RAPID COMMUNICATIONS

PHYSICAL REVIEW A VOLUME 41, NUMBER 9 1 MAY 1990

QED contributions to the 3s-3p transitions in highly charged Na-like ions

J. F. Seely
E. O. Hulburt Center for Space Research, Naval Research Laboratory, Washington, D.C. 20375-5000

R. A. Wagner
Strategic Defense Initiative Organization, Pentagon, Washington, D.C. 20301-7100

(Received 9 January 1990)

The QED contributions to the energy intervals $3s_{1/2}$-$3p_{1/2}$, $3p_{1/2}$-$3p_{3/2}$, and $3s_{1/2}$-$3p_{3/2}$ in highly charged Na-like ions were determined by comparing the transition energies derived from the observations with the relativistic many-body perturbation-theory calculations of Johnson, Blundell, and Sapirstein [Phys. Rev. A **38**, 2699 (1988)] that do not include QED effects. The determined QED contributions differ considerably from the one-electron QED contributions and are in better agreement with screened-nucleus QED contributions. Predicted transition energies and wavelengths are presented for the Na-like ions with atomic numbers up to $Z=92$.

I. INTRODUCTION

The $3s_{1/2}$-$3p_{1/2}$ and $3p_{1/2}$-$3p_{3/2}$ transition energies for highly charged Na-like ions were calculated by Johnson, Blundell, and Sapirstein[1] using the relativistic many-body perturbation theory (MBPT). The calculations included second- and third-order Coulomb correlation corrections, first-order corrections for transverse photon exchange, and correlation corrections of second- and third-order to one transverse photon exchange. Finite nuclear size, reduced mass, and mass polarization corrections were also included, but quantum electrodynamic (QED) contributions such as the electron self-energy and vacuum polarization were omitted. The uncertainties in the calculated corrections were estimated to be much smaller than the QED contributions at higher Z. Contributions from QED were inferred by comparing the calculated transition energies with the transition energies that were derived from the experimental wavelengths for the $3s_{1/2}$-$3p_{1/2}$ and $3s_{1/2}$-$3p_{3/2}$ transitions. The $3s_{1/2}$-$3p_{1/2}$ transition had been observed for most of the elements with atomic numbers up to $Z=42$ and for $Z=47$, and the $3s_{1/2}$-$3p_{3/2}$ transition had been observed for the elements up to $Z=47$ and for $Z=50$.[2]

More recently, the $3s_{1/2}$-$3p_{1/2}$ and $3s_{1/2}$-$3p_{3/2}$ transitions were observed for $Z=54$ in spectra from the Princeton Large Torus (PLT) tokamak.[3] The $3s_{1/2}$-$3p_{3/2}$ transition was observed in spectra from laser-produced plasmas for the elements $Z=49$, 51, 53, and 55 (Ref. 4) and for $Z=48$, 49, 50, and 64 (Ref. 5). The observation of the $3s_{1/2}$-$3p_{1/2}$ transition for $Z=48$ and 50 was also reported in Ref. 5. By comparing the experimentally determined $3s_{1/2}$-$3p_{1/2}$ and $3s_{1/2}$-$3p_{3/2}$ transition energies with the transition energies that were calculated using Grant and co-worker's[6,7] multiconfiguration Dirac-Fock (MCDF) program, semiempirical corrections to the observed transition energies were derived, and semiempirically corrected transition energies were predicted for the elements with atomic numbers up to $Z=92$.[5]

In this paper, we compare the MBPT calculations of Ref. 1 with the recently available observations for the elements with atomic numbers up to $Z=64$ and with the

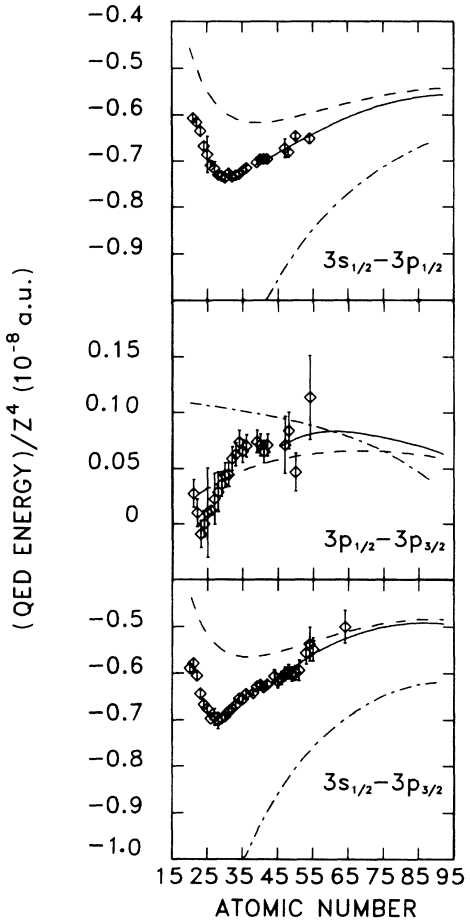

FIG. 1. The QED energy divided by Z^4 (in units of 10^{-8} a.u.) for the Na-like transitions $3s_{1/2}$-$3p_{1/2}$, $3s_{1/2}$-$3p_{3/2}$, and $3p_{1/2}$-$3p_{3/2}$. The data points are the differences between the observed transition energies (Refs. 2–5) and the MBPT energies (Ref. 1). The error bars represent the uncertainties in the observed transition energies. The solid curves are the differences between the semiempirically corrected predictions (Ref. 5) and the MBPT energies. The dashed curves are the screened-nucleus QED contributions calculated using Grant's program. The dash-dotted curves are the one-electron QED contributions (Ref. 1).

semiempirically corrected predictions for the elements up to $Z=92$. The QED contributions to the transition energies are determined by subtracting the MBPT energies from the observed and semiempirically corrected energies. These QED contributions are then compared with the calculated one-electron and screened-nucleus QED contributions.

II. TRANSITION ENERGIES

The $3s_{1/2}$-$3p_{1/2}$ and $3p_{1/2}$-$3p_{3/2}$ transition energies were calculated by Johnson, Blundell, and Sapirstein[1] for $Z=11$, 14, 17, 20, 26, 34, 42, 54, 74, and 92. In order to compare these transition energies with the observations and with the semiempirically corrected energies, the transition energies of Ref. 1 were interpolated using polynomials determined by the least-squares technique. The $3s_{1/2}$-$3p_{1/2}$ transition energy was fitted to a fourth-order polynomial in the atomic number Z. For the $3p_{1/2}$-$3p_{3/2}$ transition the quantity E/Z^3 was fitted to a fourth-order polynomial in Z. This is similar to the technique used in Ref. 8 for the Li-like $2s_{1/2}$-$2p_{1/2}$ and $2p_{1/2}$-$2p_{3/2}$ transitions. The interpolated transition energies were then subtracted from the observations of Refs. 2–5 and from the semiempirically corrected energies of Ref. 5. The resulting quantities are dominated by the QED contributions to the transition energies. The QED contributions derived in this manner from the observations of Refs. 2–5 are indicated by the data points in Fig. 1. The error bars in Fig. 1 represent the experimental uncertainties in the observations. The QED contributions derived from the semiempirically corrected energies of Ref. 5 are shown by the solid curves in Fig. 1. The dash-dotted curves in Fig. 1 are the one-electron QED contributions quoted in Ref. 1.

The electron self-energy (SE) contributions to the transition energies, and the smaller vacuum polarization contributions, were calculated using the optimal level option of Grant's program.[6,7] The Grant program derives the SE contributions to transition energies in multielectron ions from the one-electron contributions using a screened nuclear charge. The expectation value $\langle r\rangle$ of the radius r is calculated for the $3s$ and $3p$ orbitals under consideration, and the nuclear charge Z is varied to determine the effective charge Z_{eff} that would result in a relativistic Coulomb orbital of the same character and $\langle r\rangle$. The SE contribution from an orbital in the field of a point-charge Z_{eff} is determined by interpolation among the one-electron values of Mohr.[9] The calculated QED contributions to the Li-like $2s$-$2p$ and Cu-like $4s$-$4p$ transitions were compared to the observations in Refs. 8 and 10.

Using Grant's program, the QED contributions to the Na-like energies were calculated for all of the elements with atomic numbers $Z=20$–92 and are shown by the dashed curves in Fig. 1. The QED contributions derived from the observations are in better agreement with the screened-nucleus QED contributions than with the one-electron QED contributions. For higher Z, the QED contributions derived from the semiempirically corrected energies of Ref. 5 approach the screened-nucleus contributions.

TABLE I. The calculated and observed transition energies and QED contributions (in eV). For each ion, the first row is $3s_{1/2}$-$3p_{1/2}$, the second row is $3p_{1/2}$-$3p_{3/2}$, and the third row is $3s_{1/2}$-$3p_{3/2}$.

	Calculated[a]						QED		
Z Ion	Coulomb[b]	Corr.[c]	Breit[d]	Red. mass[e]	Total[f]	Fitted[g]	Total and observed[h]	Screened Nucl.[i]	One-*el.*[j]
42 Mo^{31+}	70.4673	−0.2010	0.5132	−0.0046	70.775 ± 0.001	70.185 ± 0.002	−0.590 ± 0.002	−0.52	−0.84
	27.1731	0.0499	−0.5018	−0.0001	26.721 ± 0.001	26.774 ± 0.004	0.053 ± 0.004	0.05	0.08
	97.6405	−0.1512	0.0113	−0.0047	97.496 ± 0.001	96.960 ± 0.004	−0.536 ± 0.004	−0.47	−0.76
54 Xe^{43+}	100.4848	−0.2400	1.3100	−0.0060	101.549 ± 0.002	100.054 ± 0.004	−1.495 ± 0.004	−1.38	−1.98
	87.1201	0.0909	−1.3162	−0.0003	85.895 ± 0.002	86.082 ± 0.015	0.187 ± 0.015	0.15	0.21
	187.6049	−0.1491	−0.0063	−0.0063	187.443 ± 0.002	186.136 ± 0.014	−1.307 ± 0.014	−1.24	−1.78
74 W^{63+}	160.5348	−0.2963	4.1609	−0.0082	164.391 ± 0.006	159.65 ± 0.06	−4.74 ± 0.06	−4.57	−5.87
	377.5664	0.2038	−4.6752	−0.0005	373.094 ± 0.004	373.74 ± 0.1	0.65 ± 0.1	0.53	0.55
	538.1012	−0.0925	−0.5143	−0.0087	537.486 ± 0.006	533.38 ± 0.1	−4.11 ± 0.1	−4.04	−5.32
92 U^{81+}	230.0909	−0.3676	9.5279	−0.0084	239.242 ± 0.013	228.38 ± 0.2	−10.86 ± 0.2	−10.59	−12.68
	1088.2781	0.3899	−12.3500	−0.0014	1076.317 ± 0.009	1077.55 ± 0.3	1.23 ± 0.3	1.15	0.60
	1318.3691	0.0223	−2.8221	−0.0098	1315.559 ± 0.015	1305.93 ± 0.2	−9.63 ± 0.2	−9.44	−12.07

[a]MBPT calculations of Ref. 1.
[b]Dirac-Fock energy.
[c]Second- and third-order Coulomb correlation corrections.
[d]Lowest-order Breit correction and the second- and third-order correlation corrections.
[e]Reduced mass and mass polarization corrections.
[f]Total calculated energy (sum of columns b–e).
[g]Transition energy derived from the semiempirically corrected wavelengths of Ref. 5.
[h]QED contribution derived from total and fitted columns.
[i]Screened-nucleus QED contribution calculated using Grant's program (Refs. 6 and 7).
[j]One-electron QED contribution from Ref. 1.

TABLE II. The calculated and observed wavelengths (in Å) for the $3s_{1/2}$-$3p_{1/2}$ and $3s_{1/2}$-$3p_{3/2}$ transitions in Na-like ions.

	$3s_{1/2}$-$3p_{1/2}$				$3s_{1/2}$-$3p_{3/2}$			
	Calculated				Calculated			
Z	Without QED	With QED	Fitted	Observed	Without QED	With QED	Fitted	Observed
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)
39	194.851	196.047	196.219	196.215 ± 0.010	150.310	150.961	151.033	151.035 ± 0.010
40	187.886	189.117	189.284	189.277 ± 0.010	142.126	142.768	142.845	142.839 ± 0.010
41	181.348	182.614	182.775	182.777 ± 0.010	134.428	135.061	135.135	135.138 ± 0.010
42	175.196	176.497	176.654	176.666 ± 0.010	127.180	127.802	127.873	127.873 ± 0.010
43	169.397	170.732	170.885		120.349	120.959	121.025	
44	163.920	165.289	165.440		113.905	114.503	114.566	114.556 ± 0.015
45	158.737	160.139	160.288		107.824	108.409	108.467	108.474 ± 0.015
46	153.825	155.260	155.408		102.082	102.652	102.706	102.711 ± 0.015
47	149.161	150.628	150.775	150.78 ± 0.05	96.658	97.212	97.263	97.263 ± 0.015
48	144.727	146.226	146.374	146.407 ± 0.015	91.532	92.070	92.118	92.118 ± 0.015
49	140.505	142.036	142.184		86.687	87.209	87.254	87.262 ± 0.015
50	136.479	138.043	138.191	138.149 ± 0.015	82.106	82.612	82.654	82.663 ± 0.015
51	132.636	134.231	134.380		77.774	78.263	78.303	78.311 ± 0.020
52	128.963	130.588	130.739		73.677	74.150	74.187	
53	125.449	127.103	127.254		69.803	70.259	70.293	70.276 ± 0.020
54	122.082	123.766	123.918	123.92 ± 0.03	66.138	66.578	66.610	66.58 ± 0.03
55	118.853	120.566	120.718		62.672	63.095	63.124	63.108 ± 0.020
56	115.754	117.495	117.649		59.393	59.799	59.826	
57	112.776	114.546	114.699		56.291	56.681	56.706	
58	109.912	111.710	111.861		53.357	53.731	53.754	
59	107.156	108.981	109.130		50.582	50.940	50.960	
60	104.502	106.352	106.501		47.956	48.299	48.317	
61	101.942	103.819	103.965		45.472	45.800	45.815	
62	99.474	101.375	101.522		43.122	43.436	43.450	
63	97.090	99.016	99.159		40.899	41.199	41.211	
64	94.788	96.738	96.880		38.796	39.082	39.093	39.075 ± 0.020
65	92.562	94.535	94.673		36.806	37.078	37.087	
66	90.409	92.406	92.539		34.922	35.182	35.191	
67	88.326	90.344	90.472		33.141	33.388	33.395	
68	86.308	88.349	88.471		31.454	31.690	31.696	
69	84.354	86.415	86.529		29.858	30.083	30.087	
70	82.459	84.541	84.650		28.348	28.561	28.566	
71	80.622	82.723	82.823		26.918	27.121	27.124	
72	78.839	80.960	81.053		25.564	25.757	25.760	
73	77.108	79.248	79.332		24.282	24.466	24.469	
74	75.428	77.586	77.661		23.069	23.243	23.245	
75	73.795	75.971	76.035		21.919	22.085	22.087	
76	72.208	74.401	74.459		20.830	20.988	20.990	
77	70.666	72.875	72.922		19.799	19.949	19.951	
78	69.165	71.391	71.429		18.822	18.964	18.966	
79	67.706	69.947	69.973		17.895	18.030	18.032	
80	66.285	68.541	68.560		17.018	17.146	17.148	
81	64.902	67.173	67.185		16.186	16.307	16.310	
82	63.556	65.840	65.846		15.397	15.512	15.515	
83	62.244	64.542	64.539		14.649	14.758	14.762	
84	60.966	63.276	63.261		13.940	14.043	14.046	
85	59.720	62.043	62.020		13.267	13.365	13.368	
86	58.506	60.841	60.843		12.628	12.722	12.726	
87	57.322	59.669	59.667		12.022	12.111	12.114	
88	56.167	58.526	58.529		11.448	11.532	11.535	
89	55.041	57.410	57.416		10.902	10.982	10.984	
90	53.942	56.322	56.347		10.384	10.459	10.462	
91	52.869	55.259	55.286		9.892	9.964	9.966	
92	51.822	54.223	54.288		9.424	9.493	9.494	

Based on the isoelectronic analysis of the Na-like transitions in the elements with atomic numbers up to $Z=42$, Edlén[11] found that the contributions to the $3s$ and $3p$ energy levels can be expressed as functions of $Z_{\text{eff}}=Z-s$, where s is a screening parameter that has values in the range 4–10. For increasing Z, the ratio s/Z decreases, and the screening corrections diminish in importance. In general, the transition energies in highly charged ions tend to approach the hydrogenic values in the limit of high Z.[12] Thus the Z scaling of the screened nucleus and hydrogenic QED contributions shown in Fig. 1 is consistent with the expected behavior of screening effects in highly charged ions.

Considering the high accuracy of the transition energies of Ref. 1, the differences between the QED contributions derived from the observations and the screened-nucleus QED contributions may be attributed to inaccuracies in the calculation of the screened-nucleus QED contributions. It is clear that an *ab initio* treatment of QED contributions to transition energies in highly charged multielectron ions is needed.

The results for the elements with atomic numbers $Z=42$, 54, 74, and 92 are listed in Table I. The last three columns in Table I give the values for the QED contributions derived from the observations, the screened-nucleus QED contributions, and the one-electron QED contributions. For $Z=74$ and 92, the screened-nucleus QED contributions are consistent with the QED contributions derived from the semiempirically corrected predictions of Ref. 5.

The wavelengths for the $3s_{1/2}$-$3p_{1/2}$ and $3s_{1/2}$-$3p_{3/2}$ transitions were derived from the transition energies and are listed in Table II. Columns numbers (2) and (6) in Table II give the wavelengths based on the polynomial fit to the MBPT calculations of Ref. 1, columns (3) and (7) give the wavelengths based on the MBPT calculations and the screened-nucleus QED contributions, columns (4) and (8) give the semiempirically corrected wavelengths of Ref. 5, and columns (5) and (9) give the observed wavelengths of Refs. 2–5. The wavelengths in columns (3), (4), (7), and (8) should be useful for the experimental identification of the $3s_{1/2}$-$3p_{1/2}$ and $3s_{1/2}$-$3p_{3/2}$ transitions in high-Z ions.

III. CONCLUSION

The QED contributions to the $3s_{1/2}$-$3p_{1/2}$, $3p_{1/2}$-$3p_{3/2}$, and $3s_{1/2}$-$3p_{3/2}$ energy intervals were determined for the elements with atomic numbers up to $Z=92$. For the $3s_{1/2}$-$3p_{1/2}$ and $3s_{1/2}$-$3p_{3/2}$ intervals, the one-electron QED contributions dramatically underestimate the magnitude of the QED corrections for all atomic numbers Z, and the screened-nucleus contributions slightly overestimate the QED corrections for the higher-Z ions. These results should be a stimulus for making improvements to the calculation of QED contributions to transitions in highly charged multielectron ions.

ACKNOWLEDGMENTS

This work was supported by the Office of Naval Research and the Strategic Defense Initiative Organization.

[1] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **38**, 2699 (1988).

[2] J. Reader, V. Kaufman, J. Sugar, J. O. Ekberg, U. Feldman, C. M. Brown, J. F. Seely, and W. L. Rowan, J. Opt. Soc. Am. B **4**, 1821 (1987).

[3] J. F. Seely, U. Feldman, A. W. Wouters, J. L. Schwob, and S. Suckewer (unpublished).

[4] J. F. Seely, U. Feldman, C. M. Brown, M. C. Richardson, D. D. Dietrich, and W. E. Behring, J. Opt. Soc. Am. B **5**, 785 (1988).

[5] J. F. Seely, C. M. Brown, U. Feldman, J. O. Ekberg, C. J. Keane, B. J. MacGowan, D. R. Kania, and W. E. Behring, At. Data Nucl. Data Tables (to be published).

[6] I. P. Grant, B. J. McKenzie, P. H. Norrington, D. F. Mayers, and N. C. Pyper, Comput. Phys. Commun. **21**, 207 (1980).

[7] B. J. McKenzie, I. P. Grant, and P. H. Norrington, Comput. Phys. Commun. **21**, 233 (1980).

[8] J. F. Seely, Phys. Rev. A **39**, 3682 (1989).

[9] P. J. Mohr, Ann. Phys. (N.Y.) **88**, 52 (1974); Phys. Rev. Lett. **34**, 1050 (1976).

[10] J. F. Seely, U. Feldman, A. W. Wouters, J. L. Schwob, and S. Suckewer, Phys. Rev. A **40**, 5020 (1989).

[11] B. Edlén, Phys. Scr. **17**, 565 (1978).

[12] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981), p. 570.