the relativistic corrections: mass correction, Darwin term, and spin-spin contact term.[11] They do not consider retardation and mass polarization which are included in the present work.

Agentoft *et al.*[1] also discuss a weak line at 3285 Å. They remark that Mannervik has pointed out that this line could be assigned to the $[(1s\,2p)^3P,4d]^2D^o \rightarrow [(1s\,2p)^3P,3p]^2P$ transition. Our calculated result for this transition, 3284.5 Å, confirms this assignment.

Agentoft *et al.*[1] observe two lines relatively close to each other at 2828.8 and 2845.3 Å. They identify the line at 2828.8 Å with the $(1s\,2p\,2p)^2P \rightarrow [1s\,(2s\,2p)^3P]^2P$ transition. The fact that this line has a relatively larger line width supports the observation that the lower state is an autoionizing level. However, our calculated result for this transition, 2846.4 Å, deviates from the reported wavelength by 17 Å. This calculated result, along with our

TABLE V. Radiative lifetimes for the core-excited metastable-autoionizing Be^+ doublets (in 10^{-9} sec).

State	This work	MCHF (Ref. 1)	Experiment (Ref. 1)
$[1s(2p\,2p)^3P]^2P$	0.007 67	0.008	
$[(1s\,2p)^3P,3p]^2P$	0.049 0	0.05	
$[(1s\,2p)^1P,3p]^2P$	0.009 30		
$[(1s\,2p)^3P,3d]^2D^o$	0.472	0.74	0.55±0.07
$[(1s\,2p)^1P,3d]^2D^o$	0.008 51	0.43	
$[(1s\,2p)^3P,4d]^2D^o$	0.517	1.55	1.0 ±0.2
$[(1s\,2p)^3P,4f]^2F^e$	3.29	4.2	3.6 ±0.3
$[(1s\,2p)^3P,5f]^2F^e$	7.29	8.0	7 ±1

result of 2847.1 Å for the $[(1s\,2p)^3P,5f]^2F \rightarrow [(1s\,2p)^3P,3d]^2D^o$ transition, lie much closer to the observed line at 2845.3 Å. On the other hand, the calculated transitions to the autoionizing $1s\,2p\,2p\,^2D$ from $[(1s\,2p)^3P,3d]^2D^o$ at 1114.3 Å and from $[(1s\,2p)^3P,4d]^2D^o$ at 879.49 Å agree well with the reported 1111.8 ± 0.5 Å and 877.5 ± 0.5 Å, respectively.

The calculated lifetimes for the core-excited metastable autoionizing states are given in Table V together with the experimental and theoretical result of Ref. 1. Out of the four observed lifetimes, the agreement between theory and experiment is improved for three states. However, our calculated lifetime for the $[(1s\,2p)^3P,4d]^2D^o$ is too short compared with that of the experiment. Another serious disagreement with the calculated lifetime in Ref. 1 is for the $[(1s\,2p)^1P,3d]^2D^o$. In this case, our calculation shows that the transition to the $1s^2 3d\,^2D$ makes the lifetime of this state much shorter than the results given in Ref. 1.

IV. SUMMARY

In this work seventeen bound and core-excited Be^+ doublet states were calculated along with the relativistic and mass-polarization corrections using configuration-interaction wave functions. The calculated transition wavelengths among the bound states and their fine structures were compared to the experimental data tabulated by Bashkin and Stoner.[5] The agreement between this work and the experiment for these states was found to be good except for two transition wavelengths: $(1s\,1s\,4p)^2P^o$-$(1s\,1s\,3d)^2D$ (theory 4786 Å, expt. 4828 Å) and $(1s\,1s\,4d)^2D$-$(1s\,1s\,3p)^2P^o$ (theory 4388 Å, expt. 4360 Å). This probably indicates that these calculated $^2P^o$ states are too high.

The purpose of this work was to compare our theoretical results for the optical transitions from the core-excited Be^+ doublet states with the recent experimental and theoretical results of Agentoft *et al.*[1] The calculated transition wavelengths of this work improve the agreement between theory and experiment for all of the Be^+ doublet lines observed by Agentoft *et al.* The line at 3285 Å is identified with the $[(1s\,2p)^3P,4d]^2D^o$ -$[(1s\,2p)^3P,3p]^2P$ transition in this work. Most of the lifetimes calculated agree well with that of Ref. 1 with two exceptions. The reported fine structures for the core-excited states in this work have not been measured in the literature. We hope that these measurements can be done in the near future.

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