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Relativistic many-body perturbation theory applied to $n = 2$ triplet states of heliumlike ions

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Relativistic many-body perturbation theory calculations of the energies of the 2^3P_0, 2^3P_2, and 2^3S_1 states of heliumlike ions with nuclear charges Z in the range 10–36 are presented. These calculations include Coulomb correlation corrections through third order, correlation corrections of first order in the Breit interaction and zeroth, first, and second order in the Coulomb interaction, together with second-order Breit-Breit corrections and first-order corrections for retardation of the Breit interaction. At $Z = 10$, the calculated energies of the 2^3P_0, 2^3P_2, and 2^3S_1 states differ by 2.9, 0.02, and 0.3 cm^{-1}, respectively, from benchmark calculations based on variational wave functions. For higher Z, the difference between the present calculations and the benchmark calculations increases smoothly. Radiative and mass-polarization corrections are added to the many-body calculations and comparisons are made with measured 2^3P_0-2^3S_1 and 2^3P_2-2^3S_1 intervals.

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I. INTRODUCTION

Relativistic many-body perturbation theory (MBPT) is particularly well suited for calculations of the properties of highly charged many-electron ions because of the rapid convergence associated with the $1/Z$ expansion [1]. The study of the spectra of these ions allows QED tests to be extended from the weak fields in which they are usually made to the intense electrostatic fields of highly charged nuclei. However, the complexity of the wave functions of many-electron atoms interferes with the study of QED effects as long as wave-function uncertainties are larger than or comparable to the QED corrections.

The most accurately known many-electron wave functions are those for helium-like ions. Precise variational calculations have been done for S and P states of heliumlike ions with $Z \leq 10$, and the dominant relativistic corrections were determined two decades ago by Accad, Pekeris, and Schiff [2]. More recently, multiconfiguration Dirac-Fock (MCDF) calculations have been reported by Hata and Grant [3] and by Indelicato and co-workers [4]. The most accurate recent calculations are the unified calculations of Drake [5], which have an estimated uncertainty of $\pm 1.2(Z/10)^4$ cm^{-1}.

In this paper, we apply relativistic MBPT to three states 2^3P_0, 2^3P_2 and 2^3S_1 of heliumlike ions that are given by single-configuration wave functions in the jj coupling scheme. For two of these states, 2^3P_2 and 2^3S_1, we obtain energies that agree with [5] to well within the above error estimate, while for the 2^3P_0 state we differ from [5] by over two times that estimate.

For the three single-configuration states, we derive formal solutions to the two-electron Schrödinger equation based on the *no-pair* Hamiltonian of QED [6–9]. By iterating these formal solutions, we obtain successive approximations to wave functions and energies that are identical to results of a many-body perturbation theory expansion, with negative-energy states excluded from intermediate-state summations.

The lowest approximation to the energy scales as Z^2, and each successive iteration scales as a corresponding power of $1/Z$, so that $E^{(n)} \propto Z^{2-n}$. For high Z, the iteration sequence converges rapidly and is therefore suitable for precise atomic structure calculations. In the present work, we iterate the relativistic equations to third order and add corrections of fourth and higher orders from a nonrelativistic $1/Z$ expansion [10]. The differences between the present calculations and those of [5] arise primarily because relativistic corrections to the second-order energy of order $(Z\alpha)^4$ as well as Breit-Breit corrections, which also grow as $(Z\alpha)^4$, were not included in [5].

The present work represents an attempt to include all corrections which could mask the leading QED corrections for ions with $Z \geq 10$. Of course, the separation of QED corrections from atomic structure corrections is artificial. In the present paper, we define the "atomic structure" part of the calculation to be the part arising from the no-pair Hamiltonian, including retardation corrections to the Breit interaction only in lowest order, and we define the "QED" part to be the remaining corrections from quantum electrodynamics. The atomic structure part of the calculation is done in the present paper. For comparison with measured intervals, we include the QED corrections determined in [5].

II. CALCULATION

The no-pair Hamiltonian is given in second-quantized form as

$$H = \sum_i \varepsilon_i a_i^\dagger a_i + \frac{1}{2} \sum_{i,j,k,\ell} (g_{ijk\ell} + b_{ijk\ell}) a_i^\dagger a_j^\dagger a_\ell a_k \,, \qquad (1)$$

where ε_i is the ith energy eigenvalue of the single-particle Dirac equation for an electron in the Coulomb field of the nucleus, and where $g_{ijk\ell}$ and $b_{ijk\ell}$ are two-particle matrix elements of the Coulomb and Breit interactions, respectively. The operators a_i and $a_i^\dagger$ are electron annihilation and creation operators. Nuclear finite-size corrections

are included by replacing the nuclear Coulomb field in the single-particle Dirac equation by the field of a Fermi charge distribution. The parameters of the Fermi distribution are chosen to give the nuclear charge radii listed in [11].

We describe each of our $n = 2$ states in lowest order as

$$\Psi_0 = a_v^\dagger a_a^\dagger |0\rangle, \tag{2}$$

where v refers to a $2s_{1/2}$, $2p_{1/2}$, or $2p_{3/2}$ single-particle state, and where a refers to a $1s_{1/2}$ state. The exact wave function is taken to be $\Psi = \Psi_0 + \Delta\Psi$, where

$$\Delta\Psi = \sum_{i,j(\neq a,v)} \rho_{ijva} a_i^\dagger a_j^\dagger |0\rangle \, . \tag{3}$$

The corresponding energy is $E = E^{(0)} + \Delta E$, where $E^{(0)} = \varepsilon_v + \varepsilon_a$. Substituting into the Schrödinger equation, one obtains

$$(\varepsilon_i + \varepsilon_j - \varepsilon_v - \varepsilon_a - \Delta E_J)\rho_{ijva} = -g_{ijva} - \sum_{m,n(\neq a,v)} g_{ijmn}\rho_{mnva} \, , \tag{4}$$

where ΔE_J is an eigenvalue of the energy matrix:

$$\langle \Delta E \rangle_{wb,va} = g_{wbva} - g_{wbav} + \sum_{i,j(\neq a,v)} (g_{wbij} - g_{wbji})\rho_{ijva} \, . \tag{5}$$

The states w and b in Eq. (5) are the same as the states v and a, respectively, except for magnetic quantum numbers. By coupling the states v and a to states of total angular momentum J, one can diagonalize the energy matrix in Eq. (5). For each eigenvalue ΔE_J, Eq.(4) can be reduced to a set of coupled radial equations suitable for iterative solution.

In the present calculation, the single-particle states are formed using a finite basis set constructed from B splines [12]. We iterate Eqs. (4)–(5) in powers of $g_{ijk\ell}$ to obtain wave-function corrections $\rho^{(1)}_{ijva}$ and $\rho^{(2)}_{ijva}$ and energy corrections $E^{(1)}$, $E^{(2)}$, and $E^{(3)}$, where $\rho_{ijva} = \rho^{(1)}_{ijva} + \rho^{(2)}_{ijva} + \cdots$ and $\Delta E_J = E^{(1)} + E^{(2)} + \cdots$. In the first four rows of Table I, we give the values of $E^{(n)}$, $n = 0-3$ obtained for the three triplet states of heliumlike neon, $Z = 10$. In the row labled $E^{(4)}_+$, we give an estimate of the Coulomb corrections of fourth and higher order, determined by summing fourth and higher-order terms in the nonrelativistic $1/Z$ expansion [10]. By using the nonrelativistic values, we are assuming that relativistic corrections to the fourth- and higher-order Coulomb energies are negligible for the states considered here. This assumption has been verified for the leading relativistic corrections to the fourth- and fifth-order energies, which are proportional to α^2 and α^2/Z, respectively.

The first-order Breit correction $B^{(1)}$ is obtained by evaluating the matrix element of the Breit interaction term in the no-pair Hamiltonian using the coupled lowest-order wave function. With the aid of $\rho^{(1)}_{ijva}$ and $\rho^{(2)}_{ijva}$, one obtains the higher-order corrections to the wave function which are used to evaluate the corrections $B^{(2)}$ and $B^{(3)}$ associated with one Breit interaction and one or two Coulomb interactions, respectively. These Breit corrections are listed in the sixth through eighth rows of Table I. The leading terms in the fourth- and fifth-order Breit interaction have been examined and found to be insignificant. The unretarded Breit interaction is used for each of these terms.

TABLE I. Contributions to the energies (a.u.) of the 2^3S_1, 2^3P_0, and 2^3P_2 states of heliumlike neon, Z = 10.

Term	2^3S_1	2^3P_0	2^3P_2
$E^{(0)}$	-12.5208568	-12.5208597	-12.5041630
$E^{(1)}$	1.8833955	2.2641034	2.2591589
$E^{(2)}$	-0.0476275	-0.0736296	-0.0731857
$E^{(3)}$	-0.0004838	-0.0016472	-0.0016593
$E^{(4)}_+$	-0.0000368	-0.0001092	-0.0001092
$B^{(1)}$	-0.0000002	0.0049183	0.0002863
$B^{(2)}$	-0.0000104	-0.0009956	-0.0000663
$B^{(3)}$	0.0000022	0.0000389	0.0000030
$\Delta B^{(1)}$	0.0000002	-0.0000004	-0.0000040
$[B \times B]^{(2)}$	-0.0000001	-0.0000048	-0.0000001
Mass pol.[a]	0.0000025	-0.0001756	-0.0001756
QED[a]	0.0005992	-0.0000509	-0.0000290
Sum	-10.6850161	-10.3284123	-10.3199440
Drake[a]	-10.6850148	-10.3283993	-10.3199439

[a]Reference [5].

In the ninth row of Table I, we give values of the retardation corrections to the first-order Breit interaction, $\Delta B^{(1)}$. These retardation corrections grow as $Z^5\alpha^4$. Retardation corrections to the second- and higher-order Breit interactions are neglected here. In the tenth row we give the results of a second-order calculation with two unretarded Breit interactions; this correction grows as $(Z\alpha)^4$.

The eleventh and twelfth lines of Table I contain mass-polarization and QED corrections from [5]. The resulting sum differs slightly from the values given by Drake [5], which are listed in the final row of the table. We have attempted to control the numerical accuracy well enough that all of the figures presented in Table I are significant. The small differences in the final results reflect the differences in the treatment of relativistic corrections to the atomic structure.

III. RESULTS AND CONCLUSIONS

It is of interest to compare our results first with other theoretical calculations and then with experiment. For the case of argon ($Z = 18$) we find excellent agreement between our value of the 2^3S_1 energy and that obtained in an MBPT calculation by Lindroth and Salomonson [13]. The agreement between our calculation and that of Ref. [5] for the $2^3P_2 - 2^3S_1$ transition, shown in Table II, is excellent; the difference remains less than 4cm^{-1} for the entire range $Z = 10$–36. On the other hand, the difference for the $2^3P_0 - 2^3S_1$ transition, given in Table III, increases from 3 to 500 cm^{-1} over the same range. This difference can be explained as a $-2.6(\text{Z}/10)^4$ cm^{-1} term arising from $(Z\alpha)^4$ corrections evaluated here but not included by Drake. The estimate of the size of this omitted term $\pm 1.2(Z/10)^4$ cm^{-1} given in Ref. [5] is thus seen to be too small by a factor of 2.2. We note

finally that our theory is consistent with the screened $1/Z$ expansion calculations of Vainshtein and Safronova [14], but the results of these authors are of lower precision.

We find serious discrepancies with the most recent MCDF results of Indelicato [4]. The disagreements occur in several distinct parts of the calculation, which we illustrate for the $2\,^3P_2$–$2\,^3S_1$ transition at Z=26. When we compare the sum of our Coulomb energies with the Coulomb energies from Ref. [4] a discrepancy of -9 wave numbers is found. Our magnetic energies disagree even more strongly with those from Ref. [4], differing by -57 wave numbers. While our mass polarization correction agrees well with the specific mass shift in Ref. [4], there are again significant discrepancies with the QED values: for the transition being considered here the difference is 17 wave numbers. It should be possible to eliminate the discrepancies in the structure part of the calculation by including a sufficient number of configurations in the MCDF approach: we note that Parpia and Grant [15] have achieved excellent agreement between an MCDF calculation and MBPT and the unified theory for ground-state helium.

Turning to the comparison with experiment, we first discuss the $2\,^3P_2$–$2\,^3S_1$ transition. While we have close agreement with the results of Ref. [5] for this transition, both theoretical results seem to be one or two experimental standard deviations below experiment. A possible explanation for this trend may be the need for higher-order QED corrections, as will be discussed in the conclusion. An extra negative QED contribution to the $2\,^3S_1$ energy entering at the level $0.1(Z\alpha)^4$ is certainly not excluded

TABLE II. Comparison of theory and experiment for the $2\,^3P_2$–$2\,^3S_1$ transition in heliumlike ions: units cm^{-1}.

Nuclear charge	Present theory	Experiment	Drake[a]	Indelicato[b]
10	80121.9	80123.3(0.8)[c] 80121.1(1.9)[d]	80121.6	80110.2
12	100252	100263(6)[e]	100253	100236
13	111152	111157(6)[e]	111152	111133
14	122743	122746(3)[f]	122743	122723
15	135151	135153(18)[g]	135152	135129
16	148496	148494(4)[h] 148493(5)[f]	148497	148472
17	162922	162929(4)[i] 162923(6)[f]	162923	162896
18	178576	178591(31)[j]	178577	178546
20	214170	214225(45)[k]	214172	214136
22	256683	256746(46)[l]	256685	256642
26	368742	368976(125)[m]	368745	368692
28	441907	441944(39)[n]	441910	441854
36	900008	900009(240)[o]	900012	899983

[a]Reference [5].
[b]Reference [4].
[c]N.J. Peacock, M.F. Stamp, and J.D. Silver, Phys. Scr. T**8**, 10 (1984).
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TABLE III. Comparison of theory and experiment for the $2\,^3P_0$–$2\,^3S_1$ transition in heliumlike ions: units cm^{-1}.

Nuclear charge	Present theory	Experiment	Drake[a]	Indelicato[b]
10	78263.3	78265.0(1.2)[c] 78262.6(3.1)[d]	78265.9	78244.6
12	95848	95851(8)[e]	95853	95825
13	104778	104778(11)[e]	104787	104755
14	113809	113815(4)[f]	113820	113785
15	122955	122941(30)[g]	122970	122932
16	132219	132219(4)[h] 132198(10)[f]	132238	132195
17	141616	141621(4)[i]	141640	141592
18	151155	151204(9)[j]	151186	151130
36	356823	357400(255)[k]	357330	356911

[a]Reference [5].
[b]Reference [4].
[c]N.J. Peacock, M.F. Stamp, and J.D. Silver, Phys. Scr. T**8**, 10 (1984).
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by the data.

The situation for the $2\,^3P_0$–$2\,^3S_1$ transition is complicated by some inconsistency between different experimental results above Z=17. For $Z = 10$ through 17 our theory is sometimes in agreement with experiment, but sometimes somewhat below. We note the important role of the recent accurate measurements at Z=16 and 17 [16] in confirming the relatively large $(Z\alpha)^4$ corrections included in our calculation. Note that if the 2^3S_1 Lamb shift has an uncalculated term that would explain the trend of our $2\,^3P_2$–$2\,^3S_1$ results being below experiment, the same effect would predict this transition to be somewhat low. It is obvious that more precision experiments for higher values of Z would greatly help to clarify the situation.

At the present level of experimental accuracy we can claim that relativistic MBPT taken together with the standard theory of helium QED effects is quite successful. In particular, we believe we have identified all MBPT contributions through order $(Z\alpha)^4$. However, it is likely that as the experimental accuracy improves, systematic discrepancies with the theory presented here will emerge. This is because the QED contributions are not complete at the $(Z\alpha)^4$ level. While we claim to have evaluated all $(Z\alpha)^4$ corrections associated with atomic structure, there is another source of such terms from QED, binding corrections to the screening of the Lamb shift. These arise from corrections of order $Z\alpha$ to the two-electron part of the Lamb shift, which itself enters in order $(Z\alpha)^3$. While binding corrections to the one-electron Lamb shift are included to all orders by using the exact results of Mohr [17], the analogous calculation has not been carried out for the two-electron Lamb shift. Such corrections can automatically be obtained, however, by evaluating the Feynman diagrams associated with them, vertex correction and two-photon exchange graphs, using exact relativistic propagators in a Coulomb field. When this project is carried out the largest theory error should be of order $Z^3\alpha^4$, which would come from correlation corrections to the Breit-Breit part of the calculation. While considerable experimental effort will be required to reach this level, our understanding of relativistic and QED effects in intense Coulomb fields in the simplest many-electron atom promises to be significantly advanced by such work.

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