Energy levels of the low-lying states of mid-Z heliumlike ions

K. T. Cheng and M. H. Chen
Lawrence Livermore National Laboratory, University of California, Livermore, California 94550
(Received 22 November 1999; revised manuscript received 10 January 2000; published 13 March 2000)

Energy levels of the ground state and $n=2$ excited states of heliumlike ions with $22\leqslant Z\leqslant 36$ are calculated using a large-scale, relativistic configuration-interaction method. Quantum electrodynamic corrections are evaluated in Dirac-Kohn-Sham (DKS) potentials to account for screening and relaxation effects, and results are shown to be quite reliable as long as the Latter correction to the DKS potentials is excluded. We also find good agreements among different high-precision calculations and between theory and experiment in this Z range.

PACS number(s): 31.30.Jv, 31.25.−v, 31.10.+z, 31.15.Ar

In our previous works [1,2], we have calculated the energy levels of the ground state and $n=2$ excited states of selected heliumlike ions using a large-scale, relativistic configuration-interaction (RCI) method with B-spline basis functions. Quantum electrodynamic (QED) corrections, which are calculated in external model potentials to account for screening and orbital relaxation effects, were also included. For the correlation energies, our RCI method is in excellent agreement with the relativistic many-body all-order theory of Plante *et al.* [3]. Both theories disagree slightly with the unified theory of Drake [4] and these differences are due mainly to relativistic correlation corrections, of orders $(\alpha Z)^4$ and higher, which are included in our RCI and the all-order method but not in the unified theory. As for the QED energies, there are also discrepancies between our RCI and the unified theory which can exceed those of the correlation energies.

At this time, existing measurements on transition energies are not accurate enough to test these QED differences. This can be seen, for example, in Fig. 5 of Ref. [2], where $K\alpha_1$ x-ray energies are compared between theory and experiment: In spite of the discrepancy between RCI and the unified theory in the mid-Z range, existing experiments agree either with both theories, as in the case of $Z=22$ and 24, or with neither, as in the case of $Z=26$, 32, and 36. Indeed, for Kr^{34+}, the experimental value of 13 115.31±0.30 eV [5] is higher than both the RCI value of 13 114.70 eV and the unified theory value of 13 114.34 eV. While the difference in QED corrections between the two theories amounts to 0.24 eV, which is nearly twice the 0.13 eV difference in correlation energies, the discrepancy between theory and experiment is simply too large to shed any light on these two QED calculations.

Since the publication of our work [1,2], there have been new developments in theory and experiment. On the experimental side, there are two new high-precision, electron beam ion trap (EBIT) measurements of the $K\alpha$ x-ray energies: one by Chantler *et al.* [6] for V^{21+}, and the other by Widmann *et al.* [7] for Kr^{34+}. While these new data are still not accurate enough to test different QED calculations, they are in good agreement with theory and resolve the above mentioned discrepancy between theory and experiment for Kr^{34+}. On the theoretical side, we have since discovered that differences between our QED results and those of the unified theory are due largely to the use of the Latter correction in the Dirac-Kohn-Sham (DKS) potentials used in our QED calculations. Without this correction, the two QED results are in much better agreement for mid-Z ions. Since the Latter correction is just an *ad hoc* correction to force DKS potentials to behave asymptotically like $-(Z-N+1)e^2/r$ instead of $-(Z-N)e^2/r$, there is really no compelling reason to use it for QED calculations. Indeed, as we shall show later, there is new evidence that suggests that this correction probably should not be used at all.

In view of this recognition, and in view of recent experimental interest in high-precision $K\alpha$ x-ray measurements for mid-Z ions as potential tests of QED, we present, in this paper, updated RCI results for the ground state and $n=2$ excited states of heliumlike ions with $22\leqslant Z\leqslant 36$. For the $K\alpha$ x-ray energies, our new RCI results are in much better agreement with the all-order calculations [3] and the unified theory [4]. Furthermore, all three theories are consistent with the two new EBIT measurements at $Z=23$ [6] and $Z=36$ [7].

Details of our RCI method have been given in Refs. [1,2] before. Here, we outline only the essential features. Briefly, the calculations are based on the relativistic no-pair Hamiltonian. Retarded Breit energies are calculated from the full frequency-symmetrized Breit operator [8]. B-spline basis functions used here are Dirac orbitals for an electron in a Coulomb field constrained to a cavity of finite radius and are obtained with the method of Johnson *et al.* [9]. Our RCI matrices are large and can include over 8000 configurations. The iterative Davidson method [10,11] is used here to solve these large eigenvalue problems for the first few eigenstates.

In this work, QED corrections are obtained in the same way as in Ref. [2]. Self-energies are calculated in external potentials using the method of Cheng *et al.* [12]. Vacuum polarizations are evaluated from the expectation values of the Uehling potential, with Wichmann and Kroll corrections obtained from Johnson and Soff [13]. Total QED corrections are then given by the sum of these one-electron QED contributions, weighted by the fractional occupation number of each orbital. In these QED calculations, the effects of screening and orbital relaxation are included by using DKS potentials specific to each state. In contrast to our previous work [2], the Latter correction to the DKS potentials is no longer used here.

In Table I, we present the ionization energies of the ground state and $n=2$ excited states for heliumlike ions with

TABLE I. Ionization energies (eV) of the ground state and $n=2$ excited states of heliumlike ions. RCI results include Coulomb and frequency-dependent Breit energies. MP are the mass polarization contributions from the unified theory [4].

Z	Energy	1^1S_0	2^1S_0	2^1P_1	2^3S_1	2^3P_0	2^3P_1	2^3P_2
22	RCI	−6251.1083	−1521.5709	−1499.3968	−1547.3294	−1523.3596	−1522.0628	−1515.2149
	MP	0.0009	0.0001	0.0097	0.0001	−0.0108	−0.0099	−0.0108
	QED	2.0437	0.2506	−0.0245	0.2503	−0.0419	−0.0386	−0.0212
	Total	−6249.0637	−1521.3202	−1499.4116	−1547.0791	−1523.4123	−1522.1113	−1515.2470
23	RCI	−6853.7436	−1670.5982	−1646.1661	−1697.7438	−1672.4394	−1670.9600	−1662.5677
	MP	0.0009	0.0001	0.0098	0.0001	−0.0111	−0.0100	−0.0111
	QED	2.3831	0.2948	−0.0259	0.2944	−0.0471	−0.0436	−0.0223
	Total	−6851.3597	−1670.3033	−1646.1821	−1697.4493	−1672.4976	−1671.0135	−1662.6012
24	RCI	−7484.6755	−1826.7646	−1799.8184	−1855.3173	−1828.6490	−1826.9866	−1816.7872
	MP	0.0009	0.0001	0.0103	0.0001	−0.0119	−0.0104	−0.0119
	QED	2.7594	0.3441	−0.0270	0.3437	−0.0526	−0.0489	−0.0233
	Total	−7481.9152	−1826.4204	−1799.8351	−1854.9736	−1828.7135	−1827.0460	−1816.8224
25	RCI	−8144.0234	−1990.1062	−1960.3569	−2020.0850	−1992.0220	−1990.1801	−1977.8810
	MP	0.0009	0.0001	0.0103	0.0001	−0.0123	−0.0105	−0.0123
	QED	3.1747	0.3989	−0.0280	0.3985	−0.0586	−0.0547	−0.0241
	Total	−8140.8478	−1989.7073	−1960.3746	−2019.6864	−1992.0929	−1990.2453	−1977.9174
26	RCI	−8831.8852	−2160.6545	−2127.7849	−2192.0810	−2162.5910	−2160.5772	−2145.8543
	MP	0.0009	0.0001	0.0107	0.0001	−0.0131	−0.0108	−0.0131
	QED	3.6311	0.4595	−0.0285	0.4591	−0.0649	−0.0609	−0.0245
	Total	−8828.2532	−2160.1949	−2127.8027	−2191.6218	−2162.6690	−2160.6489	−2145.8919
27	RCI	−9548.3886	−2338.4484	−2302.1055	−2371.3439	−2340.3930	−2338.2185	−2320.7150
	MP	0.0009	0.0001	0.0107	0.0001	−0.0134	−0.0108	−0.0134
	QED	4.1307	0.5264	−0.0287	0.5260	−0.0716	−0.0675	−0.0246
	Total	−9544.2571	−2337.9219	−2302.1235	−2370.8178	−2340.4780	−2338.2968	−2320.7531
28	RCI	−10293.6435	−2523.5228	−2483.3221	−2557.9105	−2525.4631	−2523.1433	−2502.4681
	MP	0.0009	0.0001	0.0113	0.0001	−0.0147	−0.0115	−0.0147
	QED	4.6755	0.5999	−0.0285	0.5993	−0.0786	−0.0745	−0.0243
	Total	−10288.9670	−2522.9229	−2483.3393	−2557.3111	−2525.5565	−2523.2292	−2502.5072
29	RCI	−11067.7875	−2715.9209	−2671.4429	−2751.8247	−2717.8445	−2715.3976	−2691.1246
	MP	0.0009	0.0001	0.0109	0.0001	−0.0146	−0.0110	−0.0146
	QED	5.2678	0.6802	−0.0277	0.6797	−0.0860	−0.0819	−0.0236
	Total	−11062.5188	−2715.2406	−2671.4598	−2751.1449	−2717.9451	−2715.4905	−2691.1628
30	RCI	−11870.9450	−2915.6811	−2866.4694	−2953.1259	−2917.5742	−2915.0218	−2886.6883
	MP	0.0009	0.0001	0.0111	0.0001	−0.0154	−0.0112	−0.0154
	QED	5.9100	0.7679	−0.0264	0.7674	−0.0937	−0.0896	−0.0224
	Total	−11865.0341	−2914.9131	−2866.4847	−2952.3585	−2917.6833	−2915.1227	−2886.7260
31	RCI	−12703.2658	−3122.8497	−3068.4105	−3161.8618	−3124.6980	−3122.0647	−3089.1701
	MP	0.0009	0.0001	0.0107	0.0001	−0.0153	−0.0108	−0.0153
	QED	6.6036	0.8634	−0.0245	0.8628	−0.1016	−0.0977	−0.0205
	Total	−12696.6613	−3121.9863	−3068.4243	−3160.9989	−3124.8150	−3122.1731	−3089.2059
32	RCI	−13564.8814	−3337.4693	−3277.2717	−3378.0764	−3339.2593	−3336.5718	−3298.5767
	MP	0.0008	0.0001	0.0104	0.0001	−0.0154	−0.0105	−0.0154
	QED	7.3512	0.9669	−0.0218	0.9663	−0.1099	−0.1060	−0.0180
	Total	−13557.5293	−3336.5023	−3277.2831	−3377.1101	−3339.3846	−3336.6883	−3298.6101
36	RCI	−17307.4871	−4271.4460	−4182.0624	−4318.7245	−4272.8401	−4270.2423	−4205.6223
	MP	0.0008	0.0001	0.0101	0.0001	−0.0171	−0.0102	−0.0171
	QED	10.9257	1.4702	−0.0031	1.4694	−0.1453	−0.1420	0.0003
	Total	−17296.5605	−4269.9758	−4182.0554	−4317.2550	−4273.0025	−4270.3945	−4205.6391

$Z=22$–32 as well as $Z=36$. Here, the RCI energies include Coulomb and frequency-dependent Breit energies and are newly calculated, except for some of the even-Z ions where data are available from our previous work [1,2]. QED corrections are completely recalculated. As before, mass polarization (MP) contributions are taken from the unified theory [4].

Between the $n=2$ states, the effect of our new QED corrections on transition energies is not significant. More obvious changes can be found in transitions between the $n=1$ and 2 states. As an example, we compare, in Table II, $K\alpha_1$ x-ray energies between theory and experiment. It can be seen that, without the Latter correction in our QED calculations, the present RCI results are in much better agreement with the all-order method [3] and the unified theory [4] than our previous results in Ref. [2]. Nevertheless, changes in our RCI results are small enough that they do not alter the agreement between theory and experiment, which is very good overall.

TABLE II. Theoretical and experimental $K\alpha_1$ x-ray energies (eV) for heliumlike ions.

Z	Previous RCI[a]	Present RCI	All order[b]	Unified theory[c]	Experiment	Reference
22	4749.71	4749.65	4749.64	4749.63	4749.74(0.17)	[16]
23		5205.18	5205.16	5205.15	5205.10(0.14)	[6]
24	5682.15	5682.08	5682.06	5682.05	5682.32(0.40)	[16]
25		6180.47		6180.43		
26	6700.54	6700.45	6700.43	6700.40	6700.73(0.20)	[16]
					6700.90(0.25)	[17]
					6700.08(0.24)	[18]
27		7242.13		7242.08		
28		7805.63	7805.59	7805.56		
29		8391.06		8390.98		
30		8998.55	8998.50	8998.46		
31		9628.24		9628.14		
32	10280.39	10280.25	10280.19	10280.14	10280.70(0.22)	[19]
36	13114.70	13114.51	13114.42	13114.34	13115.31(0.30)	[5]
					13114.68(0.36)	[7]

[a]Reference [2].
[b]Reference [3].
[c]Reference [4].

Exceptions are $Z=26$ and 32, where theoretical values lie slightly outside experimental uncertainties. But the large discrepancy between theory and experiment at $Z=36$ is clearly removed by the new EBIT measurement [7].

In Fig. 1, differences between our RCI and the unified theory on $K\alpha_1$ correlation and QED energies as scaled by $(\alpha Z)^4$ are shown. As pointed out in Refs. [2,3], QED energies of the singlet states from the unified theory contain $(\alpha Z)^3$ terms that come from the no-pair Hamiltonian and not from radiative corrections. They are given by $\delta(\alpha Z)^3$ a.u., where $\delta=0.189\,50$, $0.037\,43$, and $0.012\,48$ for the 1^1S_0, 2^1S_0, and 2^1P_1 states, respectively. For more meaningful comparisons with our RCI results here, these terms are removed from the QED energies of the unified theory and added to its correlation energies.

As seen in Fig. 1, differences in the scaled correlation energy are almost constant in this Z range. This is due mainly to the missing relativistic correlation energies in the unified theory, which are of order $(\alpha Z)^4$ and higher in the perturbation expansion. But the most striking feature here is the effect of the Latter correction on our QED results. With this correction in the DKS potentials, our previous QED results differ significantly from those of the unified theory and the scaled discrepancy actually increases as Z decreases. Without this correction, however, our new QED results agree much better with the unified theory, especially at the low-Z end.

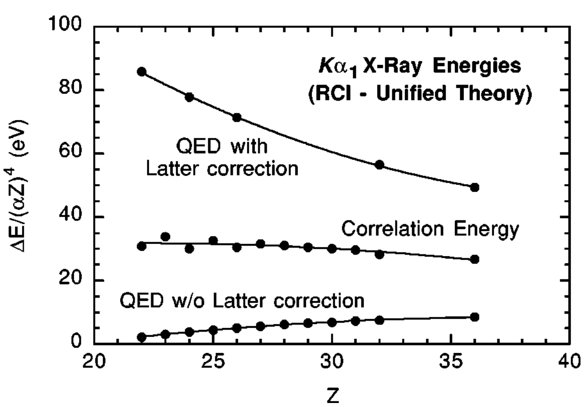

FIG. 1. Differences in scaled $K\alpha_1$ correlation and QED energies between the RCI and the unified theory [4].

In the unified theory, screening corrections to the hydrogenic QED energies are included by evaluating leading αZ-expansion terms from higher-order QED diagrams. This method may not be suitable for high-Z ions, but should work reasonably well for low- to mid-Z ions. Our method is based on nonperturbative calculations of the one-loop self-energy and vacuum polarization diagrams and should work for any ion. But as screening corrections are included by the use of model potentials in evaluating these one-loop radiative diagrams, the results are nevertheless potential dependent. In principle, it should not matter what potential is used if higher-order QED calculations are also carried out. But until that can be accomplished, the fact that QED energies calculated with the Latter correction actually diverge from those of the unified theory at low Z suggests that this is probably not a very good approximation for lowest-order QED calculations.

In fact, higher-order QED calculations for the $1s^2$ ground state have been carried out by Persson *et al.* [14] and by Yerokhin *et al.* [15]. In Table III, two-electron QED correlation energies are compared between different theories. They are given by the differences between QED ionization energies of the $1s^2$ ground state and QED energies of the hydrogenic $1s$ state. Comparisons are also made in Fig. 2 where QED correlation energies relative to the higher-order results of Yerokhin *et al.* are scaled by α^4Z^3 and plotted as functions of Z. It can be seen that without the Latter correc-

TABLE III. Two-electron QED correlation energies (eV).

Z	Previous RCI[a]	Present RCI	Unified theory[b]	Higher order Persson[c]	Higher order Yerokhin[d]
32	−0.64	−0.47	−0.37	−0.4	−0.43
54	−2.20	−1.61	−1.12	−1.6	−1.56
66		−2.62	−1.73	−2.7	−2.66
74		−3.50	−2.28	−3.7	−3.68
83		−4.72	−3.19	−5.2	−5.18
92	−8.36	−6.28	−4.68	−7.1	−7.15

[a]Reference [2].
[b]Reference [4].
[c]Reference [14].
[d]Reference [15].

tion in the DKS potentials, our new QED results consistently agree better with the higher-order results than do our previous results calculated with this correction. Our new QED results also appear to be better than those of the unified theory in this Z range. To our knowledge, there is as yet no report of higher-order QED calculations for the excited states of heliumlike ions.

Even though our QED results are potential dependent, it does appear that screening and orbital relaxation effects can be well accounted for by the DKS potential. We note that there is nothing wrong with our previous QED results, as there is no *a priori* reason to prefer one model potential over the other. It just happens that DKS potentials *without* the Latter correction give slightly better lowest-order QED energies.

In summary, we have calculated the energy levels of the ground state and $n=2$ excited states of heliumlike ions with $22 \leqslant Z \leqslant 36$ using a large-scale relativistic configuration-interaction method. We believe that relativistic correlation energies for two-electron ions are well under control, but QED energies remain uncertain. Further improvements in theory will have to come from *ab initio* higher-order QED calculations for both the ground and excited states. It is also desirable to have new measurements that are accurate enough to sort out different theoretical predictions.

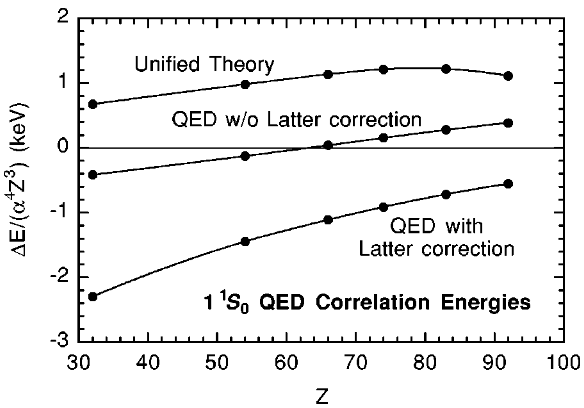

FIG. 2. Scaled two-electron QED correlation energies for the 1^1S_0 ground state relative to the higher-order results of Yerokhin *et al.* [15].

This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-ENG-48. We thank Dr. C. T. Chantler and Dr. D. Paterson for helpful discussions.

[1] M. H. Chen, K. T. Cheng, and W. R. Johnson, Phys. Rev. A **47**, 3692 (1993).
[2] K. T. Cheng, M. H. Chen, W. R. Johnson, and J. Sapirstein, Phys. Rev. A **50**, 247 (1994).
[3] D. R. Plante, W. R. Johnson, and J. Sapirstein, Phys. Rev. A **49**, 3519 (1994).
[4] G. W. F. Drake, Can. J. Phys. **66**, 586 (1988).
[5] P. Indelicato, J. P. Briand, M. Tavernier, and D. Liesen, Z. Phys. D: At., Mol. Clusters **2**, 249 (1986).
[6] C. T. Chantler, D. Paterson, L. T. Hudson, F. G. Serpa, J. D. Gillaspy, and E. Takács (unpublished).
[7] K. Widmann, P. Beiersdorfer, V. Decaux, and M. Bitter, Phys. Rev. A **53**, 2200 (1996).
[8] M. H. Mittleman, Phys. Rev. A **4**, 893 (1971); **5**, 2395 (1972); **24**, 1167 (1981).
[9] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 307 (1988).
[10] E. R. Davidson, J. Comput. Phys. **17**, 87 (1975).
[11] A. Stathopoulos and C. F. Fischer, Comput. Phys. Commun. **79**, 1 (1994).
[12] K. T. Cheng, W. R. Johnson, and J. Sapirstein, Phys. Rev. A **47**, 1817 (1993); Phys. Rev. Lett. **66**, 2960 (1991).
[13] W. R. Johnson and G. Soff, At. Data Nucl. Data Tables **33**, 405 (1985).
[14] H. Persson, S. Salomonson, P. Sunnergren, and I. Lindgren, Phys. Rev. Lett. **76**, 204 (1996).
[15] V. A. Yerokhin, A. N. Artemyerv, and V. M. Shabaev, Phys. Lett. A **234**, 361 (1997).
[16] P. Beiersdorfer, M. Bitter, S. von Goeler, and K. W. Hill, Phys. Rev. A **40**, 150 (1989).
[17] J. P. Briand, M. Tavernier, R. Marrus, and J. P. Desclaux, Phys. Rev. A **29**, 3143 (1984).
[18] C. T. Chantler, D.Phil. thesis, Oxford University, 1990 (unpublished).
[19] S. MacLaren, P. Beiersdorfer, D. A. Vogel, D. Knapp, R. E. Marrs, K. Wong, and R. Zasadzinski, Phys. Rev. A **45**, 329 (1992).