Relativistic many-body calculations of the energies of $n=2$ states for the berylliumlike isoelectronic sequence

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(Received 4 December 1995; revised manuscript received 6 February 1996)

Energies of the ten $(2l2l')$ states of ions of the beryllium isoelectronic sequence are determined to second order in relativistic many-body perturbation theory. Both the second-order Coulomb interaction and the second-order Breit-Coulomb interaction are included. Corrections for the frequency-dependent Breit interaction are taken into account in lowest order only. The effect of the Lamb shift is also estimated and included. Comparison with experiment and other theoretical data is made. [S1050-2947(96)08106-1]

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

I. INTRODUCTION

Berylliumlike ions are the simplest examples of atomic systems for which both intrashell and intershell interactions are important. Heliumlike ions and lithiumlike ions provide examples for which intrashell (heliumlike) and intershell (lithiumlike) interactions are separately important. These latter two isoelectronic sequences have been studied in more detail than the beryllium sequence. Moreover, all of the difficulties of heliumlike systems (two-electron interactions) and lithiumlike systems (core-valence interactions) occur for berylliumlike ions.

One of the first to identify lines of berylliumlike systems in observed spectra was Edlén in his 1933 thesis [1]. A detailed comparison of theoretical and experimental data for energies of berylliumlike ions was given 50 years later by Edlén in Ref. [2]. On the basis of this comparison, he suggested a simple formula for predicting energy levels as functions of Z in high-Z ions. This formula was used by Denne and Hinnov [3] to identify spectra obtained from high-temperature Tokamak plasmas. The $(2s^2)$-$(2s2p)^1P$ and $(2s^2)$-$(2s2p)^3P$ lines for ions with $Z=22,24,26,28,29,32,34,36$ were observed. Recently, highly charged uranium and thorium ions were produced in a high-energy electron beam ion trap (SuperEBIT) at the Lawrence Livermore National Laboratory [4]. Thirteen $2s_{1/2}$-$2p_{3/2}$ transitions (lithiumlike through neonlike) were identified and measured with high accuracy. Nearly all experimental results obtained by different authors were gathered and critically evaluated for reliability by a group at the National Institute of Standards and Technology (NIST). We have used the resulting data [5–23] for comparison. We will return to this comparison later.

Nonrelativistic perturbation theory was previously used to calculate energy levels of $(2l2l')$ terms for berylliumlike ions in Refs. [24–26]. Contributions of Breit operators, calculated with exact nonrelativistic functions and represented as a power series in $1/Z$, were given in Refs. [27,28]. In those papers, accurate data for ions with $Z = 6$–54 were obtained by introducing screening constants and including radiative and higher-order relativistic effects. The $1/Z$ expansion used in that work is referred to as the MZ method. The most precise theoretical studies of $(2snl)$ states of berylliumlike ions are those of Chung and Zhu [29,30] who determined the energies of such states in neutral beryllium to an accuracy of 1 cm^{-1} and in ions with $Z = 5$–14 to an accuracy of a few cm^{-1} using a ''full core plus correlation'' method including relativistic and QED corrections perturbatively.

The multiconfiguration Dirac-Fock (MCDF) method was used to calculate energies for the first excited states of Li-, Be-, B-, C-, N-, O-, and F-like ions with $Z = 6$–92 in Ref. [31]. This method was improved later by adding the second-order correlation energy for the above mentioned ions and for $Z=26$ [32]. Systematic multiconfiguration Hartree-Fock (MCHF) results in the Breit-Pauli approximation were obtained recently for the $(2l2l')$ states of berylliumlike carbon in Ref. [33]. We also note that multiconfiguration Dirac-Fock (MCDF) calculations of the $(2s^2)^1S_0$-$(2s2p)^{1,3}P_1$ transitions for ions with $Z=6,8,14,26$ were reported recently in Ref. [34]. Relativistic many-body calculations similar in spirit to those presented here were carried out previously by Liu and Kelly [35] for the ground state of beryllium and by Lindroth and Hvarfner [36] for the ground state and the $(2s2p)$ $J=1$ excited states of berylliumlike iron and molybdenum, $Z=26$ and 42.

In the present paper, we use relativistic many-body perturbation theory (MBPT) to determine the energies of $n=2$ states of berylliumlike ions with nuclear charges ranging from $Z=4$ to 100. Energies are calculated for the $(2s^2)$ ground state, the four odd-parity $(2s2p)$ excited states, and the five even-parity $(2p2p')$ excited states. Our calculations are carried out to second order in perturbation theory and include both the second-order Coulomb interaction and the second-order Breit-Coulomb interaction. Corrections for the frequency-dependent Breit interaction are included in lowest order only. The effect of the Lamb shift is also estimated and included.

Two distinct starting points are used for the perturbation expansion. First, we start our calculations using relativistic Coulomb wave functions and obtain the first three terms in a

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relativistic version of the $1/Z$ expansion. The resulting perturbation expansion can be compared with its nonrelativistic counterpart to obtain $O(\alpha^2 Z^2)$ corrections to the expansion coefficients. Second, we use one-electron orbitals calculated in the Hartree-Fock (HF) potential of the $1s^2$ ionic core to start the perturbation expansion. Two-particle perturbation theory takes its simplest form in this potential. Furthermore, the dominant third-order corrections occurring in the Coulomb case are accounted for automatically in the HF case.

We make detailed comparisons of the values obtained from the present calculations with experiment. For the HF case, we obtain agreement with experiment for intermediate Z at the level of 50 cm^{-1} for triplet states and 500 cm^{-1} for singlet states.

II. METHOD

We use MBPT starting from the ''no-pair'' Hamiltonian [37] of QED, $H=H_0+V_I$, with

$$H_0=\sum_i \epsilon_i a_i^\dagger a_i,$$

$$V_I=\frac{1}{2}\sum_{ijkl} v_{ijkl} a_i^\dagger a_j^\dagger a_l a_k,$$

where the quantities ϵ_i are eigenvalues of the one-electron Dirac equation, and where the creation and annihilation operators, $a_i^\dagger$ and a_j, are restricted to positive-energy (electron) states only. The two-particle matrix element $v_{ijkl}=g_{ijkl}+b_{ijkl}$ is the sum of the two-particle Coulomb matrix element g_{ijkl} and the two-particle matrix element of the instantaneous Breit interaction, b_{ijkl}.

An effective Hamiltonian for the two-valence-electron atom is found in terms of a correlation operator χ following the procedure outlined in Chap. 9 of Ref. [38]. Specifically, the Bloch equation

$$[\chi,H_0]P=QV\Omega P-\chi PV\Omega P\approx QVP \tag{2.1}$$

is solved to obtain the first-order correlation operator $\chi^{(1)}$, and the first-order correlation operator is then used to obtain a second-order effective Hamiltonian. The effective Hamiltonian is given in terms of the correlation operator by

$$H^{\rm eff}=PHP+PV\chi P. \tag{2.2}$$

The eigenvalues of $H^{\rm eff}$ are the exact energies.

A. Model space

For atoms with two electrons beyond closed shells, the model space is formed from two-particle states of the type $a_v^\dagger a_w^\dagger|0\rangle$, where $|0\rangle$ is the ground state of the closed-shell, $(N-2)$-electron, ionic core. The single-particle indices v and w range over states in the valence shell. For our study of low-lying states of berylliumlike ions, v and w are $2s_{1/2}$, $2p_{1/2}$, and $2p_{3/2}$ single-particle states. To obtain orthonormal model states, we consider the coupled states $\Phi_{JM}(vw)$ defined by

$$\Phi_{JM}(vw)=\eta_{vw}\sum_{m_v m_w} -\!\!\left|\begin{array}{l} vm_v \\ \\ JM \\ \\ wm_w \end{array}\right\rangle\!\!- a_{vm_v}^\dagger a_{wm_w}^\dagger|0\rangle, \tag{2.3}$$

where η_{vw} is a normalization factor

$$\eta_{vw}=\begin{cases} 1 & \text{for } w\neq v, \\ 1/\sqrt{2} & \text{for } w=v, \end{cases}$$

and where the graph represents a Clebsch-Gordan coefficient in the notation of Ref. [38]. Combining the $n=2$ orbitals in beryllium, we obtain four odd-parity states consisting of one $J=0$ state, two $J=1$ states, and one $J=2$ state. These states have a total of $1\times1+2\times3+1\times5=12$ magnetic substates. Additionally, there are six even-parity states consisting of three $J=0$ states, one $J=1$ state, and two $J=2$ states, with a total of $3\times1+1\times3+2\times5=16$ magnetic substates. The distribution of the 28 magnetic substates in the model space is summarized in the following table.

Parity	(vw)	$J=0$	$J=1$	$J=2$
odd	$2s_{1/2}2p_{1/2}$	1	3	
odd	$2s_{1/2}2p_{3/2}$		3	5
even	$2s_{1/2}2s_{1/2}$	1		
even	$2p_{1/2}2p_{1/2}$	1		
even	$2p_{1/2}2p_{3/2}$		3	5
even	$2p_{3/2}2p_{3/2}$	1		5

The projection operators P and Q used in Eqs. (2.1) and (2.2) are defined in terms of the model-space functions by

$$P=\sum_{\substack{JM \\ v\leq w}} \Phi_{JM}(vw)\Phi_{JM}^\dagger(vw), \tag{2.4}$$

with $Q=1-P$.

The effective Hamiltonian matrix is block diagonal in J and independent of M. There are $1\times1+2\times2+1\times1=6$ distinct odd-parity matrix elements and $3\times3+1\times1+2\times2=14$ distinct even-parity matrix elements. As discussed in [38], the effective Hamiltonian is non-Hermitian.

B. Correlation operator — effective Hamiltonian

From the Bloch equation, we obtain in first order

$$\chi^{(1)}\Phi_{JM}(vw) = -\eta_{vw}\sum_{m_v m_w} -\left|\begin{matrix} v m_v \\ \\ w m_w \end{matrix}\right.^{JM} \left\{ \frac{1}{2}\sum_{mnbc}\frac{v_{mnbc}}{\epsilon_{mn}-\epsilon_{bc}}a_m^\dagger a_n^\dagger a_c a_b + \sum_{mnc}\frac{v_{mnvc}}{\epsilon_{mn}-\epsilon_{vc}}a_m^\dagger a_n^\dagger a_c a_v \right.$$
$$+\sum_{mnb}\frac{v_{mnbw}}{\epsilon_{mn}-\epsilon_{bw}}a_m^\dagger a_n^\dagger a_w a_b + \sum_{mn\neq vw}\frac{v_{mnvw}}{\epsilon_{mn}-\epsilon_{vw}}a_m^\dagger a_n^\dagger a_w a_v$$
$$\left. +\sum_{mb}\frac{\Delta_{mb}}{\epsilon_m-\epsilon_b}a_m^\dagger a_b + \sum_{m\neq v}\frac{\Delta_{mv}}{\epsilon_m-\epsilon_v}a_m^\dagger a_v + \sum_{m\neq w}\frac{\Delta_{mw}}{\epsilon_m-\epsilon_w}a_m^\dagger a_w \right\} a_v^\dagger a_w^\dagger |0\rangle. \tag{2.5}$$

Here, $\Delta_{ij}=(V_{\rm HF}-U)_{ij}$, $V_{\rm HF}=\Sigma_a(v_{iaja}-v_{iaaj})$, and U is the potential (Coulomb or HF) used to obtain the basic single-particle orbitals.

The first-order contribution to the effective Hamiltonian matrix is

$$\langle\Phi_{JM}(v'w')|H^{(1)}|\Phi_{JM}(vw)\rangle = \eta_{v'w'}\eta_{vw}\sum_{\substack{m_{v'}m_{w'}\\ m_v m_w}} -\left|\begin{matrix} v' m_{v'} \\ \\ w' m_{w'} \end{matrix}\right.^{JM} -\left|\begin{matrix} v m_v \\ \\ w m_w \end{matrix}\right.^{JM} \times\langle v'w'|H|vw\rangle$$
$$= \eta_{v'w'}\eta_{vw}\sum_{\substack{m_{v'}m_{w'}\\ m_v m_w}} -\left|\begin{matrix} v' m_{v'} \\ \\ w' m_{w'} \end{matrix}\right.^{JM} -\left|\begin{matrix} v m_v \\ \\ w m_w \end{matrix}\right.^{JM} \times[(\delta_{v'v}\delta_{w'w}-\delta_{v'w}\delta_{w'v})(\epsilon_v+\epsilon_w)$$
$$+\delta_{w'w}\Delta_{v'v}+\delta_{w'w}\Delta_{v'v}-\delta_{v'w}\Delta_{w'v}-\delta_{w'v}\Delta_{v'w}+\tilde{v}_{v'w'vw}]. \tag{2.6}$$

The second-order contribution is found to be

$$\langle\Phi_{JM}(v'w')|H^{(2)}|\Phi_{JM}(vw)\rangle = \eta_{v'w'}\eta_{vw}\sum_{\substack{m_{v'}m_{w'}\\ m_v m_w}} -\left|\begin{matrix} v' m_{v'} \\ \\ w' m_{w'} \end{matrix}\right.^{JM} -\left|\begin{matrix} v m_v \\ \\ w m_w \end{matrix}\right.^{JM} \times\langle v'w'|V\chi^{(1)}|vw\rangle$$
$$= \eta_{v'w'}\eta_{vw}\sum_{\substack{m_{v'}m_{w'}\\ m_v m_w}} -\left|\begin{matrix} v' m_{v'} \\ \\ w' m_{w'} \end{matrix}\right.^{JM} -\left|\begin{matrix} v m_v \\ \\ w m_w \end{matrix}\right.^{JM}$$
$$\times\left[(\delta_{v'v}\delta_{w'w}-\delta_{v'w}\delta_{w'v})\left\{\frac{1}{2}\sum_{bcmn}\frac{v_{mnbc}\tilde{v}_{bcmn}}{\epsilon_{bc}-\epsilon_{mn}}+\sum_{bm}\frac{\Delta_{bm}\Delta_{mb}}{\epsilon_b-\epsilon_m}\right\}\right.$$
$$+\left\{\sum_{bcn}\frac{\tilde{v}_{bcxn}v_{ynbc}}{\epsilon_{yn}-\epsilon_{bc}}+\sum_{cmn}\frac{v_{ycmn}\tilde{v}_{mnxc}}{\epsilon_{xc}-\epsilon_{mn}}-\sum_{bm}\frac{\Delta_{bm}\tilde{v}_{mybx}}{\epsilon_{ym}-\epsilon_{xb}}-\sum_{bm}\frac{\tilde{v}_{bymx}\Delta_{mb}}{\epsilon_m-\epsilon_b}+\sum_b\frac{\Delta_{bx}\Delta_{yb}}{\epsilon_y-\epsilon_b}\right.$$
$$\left.\left.+\sum_{m\neq x,y}\frac{\Delta_{ym}\Delta_{mx}}{\epsilon_x-\epsilon_m}\right\}(\delta_{v'v}\delta_{xw}\delta_{yw'}+\delta_{w'w}\delta_{xv}\delta_{yv'}-\delta_{v'w}\delta_{xv}\delta_{yw'}-\delta_{w'v}\delta_{xw}\delta_{yv'})\right.$$
$$+\sum_{bc}\frac{v_{bcvw}\tilde{v}_{v'w'bc}}{\epsilon_{bc}-\epsilon_{v'w'}}+\sum_{mn\neq wv}\frac{v_{v'w'mn}\tilde{v}_{mnvw}}{\epsilon_{vw}-\epsilon_{mn}}+\sum_{bn}\frac{\tilde{v}_{v'bvn}\tilde{v}_{w'nwb}}{\epsilon_{wb}-\epsilon_{w'n}}$$
$$+\sum_{cn}\frac{\tilde{v}_{w'cwn}\tilde{v}_{v'nvc}}{\epsilon_{vc}-\epsilon_{v'n}}+\sum_{cn}\frac{\tilde{v}_{v'cwn}\tilde{v}_{w'nvc}}{\epsilon_{w'n}-\epsilon_{vc}}+\sum_{bn}\frac{\tilde{v}_{w'bvn}\tilde{v}_{v'nwb}}{\epsilon_{v'n}-\epsilon_{wb}}$$
$$+\sum_{b}\frac{\tilde{v}_{v'bvw}\Delta_{w'b}}{\epsilon_{w'}-\epsilon_b}+\sum_{m\neq w'}\frac{\Delta_{w'm}\tilde{v}_{v'mvw}}{\epsilon_{vw}-\epsilon_{v'm}}+\sum_{c}\frac{\Delta_{cw}\tilde{v}_{v'w'vc}}{\epsilon_{w'v'}-\epsilon_{vc}}+\sum_{m\neq w}\frac{\tilde{v}_{v'w'vm}\Delta_{mw}}{\epsilon_w-\epsilon_m}$$
$$\left.+\sum_{b}\frac{\tilde{v}_{w'bwv}\Delta_{v'b}}{\epsilon_{v'}-\epsilon_b}+\sum_{m\neq v'}\frac{\Delta_{v'm}\tilde{v}_{w'mwv}}{\epsilon_{vw}-\epsilon_{w'm}}+\sum_{c}\frac{\Delta_{cv}\tilde{v}_{v'w'cw}}{\epsilon_{w'v'}-\epsilon_{wc}}+\sum_{m\neq v}\frac{\tilde{v}_{v'w'mw}\Delta_{mv}}{\epsilon_v-\epsilon_m}\right]. \tag{2.7}$$

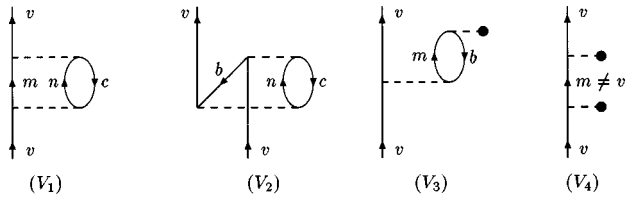

FIG. 1. Diagrams for the contributions of $E_v^{(2)}$ to the second-order two-particle energy. V_1 represents double sums, V_2 represents single sums, V_3 gives one-potential terms, and V_4 gives two-potential terms.

Here, $\epsilon_{ab}=\epsilon_a+\epsilon_b$ and $\tilde{v}_{abcd}=v_{abcd}-v_{abdc}$.

C. Angular reduction

We carry out the sum over magnetic substates to find

$$\langle\Phi_{JM}(v'w')|H^{(1)}|\Phi_{JM}(vw)\rangle=\delta_{vv'}\delta_{ww'}(E_v^{(1)}+E_w^{(1)})+V^{(1)}_{v'w'vw}, \tag{2.8}$$

where

$$E_v^{(1)}=\epsilon_v+\Delta_{vv}, \tag{2.9}$$

$$V^{(1)}_{v'w'vw}=\eta_{v'w'}\eta_{vw}Y_J(v'w'vw). \tag{2.10}$$

Here, we have introduced the notation

$$Y_J(abcd)=\sum_k(-1)^{j_b+j_c+k+J}\begin{Bmatrix}j_a & j_b & J\\ j_d & j_c & k\end{Bmatrix}X_k(abcd)+\sum_k(-1)^{j_b+j_c+k}\begin{Bmatrix}j_a & j_b & J\\ j_c & j_d & k\end{Bmatrix}X_k(abdc), \tag{2.11}$$

where

$$X_k(abcd)=(-1)^k\langle a||C_k||c\rangle\langle b||C_k||d\rangle R_k(abcd). \tag{2.12}$$

The quantities C_k are normalized spherical harmonics and $R_k(abcd)$ are Slater integrals. The functions $X_k(abcd)$ have several interesting symmetry properties:

$$X_k(cdab)=(-1)^{j_a+j_b+j_c+j_d}X_k(abcd),$$

$$X_k(badc)=X_k(abcd).$$

From these properties, it follows that

$$Y_J(cdab)=Y_J(abcd),$$

$$Y_J(badc)=(-1)^{j_a+j_b+j_c+j_d}Y_J(abcd),$$

$$Y_J(bacd)=(-1)^{j_a-j_b+J}Y_J(abcd).$$

The second-order Hamiltonian can be written

$$\langle\Phi_{JM}(v'w')|H^{(2)}|\Phi_{JM}(vw)\rangle=\delta_{vv'}\delta_{ww'}(E^{(2)}_{\rm core}+E_v^{(2)}+E_w^{(2)})+V^{(2)}_{v'w'vw}. \tag{2.13}$$

For the second-order core energy $E^{(2)}_{\rm core}$ we have

$$E^{(2)}_{\rm core}=\frac{1}{2}\sum_{\substack{kmn\\ bc}}\frac{(-1)^{j_m+j_n-j_b-j_c}}{[k]}\frac{X_k(mnbc)Z_k(bcmn)}{\epsilon_{bc}-\epsilon_{mn}}+\sum_{bm}[j_b]\delta_{\kappa_m\kappa_b}\frac{\Delta_{bm}\Delta_{mb}}{\epsilon_b-\epsilon_m}. \tag{2.14}$$

Here,

$$Z_k(bcmn)=X_k(bcmn)+\sum_{k'}[k]\begin{Bmatrix}j_b & j_m & k\\ j_c & j_n & k'\end{Bmatrix}X_{k'}(bcnm). \tag{2.15}$$

Labels b and c are used for core states and n and m for all other states. In the above equations, $[k]=2k+1$. The second-order energy for the valence electron v is found to be

$$E_v^{(2)}=\sum_{kcmn}\frac{(-1)^{j_m+j_n-j_v-j_c}}{[j_v][k]}\frac{X_k(vcmn)Z_k(mnvc)}{\epsilon_{vc}-\epsilon_{mn}}+\sum_{kbcn}\frac{(-1)^{j_v+j_n-j_b-j_c}}{[j_v][k]}\frac{Z_k(bcvn)X_k(vnbc)}{\epsilon_{vn}-\epsilon_{bc}}+2\sum_{mb}\delta_{\kappa_b\kappa_m}\sqrt{\frac{[j_b]}{[j_v]}}\frac{\Delta_{bm}Z_0(mvbv)}{\epsilon_b-\epsilon_m}+\sum_{i\neq v}\delta_{\kappa_i\kappa_v}\frac{\Delta_{vi}\Delta_{iv}}{\epsilon_v-\epsilon_i}. \tag{2.16}$$

Diagrams representing the four terms in Eq. (2.16) are given in Fig. 1. The second-order energy for the valence electron w is found by replacing v by w in the above expression. The second-order interaction energy is

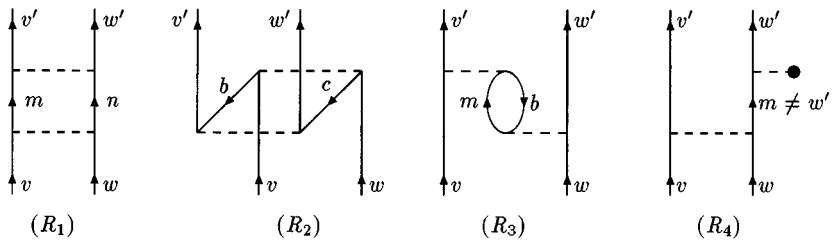

FIG. 2. Diagrams for the second-order interaction energy $V^{(2)}_{v'w'vw}$. R_1 represents double sums, R_2 represents single sums, R_3 gives random-phase approximation (RPA) terms, and R_4 gives one-potential terms.

$$V^{(2)}_{v'w'vw}=\eta_{v'w'}\eta_{vw}\Bigg[-\sum_{kmn}(-1)^{j_{w'}+j_m+k+J}\begin{Bmatrix} j_{v'} & j_{w'} & J\\ j_n & j_m & k\end{Bmatrix}\frac{X_k(v'w'mn)Y_J(mnvw)}{\epsilon_{vw}-\epsilon_{mn}}$$

$$+\sum_{kbc}(-1)^{j_v+j_c+k+J}\begin{Bmatrix} j_v & j_w & J\\ j_c & j_b & k\end{Bmatrix}\frac{X_k(bcvw)Y_J(v'w'bc)}{\epsilon_{bc}-\epsilon_{w'v'}}$$

$$-\sum_{\substack{\alpha'\beta'\\ \alpha\beta}}C_1(\alpha'\beta'\alpha\beta)\sum_{nbk}\frac{(-1)^{j_{w'}+j_v+j_n+j_b}}{[k]}\begin{Bmatrix} j_{\alpha'} & j_{\beta'} & J\\ j_\beta & j_\alpha & k\end{Bmatrix}\frac{Z_k(\alpha'b\alpha n)Z_k(\beta'n\beta b)}{\epsilon_{\beta b}-\epsilon_{\beta' n}}+\sum_{\substack{\alpha'\beta'\\ \alpha\beta}}C_2(\alpha'\beta'\alpha\beta)$$

$$\times\Bigg(\sum_b\delta_{\kappa_b\kappa_{\beta'}}\frac{Y_J(\alpha'b\alpha\beta)\Delta_{\beta' b}}{\epsilon_{\beta'}-\epsilon_b}+\sum_{m\neq\beta'}\delta_{\kappa_m\kappa_{\beta'}}\frac{\Delta_{\beta' m}Y_J(\alpha'm\alpha\beta)}{\epsilon_{\alpha\beta}-\epsilon_{m\alpha'}}+\sum_b\delta_{\kappa_b\kappa_\beta}\frac{\Delta_{b\beta}Y_J(\alpha'\beta'\alpha b)}{\epsilon_{\alpha'\beta'}-\epsilon_{\beta b}}$$

$$+\sum_{m\neq\beta}\delta_{\kappa_m\kappa_\beta}\frac{Y_J(\alpha'\beta'\alpha m)\Delta_{m\beta}}{\epsilon_\beta-\epsilon_m}\Bigg)\Bigg], \tag{2.17}$$

where

$$C_1(\alpha'\beta'\alpha\beta)=(-1)^J[\delta_{\alpha'v'}\delta_{\beta'w'}\delta_{\alpha v}\delta_{\beta w}+\delta_{\alpha'w'}\delta_{\beta'v'}\delta_{\alpha w}\delta_{\beta v}]+\delta_{\alpha'v'}\delta_{\beta'w'}\delta_{\alpha w}\delta_{\beta v}+\delta_{\alpha'w'}\delta_{\beta'v'}\delta_{\alpha v}\delta_{\beta w}, \tag{2.18}$$

$$C_2(\alpha'\beta'\alpha\beta)=\delta_{\alpha'v'}\delta_{\beta'w'}\delta_{\alpha v}\delta_{\beta w}+(-1)^{\alpha'+\beta'+\alpha+\beta}\delta_{\alpha'w'}\delta_{\beta'v'}\delta_{\alpha w}\delta_{\beta v}. \tag{2.19}$$

Diagrams representing the four classes of terms in Eq. (2.17) are given in Fig. 2. When starting calculations from the HF orbitals, we must set $\Delta_{ij}=0$ in the above formulas, and when starting from the relativistic Coulomb orbitals, we must set $\Delta_{ij}=(V_{\rm HF})_{ij}$. Specifically,

$$\Delta_{ij}=\sum_a\delta_{j_ij_j}\sqrt{\frac{[j_a]}{[j_i]}}Z_0(iaja)$$

for the Coulomb case.

III. RESULTS AND DISCUSSION

We calculated energies of ten $(2l2l')\ [J]$ states for all ions up to $Z=30$, and for 17 representative high-Z ions with $Z=$ 32,36,40,42,47,50,54,60,63,70,74,79,80,83,90,92,100. Two different potentials were used to obtain the basis orbitals for our calculation, the frozen-core HF potential and the nuclear Coulomb potential. To obtain the energies of interest, it was necessary to evaluate first- and second-order contributions from the Coulomb and Breit operators to the six independent matrix elements of $H^{\rm eff}$ for odd-parity states, and to the 14 independent matrix elements of $H^{\rm eff}$ for even-parity states.

In Tables I–III and Figs. 3–7, we give details of the second-order contributions to the energies. In Table I, we show the second-order contributions to the valence energy $E_v^{(2)}+E_w^{(2)}$, defined in Eq. (2.16), for the special case of the berylliumlike iron, $Z=26$. Contributions from each of the four distinct types of diagrams in Fig. 1 are given in this table. These contributions are calculated using both HF and Coulomb basis orbitals. In panels I(a) and I(c), HF orbitals and Coulomb orbitals, respectively, are used to evaluate second-order Coulomb contributions; and, in panels I(b) and I(d), HF and Coulomb orbitals, respectively, are used to evaluate second-order Breit×Coulomb corrections. The first diagram contributing in each of the four cases is the one corresponding to two-particle sums. We see that this diagram gives similar contributions using either HF or Coulomb orbitals. (Compare $V_1^{\rm HF}$ to $V_1^{\rm Cl}$ and $V_1^{\rm BHF}$ to $V_1^{\rm BCl}$.) A similar comment can also be made regarding diagram V_2. Only these two diagrams contribute when we use HF orbitals. The result of the present calculation, given in the last column of Table I, is in complete agreement with [39], which is devoted to energy levels along the lithium isoelectronic sequence. The contributions of diagram V_3, when evaluated using Breit-Coulomb operators, are sensitive to the type of basis function used. It should be noted that, when evaluating contributions of diagram V_3 to the second-order Breit matrix elements, terms of the type $\Delta_{ij}Z_k(klmn)$ do not automatically vanish in the HF case. The V_4 diagram contributes only when using Coulomb basis orbitals and gives the largest contribution among the four valence diagrams [see panels I(c) and I(d)]. Finally, let us note that the sum $\Sigma^{\rm BHF}$, given in the last column of I(b), agrees completely with data given in Table I of Ref. [39].

Tables II and III give the second-order interaction energy, defined in Eq. (2.17) and shown in Fig. 2, for the special case $Z=26$. These diagrams contribute for systems with two (or more) electrons above a closed core. There are ten diagonal and ten nondiagonal matrix elements for $(2l2l')\ [J]$ states in jj coupling. We calculated contributions for the 20 matrix elements using both sets of basis orbitals. Matrix elements obtained using HF orbitals are given in Tables II(a) and II(b), and those obtained using Coulomb orbitals are given in Tables III(a) and III(b). These tables include data for

TABLE I. Contributions to the valence-electron energy $E_v^{(2)}$ for $v=2s$, $2p^*$, and $2p$ for ions with a $1s^2$ core from the four diagrams V_1–V_4 evaluated for the case of iron, $Z=26$. Notation: $y[x]$ represents $y\times 10^x$, $2p\equiv 2p_{3/2}$, $2p^*\equiv 2p_{1/2}$.

(a) Hartree-Fock basis—Coulomb interaction

	$V_1^{\rm HF}$	$V_2^{\rm HF}$	$V_3^{\rm HF}$	$V_4^{\rm HF}$	$\Sigma^{\rm HF}$
$2s$	-0.896014[-2]	0.235131[-2]			-0.660883[-2]
$2p^*$	-0.144291[-1]	0.116405[-2]			-0.132650[-1]
$2p$	-0.136570[-1]	0.117396[-2]			-0.124831[-1]

(b) Hartree-Fock basis—Breit correction

	$V_1^{\rm BHF}$	$V_2^{\rm BHF}$	$V_3^{\rm BHF}$	$V_4^{\rm BHF}$	$\Sigma^{\rm BHF}$
$2s$	-0.848539[-3]	0.229586[-3]	-0.252280[-3]		-0.871223[-3]
$2p^*$	-0.869567[-3]	0.279718[-3]	-0.757397[-3]		-0.134725[-2]
$2p$	-0.555487[-3]	0.124192[-3]	-0.721159[-3]		-0.115245[-2]

(c) Relativistic Coulomb basis—Coulomb interaction

	$V_1^{\rm Cl}$	$V_2^{\rm Cl}$	$V_3^{\rm Cl}$	$V_4^{\rm Cl}$	$\Sigma^{\rm Cl}$
$2s$	-0.992285[-2]	0.259418[-2]	-0.818915[-2]	-0.243995[-0]	-0.259513[-0]
$2p^*$	-0.163688[-1]	0.137531[-2]	-0.269447[-1]	-0.348615[-0]	-0.390553[-0]
$2p$	-0.154426[-1]	0.138589[-2]	-0.256858[-1]	-0.337010[-0]	-0.376753[-0]

(d) Relativistic Coulomb basis—Breit correction

	$V_1^{\rm BCl}$	$V_2^{\rm BCl}$	$V_3^{\rm BCl}$	$V_4^{\rm BCl}$	$\Sigma^{\rm BCl}$
$2s$	-0.969508[-3]	0.260830[-3]	-0.746183[-3]	-0.2601299[-2]	-0.405615[-2]
$2p^*$	-0.106555[-2]	0.340669[-3]	-0.984698[-3]	-0.843035[-2]	-0.101399[-1]
$2p$	-0.679906[-3]	0.150897[-3]	-0.936836[-3]	-0.366439[-2]	-0.513023[-2]

three 1×1 matrices: $(2s2p_{1/2})$ [0], $(2p_{1/2}2p_{3/2})$ [1], and $(2s2p_{3/2})$ [2]; for two 2×2 matrices: $(2s2p_{1/2})+(2s2p_{3/2})$ [1] and $(2p_{1/2}2p_{3/2})+(2p_{3/2}2p_{3/2})$ [2]; and for one 3×3 matrix: $(2s2s)+(2p_{1/2}2p_{1/2})+(2p_{3/2}2p_{3/2})$ [0]. There are no large differences in the values obtained using different basis orbitals as can be seen by comparing $R_k^{\rm HF}$ with $R_k^{\rm Cl}$ and $R_k^{\rm BHF}$ with $R_k^{\rm BCl}$ for $k=1$–3. The R_4 diagrams, which contribute in the Coulomb case, are the dominant contributions to the sums $\Sigma^{\rm Cl}$ and $\Sigma^{\rm BCl}$ as can be seen from Tables III(a) and III(b), respectively. Let us note that in the HF cases [panels II(a) and II(b)], the total values of nondiagonal matrix elements are smaller by a factor of 2–3 than the values of the diagonal ones. On the other hand, in the Coulomb cases shown in Tables III(a) and III(b), the total values of nondiagonal matrix elements are 5–10 times smaller than the total values of diagonal ones.

The orbitals used in the present calculation were obtained as linear combinations of B splines. These B-spline basis orbitals were determined using precisely the method described in Ref. [39]. We used 50 B splines of order 9 for each single-particle angular momentum state and we included all orbitals with orbital angular momentum $l\leqslant 9$ in our single-particle basis.

In Figs. 3 and 4, we illustrate the Z dependence of the second-order contributions for the special case of the $(2p_{3/2})^2$-$(2p_{3/2})^2$ $[J=0]$ diagonal matrix element in four cases: 3(a) Coulomb-Coulomb with HF basis, 3(b) Breit-Coulomb with HF basis, 4(a) Coulomb-Coulomb with Coulomb basis, and 4(b) Breit-Coulomb with Coulomb basis. The labels in Figs. 3 and 4 are the same as those used in Tables I–III. We can see from Figs. 3(a) and 3(b) (HF functions) that the contributions of the R_1 diagram are larger than those of the V_1 diagram. By contrast, we see from Figs. 4(a) and 4(b) that, in the Coulomb case, contributions from diagram V_4 dominate.

For each of the second-order matrix elements, it is seen that the Z dependence of each contributing diagram is smooth. Moreover, the leading term in a power series in Z for the second-order Coulomb-Coulomb energy is a constant. We may write

$$E_{\rm Cl}^{(2)}=E_{20}+E_{22}(\alpha Z)^2+E_{24}(\alpha Z)^4+\cdots, \tag{3.1}$$

$$E_{\rm HF}^{(2)}=E_{20}+E_{22}(\alpha Z)^2+E_{24}(\alpha Z)^4+\cdots+\frac{1}{Z}\times[E'_{30}+E'_{32}(\alpha Z)^2+E'_{34}(\alpha Z)^4+\cdots]+\cdots. \tag{3.2}$$

The $1/Z$ terms in Eq. (3.2) describe the deviation from constancy in the HF case which is obvious for $Z<10$ from Fig. 3(a). The leading term in Z for the second-order Breit-Coulomb contributions is $(\alpha Z)^2$. The corresponding expansion in powers of Z is

$$B_{\rm Cl}^{(2)}=(\alpha Z)^2[B_{20}+B_{22}(\alpha Z)^2+B_{24}(\alpha Z)^4+\cdots], \tag{3.3}$$

TABLE II. Diagonal and nondiagonal contributions to the second-order interaction term in the effective Hamiltonian matrix from diagrams R_1–R_4 calculated using HF orbitals. These contributions are given for a two-electron ion with a $(1s^2)$ core, and evaluated numerically for the case of iron, $Z=26$. Notation: $y[x]$ represents $y\times10^x$, $2p\equiv2p_{3/2}$, $2p^*\equiv2p_{1/2}$.

(a) Coulomb interaction

			$R_1^{\rm HF}$	$R_2^{\rm HF}$	$R_3^{\rm HF}$	$R_4^{\rm HF}$	$\Sigma^{\rm HF}$
$2s2p^*$	$2s2p^*$	0	-0.300484[-1]		0.379127[-2]		-0.2625711[-1]
$2p^*2p$	$2p^*2p$	1	-0.409676[-1]		-0.257787[-2]		-0.4354549[-1]
$2s2p$	$2s2p$	2	-0.297469[-1]		0.368892[-2]		-0.2605796[-1]
$2s2p^*$	$2s2p^*$	1	-0.526635[-1]		0.101648[-2]		-0.5164703[-1]
$2s2p$	$2s2p$	1	-0.753983[-1]		-0.173706[-2]		-0.7713532[-1]
$2s2p^*$	$2s2p$	1	0.322853[-1]		0.388400[-2]		0.3616929[-1]
$2s2p$	$2s2p^*$	1	0.319776[-1]		0.387639[-2]		0.3585404[-1]
$2p^*2p$	$2p^*2p$	2	-0.743034[-1]		-0.140292[-2]		-0.7570627[-1]
$2p2p$	$2p2p$	2	-0.571623[-1]		-0.189193[-2]		-0.5905420[-1]
$2p^*2p$	$2p2p$	2	-0.238021[-1]		0.830084[-3]		-0.2297198[-1]
$2p2p$	$2p^*2p$	2	-0.235698[-1]		0.828127[-3]		-0.2274163[-1]
$2s2s$	$2s2s$	0	-0.383477[-1]	-0.573671[-3]	0.167006[-2]		-0.3725135[-1]
$2p^*2p^*$	$2p^*2p^*$	0	-0.673070[-1]	-0.294730[-3]	-0.845335[-3]		-0.6844702[-1]
$2p2p$	$2p2p$	0	-0.921419[-1]	-0.574195[-3]	0.110373[-2]		-0.9161237[-1]
$2s2s$	$2p^*2p^*$	0	0.191991[-1]	0.412665[-3]	0.341603[-2]		0.2302777[-1]
$2p^*2p^*$	$2s2s$	0	0.184010[-1]	0.409723[-3]	0.337404[-2]		0.2218478[-1]
$2s2s$	$2p2p$	0	0.279390[-1]	0.576684[-3]	0.470355[-2]		0.3321922[-1]
$2p2p$	$2s2s$	0	0.263656[-1]	0.571195[-3]	0.462659[-2]		0.3156343[-1]
$2p^*2p^*$	$2p2p$	0	-0.367687[-1]	-0.411875[-3]	0.257004[-2]		-0.3461058[-1]
$2p2p$	$2p^*2p^*$	0	-0.361864[-1]	-0.410883[-3]	0.256067[-2]		-0.3403657[-1]

(b) Breit corrections

			$R_1^{\rm BHF}$	$R_2^{\rm BHF}$	$R_3^{\rm BHF}$	$R_4^{\rm BHF}$	$\Sigma^{\rm BHF}$
$2s2p^*$	$2s2p^*$	0	-0.303912[-3]		0.158613[-3]	-0.166445[-2]	-0.180975[-2]
$2p^*2p$	$2p^*2p$	1	-0.682539[-3]		0.473267[-5]	-0.206845[-2]	-0.274626[-2]
$2s2p$	$2s2p$	2	-0.113697[-3]		0.209144[-4]	-0.916270[-3]	-0.100905[-2]
$2s2p^*$	$2s2p^*$	1	-0.251443[-3]		-0.281692[-4]	-0.170956[-2]	-0.198917[-2]
$2s2p$	$2s2p$	1	-0.705892[-3]		-0.574215[-4]	-0.121276[-2]	-0.197607[-2]
$2s2p^*$	$2s2p$	1	0.361081[-3]		0.967786[-4]	0.136450[-3]	0.594310[-3]
$2s2p$	$2s2p^*$	1	0.359397[-3]		0.965846[-4]	0.135166[-3]	0.591148[-3]
$2p^*2p$	$2p^*2p$	2	-0.265898[-3]		0.490395[-4]	-0.219864[-2]	-0.241550[-2]
$2p2p$	$2p2p$	2	-0.541893[-3]		0.756508[-5]	-0.131442[-2]	-0.184875[-2]
$2p^*2p$	$2p2p$	2	-0.383908[-3]		0.244986[-5]	-0.765263[-4]	-0.457984[-3]
$2p2p$	$2p^*2p$	2	-0.381689[-3]		0.243536[-5]	-0.753269[-4]	-0.454581[-3]
$2s2s$	$2s2s$	0	-0.524410[-3]	-0.439629[-4]	0.109601[-3]	-0.983188[-3]	-0.144196[-2]
$2p^*2p^*$	$2p^*2p^*$	0	-0.137227[-2]	-0.617539[-4]	0.158027[-3]	-0.312137[-2]	-0.439737[-2]
$2p2p$	$2p2p$	0	-0.235576[-2]	-0.554670[-4]	0.967601[-4]	-0.148479[-2]	-0.379926[-2]
$2s2s$	$2p^*2p^*$	0	0.593229[-3]	0.590443[-4]	-0.153902[-4]	0.810567[-4]	0.717940[-3]
$2p^*2p^*$	$2s2s$	0	0.576000[-3]	0.586234[-4]	-0.155557[-4]	0.727000[-4]	0.691768[-3]
$2s2s$	$2p2p$	0	0.100785[-2]	0.499507[-4]	-0.949262[-4]	0.340018[-3]	0.130289[-2]
$2p2p$	$2s2s$	0	0.960552[-3]	0.494752[-4]	-0.936432[-4]	0.316212[-3]	0.123260[-2]
$2p^*2p^*$	$2p2p$	0	-0.119512[-2]	-0.630430[-4]	0.128100[-3]	-0.235172[-3]	-0.136524[-2]
$2p2p$	$2p^*2p^*$	0	-0.118114[-2]	-0.628912[-4]	0.127670[-3]	-0.227803[-3]	-0.134416[-2]

$$B_{\rm HF}^{(2)}=(\alpha Z)^2\Big\{B_{20}+B_{22}(\alpha Z)^2+B_{24}(\alpha Z)^4+\cdots+\frac{1}{Z}\times[B'_{30}+B'_{32}(\alpha Z)^2+B'_{34}(\alpha Z)^4+\cdots]+\cdots\Big\}. \tag{3.4}$$

The curves for $E_{\rm HF}^{(2)}$ and $E_{\rm Cl}^{(2)}$ shown in Figs. 3(a) and 4(a) change by less than a factor of 2 over the range $Z=10$–100. The same is true of $B_{\rm Cl}^{(2)}$ and $B_{\rm HF}^{(2)}$, provided we divide out the factor $(\alpha Z)^2$.

These analytical formulas represent the second-order contributions before diagonalization. To determine the first-order energies of the states under consideration, we diagonalize the symmetric first-order effective Hamiltonian, including both the Coulomb and Breit interactions. The

TABLE III. Diagonal and nondiagonal contributions to the second-order interaction term in the effective Hamiltonian matrix from diagrams R_1–R_4 calculated using Coulomb orbitals. These contributions are given for a two-electron ion with a $(1s^2)$ core, and evaluated numerically for the case of iron, $Z=26$. Notation: $y[x]$ represents $y\times10^x$, $2p\equiv2p_{3/2}$, $2p^*\equiv2p_{1/2}$.

(a) Coulomb interaction

			R_1^{Cl}	R_2^{Cl}	R_3^{Cl}	R_4^{Cl}	Σ^{Cl}
$2s2p^*$	$2s2p^*$	0	-0.303054[-1]		0.425494[-2]	-0.215356[-0]	-0.241407[-0]
$2p^*2p$	$2p^*2p$	1	-0.404064[-1]		-0.325832[-2]	-0.282265[-0]	-0.325930[-0]
$2s2p$	$2s2p$	2	-0.299687[-1]		0.413166[-2]	-0.211690[-0]	-0.237527[-0]
$2s2p^*$	$2s2p^*$	1	-0.523910[-1]		0.110355[-2]	-0.228171[-0]	-0.279458[-0]
$2s2p$	$2s2p$	1	-0.746387[-1]		-0.202435[-2]	-0.238717[-0]	-0.315380[-0]
$2s2p^*$	$2s2p$	1	0.315840[-1]		0.441000[-2]	0.187514[-1]	0.547454[-1]
$2s2p$	$2s2p^*$	1	0.312356[-1]		0.439908[-2]	0.184622[-1]	0.540969[-1]
$2p^*2p$	$2p^*2p$	2	-0.724474[-1]		-0.187811[-2]	-0.306864[-0]	-0.381190[-0]
$2p2p$	$2p2p$	2	-0.559062[-1]		-0.243442[-2]	-0.289827[-0]	-0.348167[-0]
$2p^*2p$	$2p2p$	2	-0.228988[-1]		0.975874[-3]	-0.176180[-1]	-0.395408[-1]
$2p2p$	$2p^*2p$	2	-0.226577[-1]		0.973002[-3]	-0.173508[-1]	-0.390355[-1]
$2s2s$	$2s2s$	0	-0.387176[-1]	-0.684262[-3]	0.202434[-2]	-0.193231[-0]	-0.230609[-0]
$2p^*2p^*$	$2p^*2p^*$	0	-0.665325[-1]	-0.389341[-3]	-0.117068[-2]	-0.317745[-0]	-0.385838[-0]
$2p2p$	$2p2p$	0	-0.910576[-1]	-0.757244[-3]	0.121964[-2]	-0.339544[-0]	-0.430140[-0]
$2s2s$	$2p^*2p^*$	0	0.171591[-1]	0.516150[-3]	0.380596[-2]	0.192215[-1]	0.407028[-1]
$2p^*2p^*$	$2s2s$	0	0.171592[-1]	0.516150[-3]	0.380597[-2]	0.192217[-1]	0.407030[-1]
$2s2s$	$2p2p$	0	0.251190[-1]	0.720923[-3]	0.523094[-2]	0.299267[-1]	0.609975[-1]
$2p2p$	$2s2s$	0	0.247361[-1]	0.718736[-3]	0.520301[-2]	0.289723[-1]	0.596301[-1]
$2p^*2p^*$	$2p2p$	0	-0.364324[-1]	-0.543804[-3]	0.311873[-2]	-0.441467[-1]	-0.780042[-1]
$2p2p$	$2p^*2p^*$	0	-0.358029[-1]	-0.542154[-3]	0.310471[-2]	-0.428189[-1]	-0.760593[-1]

(b) Breit correction

			R_1^{BCl}	R_2^{BCl}	R_3^{BCl}	R_4^{BCl}	Σ^{BCl}
$2s2p^*$	$2s2p^*$	0	-0.363442[-3]		0.208030[-3]	-0.304132[-2]	-0.319673[-2]
$2p^*2p$	$2p^*2p$	1	-0.770602[-3]		-0.232693[-5]	-0.427572[-2]	-0.504865[-2]
$2s2p$	$2s2p$	2	-0.140076[-3]		0.247088[-4]	-0.142879[-2]	-0.154416[-2]
$2s2p^*$	$2s2p^*$	1	-0.269237[-3]		-0.402832[-4]	-0.175340[-2]	-0.206292[-2]
$2s2p$	$2s2p$	1	-0.761844[-3]		-0.740767[-4]	-0.198786[-2]	-0.282378[-2]
$2s2p^*$	$2s2p$	1	0.371556[-3]		0.126648[-3]	0.143511[-4]	0.512555[-3]
$2s2p$	$2s2p^*$	1	0.369604[-3]		0.126327[-3]	0.144713[-4]	0.510402[-3]
$2p^*2p$	$2p^*2p$	2	-0.316835[-3]		0.603776[-4]	-0.177143[-2]	-0.202789[-2]
$2p2p$	$2p2p$	2	-0.615100[-3]		0.605456[-5]	-0.220717[-2]	-0.281622[-2]
$2p^*2p$	$2p2p$	2	-0.439548[-3]		0.584691[-5]	-0.520448[-3]	-0.954149[-3]
$2p2p$	$2p^*2p$	2	-0.436704[-3]		0.581594[-5]	-0.513579[-3]	-0.944467[-3]
$2s2s$	$2s2s$	0	-0.575526[-3]	-0.543402[-4]	0.137713[-3]	-0.187162[-2]	-0.236377[-2]
$2p^*2p^*$	$2p^*2p^*$	0	-0.155500[-2]	-0.846961[-4]	0.200276[-3]	-0.545171[-2]	-0.689113[-2]
$2p2p$	$2p2p$	0	-0.265950[-2]	-0.756558[-4]	0.126224[-3]	-0.552676[-2]	-0.813569[-2]
$2s2s$	$2p^*2p^*$	0	0.660249[-3]	0.766358[-4]	-0.344228[-4]	0.579394[-3]	0.128186[-2]
$2p^*2p^*$	$2s2s$	0	0.660251[-3]	0.766359[-4]	-0.344228[-4]	0.579399[-3]	0.128186[-2]
$2s2s$	$2p2p$	0	0.111119[-2]	0.646393[-4]	-0.127575[-3]	0.192358[-2]	0.297183[-2]
$2p2p$	$2s2s$	0	0.109602[-2]	0.644432[-4]	-0.127021[-3]	0.187831[-2]	0.291175[-2]
$2p^*2p^*$	$2p2p$	0	-0.135219[-2]	-0.863144[-4]	0.173051[-3]	-0.131950[-2]	-0.258495[-2]
$2p2p$	$2p^*2p^*$	0	-0.133487[-2]	-0.860526[-4]	0.172328[-3]	-0.128443[-2]	-0.253302[-2]

second-order Coulomb corrections were determined by solving the nonsymmetric eigenvalue equation

$$H^{\mathrm{eff}}C=EC,$$

with the first- plus second-order effective Hamiltonian. The first- and second-order Coulomb interactions and the first-order Breit interaction are included in H^{eff}. The resulting eigenvectors are used to determine the second-order Breit correction and the QED correction. The difference between the energies obtained using the first- plus second-order Hamiltonian and those determined using only the first-order Hamiltonian give the second-order energies.

In the HF case, QED contributions for $Z\geqslant15$ were determined using one-electron Lamb shift data calculated in a $(1s^2)$ potential following the method described in Ref. [40].

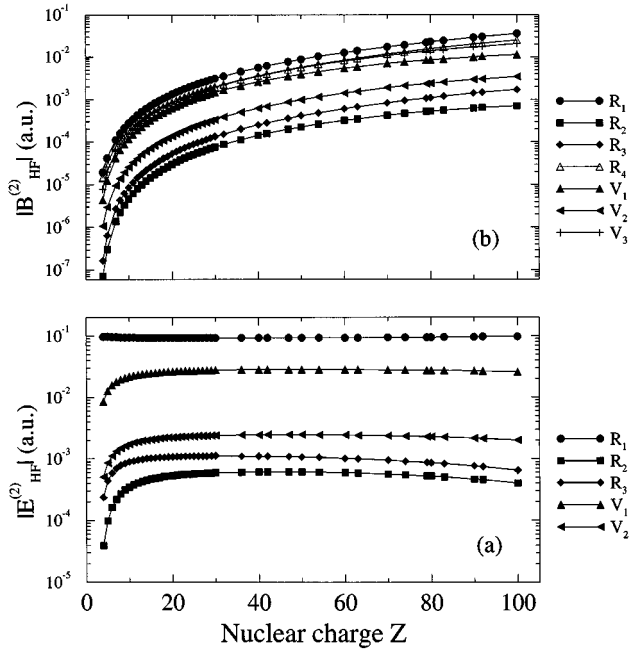

FIG. 3. Absolute values of contributions to the second-order $(2p^2_{3/2})$-$(2p^2_{3/2})$ $[J=0]$ diagonal matrix element in the HF case: (a) Coulomb interaction $E^{(2)}_{\rm HF}$; (b) Breit interaction $B^{(2)}_{\rm HF}$.

For smaller values of Z, the QED corrections in the HF case were taken from Ref. [41] with $Z\rightarrow Z-1$. In the Coulomb case, the QED corrections from [41], with Z replaced by $Z-2$, were used for all values of Z.

The first- and second-order energies are shown graphically in Figs. 5–8 and listed in Table IV. In Figs. 5(a) and 5(b), we show the Z dependence of the second-order Coulomb-Coulomb contributions for ten states. We can see

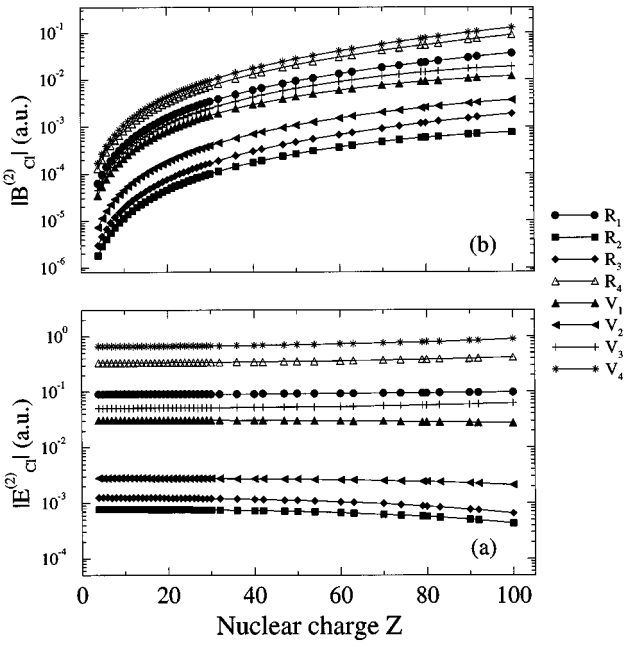

FIG. 4. Absolute values of contributions to the second-order $(2p^2_{3/2})$-$(2p^2_{3/2})$ $[J=0]$ diagonal matrix element in the Coulomb case: (a) Coulomb interaction $E^{(2)}_{\rm Cl}$; (b) Breit Interaction $B^{(2)}_{\rm Cl}$.

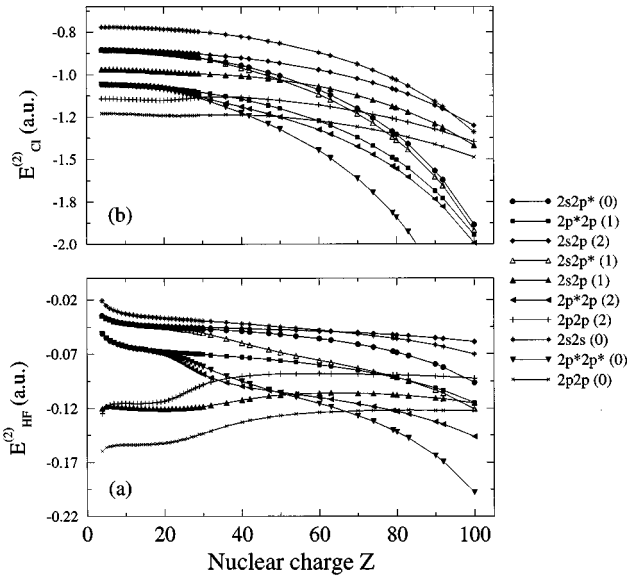

FIG. 5. Second-order Coulomb energies after diagonalization are shown as functions of nuclear charge Z for each of the ten states considered: (a) $E^{(2)}_{\rm HF}$; (b) $E^{(2)}_{\rm Cl}$.

from Figs. 5(a) and 5(b) that diagonalization essentially changes the Z dependence of the energies, especially in the Coulomb case.

The variation with Z of the second-order Coulomb energy $E^{(2)}$, the first- and second-order Breit energies $B^{(1)}$ and $B^{(2)}$, and the QED contributions $E_{\rm Lamb}$ are illustrated in Figs. 6 and 7. Data for $(2p^2)^1S_0$ and $(2s^2)^1S_0$ states, respectively, are given in Figs. 6(a) and 7(a) for the HF case, and in Figs. 6(b) and 7(b) for the Coulomb case. We can see that, in the HF case, $E^{(2)}$ is dominant up to $Z=33$ for the $(2p^2)^1S_0$ state, and up to $Z=25$ for the $(2s^2)^1S_0$ state. For the Coulomb case, $E^{(2)}$ is the most important contribution up to

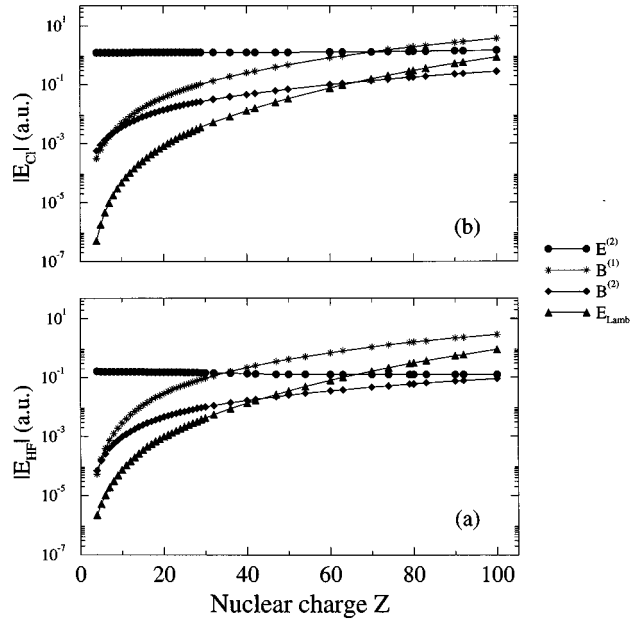

FIG. 6. Contributions to the energy of the $(2p^2)^1S_0$ state obtained using (a) HF basis set and (b) Coulomb basis set.

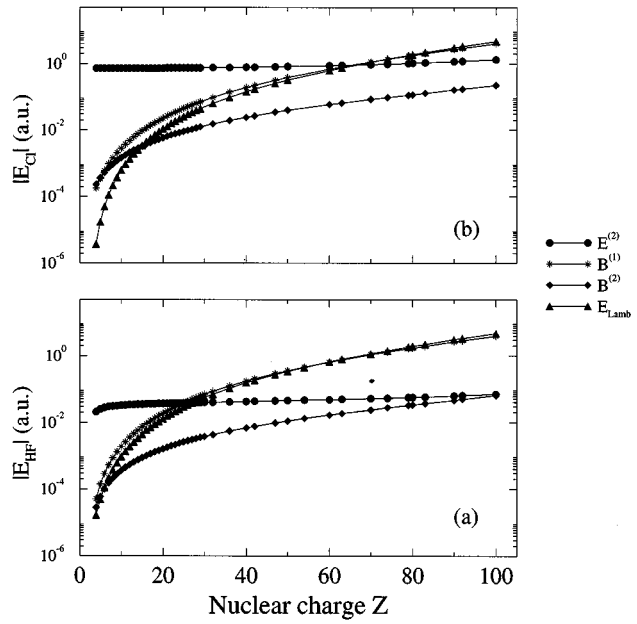

FIG. 7. Contributions to the energy of the $(2s^2)^1S_0$ state obtained using (a) HF basis set and (b) Coulomb basis set.

$Z=70$ and 65 for the $(2p^2)^1S_0$ and $(2s^2)^1S_0$ states, respectively. The QED contribution $E_{\rm Lamb}$ is smaller than all other contributions to the $(2p^2)^1S_0$ energy for $Z<43$ in the HF case as shown in Fig. 6(a), and up to $Z=65$ for the Coulomb case shown in Fig. 6(b). The situation is somewhat different for the $(2s^2)^1S_0$ state where the curve $E_{\rm Lamb}$ crosses $B^{(2)}$ first, then crosses the $E^{(2)}$ curve, and finally $B^{(1)}$, for the highest values of Z.

The final summary of our calculations is given in Table IV and in Figs. 8(a) and 8(b). In Table IV, we list energies of berylliumlike ions relative to the $(2s^2)^1S_0$ ground state. We tabulate the following separate contributions: zeroth- plus

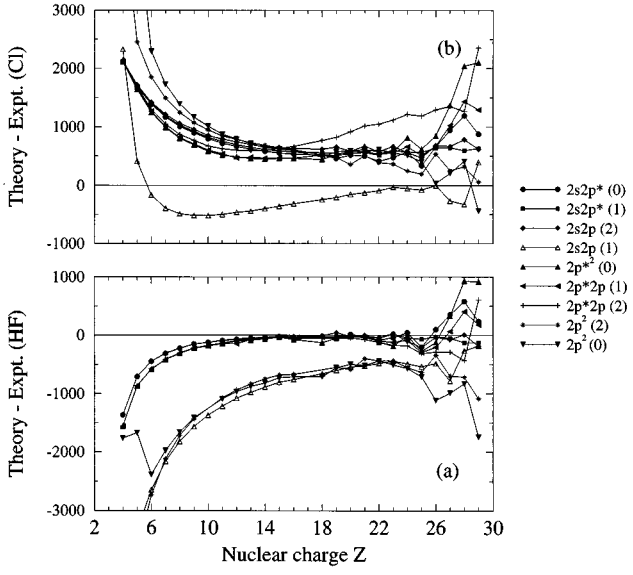

FIG. 8. Differences between theoretical and experimental energy levels ($\rm cm^{-1}$) obtained using (a) HF basis set and (b) Coulomb basis set.

first-order energy $E^{(0+1)}\equiv E^{(0)}+E^{(1)}+B^{(1)}$, the second-order Coulomb energy $E^{(2)}$, the second-order Breit correction $B^{(2)}$, the QED correction $E_{\rm Lamb}$, the total theoretical energy $E_{\rm tot}$, available experimental data $E_{\rm expt}$, and the differences between theoretical and experimental values $\delta E\equiv E_{\rm tot}-E_{\rm expt}$. The tabulation is made only for the HF case. It should be noted that for very high Z (90, 92), the HF and Coulomb cases give essentially identical results. For the experimentally observed $2s_{1/2}$-$2p_{3/2}$ transition [4], we obtain in the Coulomb case 4070.138 eV ($Z=90$) and 4502.759 eV ($Z=92$). These values differ from the corresponding values obtained in the HF case (shown in Table IV) by about 1 eV. We emphasize that both the HF and Coulomb values obtained here agree better with the measured energies than do the values from the MCDF calculations reported in [4].

The differences δE are shown in Figs. 8(a) and 8(b) for the HF and Coulomb cases, respectively. These differences are seen to be more or less smooth functions of Z. The fact that experimental data given by different authors are of different accuracy explains the variations (especially at high Z) seen in Figs. 8(a) and 8(b). The accuracy of the experimental data at high Z is estimated to be 100–300 $\rm cm^{-1}$. The peaks seen in Fig. 8 disappear if we use the data recommended by Edlén [2]. Here, we compare our *ab initio* calculations directly with experiment to illustrate the utility of these calculations as reference data for future measurements.

In Table V, we compare the present calculations of the $2\,^1P_1$-$2\,^1S_0$ and $2\,^3P_1$-$2\,^1S_0$ energy intervals for the ions $Z=26$ and $Z=42$ with the many-body calculations of Ref. [36]. The differences seen in this table arise partly from correlation corrections and partly from QED corrections. In our treatment of correlation, we ignored third- and higher-order MBPT graphs which are expected to contribute at the level of $1/Z$ of the second-order graphs. These higher-order correlation corrections are partially included in the calculations of Ref. [36]. A further difference is in the treatment of partial-wave sums. In Ref. [36], the sums over intermediate states were truncated at five or six partial waves; in the present calculations, the sums were carried out to ten partial waves. In both cases, the remainder of the partial-wave sums were estimated. Differences in higher-order correlation corrections and higher partial waves contribute to the differences seen in Table V. To help analyze the resulting differences, we compare the 2×2 effective Hamiltonian matrices for $2P_1$ states in the two calculations (considering only Coulomb and Breit corrections) for the case $Z=26$:

$$H_{\rm eff}=\begin{bmatrix} -144.856\,16 & -0.669\,18 \\ -0.669\,50 & -143.811\,02 \end{bmatrix} \text{ present,}$$

$$=\begin{bmatrix} -144.855\,07 & -0.670\,17 \\ -0.670\,47 & -143.809\,27 \end{bmatrix} \text{ Ref. [36].}$$

The corresponding eigenvalues are

$$E_{\rm Coul.+Breit}=(-145.182\,76 \quad -143.484\,42) \text{ present,}$$

$$=(-145.182\,32 \quad -143.482\,02) \text{ Ref. [36].}$$

For the first and second eigenvalues ($2\,^3P_1$ and $2\,^1P_1$ states), we see that the sum of Coulomb and Breit energies from the

TABLE IV. Energies of berylliumlike ions given relative to the ground state. Units: cm^{-1} for ions with $Z=4$–42 and eV for ions with $Z=47$–100. Notation: $2p^*\equiv 2p_{1/2}$, $2p\equiv 2p_{3/2}$, $E^{(0+1)}\equiv E^{(0)}+E^{(1)}+B^{(1)}$, and $\delta E\equiv E_{\rm tot}-E_{\rm expt}$.

	$2s2p\ ^3P_0$ $2s2p^*(0)$	$2s2p\ ^3P_1$ $2s2p^*(1)$	$2s2p\ ^3P_2$ $2s2p(2)$	$2s2p\ ^1P_1$ $2s2p(1)$	$2p^2\ ^3P_0$ $2p^*2p^*(0)$	$2p^2\ ^3P_1$ $2p^*2p(1)$	$2p^2\ ^3P_2$ $2p^*2p(2)$	$2p^2\ ^1D_2$ $2p2p(2)$	$2p^2\ ^1S_0$ $2p2p(0)$
$Z=4$									
$E^{(0+1)}$	23607.9	23607.4	23608.2	60057.5	64791.0	64791.6	64790.9	74393.8	100022.4
$E^{(2)}$	−2994.6	−2993.8	−2993.3	−21735.5	−6648.6	−6648.1	−6646.6	−22723.7	−30275.9
$B^{(2)}$	−1.6	−0.5	0.5	−3.9	−2.1	−1.8	0.3	−1.4	−8.3
$E_{\rm Lamb}$	−1.7	−1.7	−1.6	−1.6	−3.7	−3.7	−3.6	−3.7	−3.5
$E_{\rm tot}$	20610	20611	20614	38316	58137	58138	58141	51665	69735
$E_{\rm expt}$ [5]	21979	21980	21982	42565	59694	59696	59698	56432	71499
δE	−1369	−1369	−1368	−4249	−1557	−1558	−1557	−4767	−1764
$Z=5$									
$E^{(0+1)}$	39116.7	39120.2	39132.6	90407.8	104573.9	104580.4	104587.0	118978.2	154611.7
$E^{(2)}$	−2484.1	−2482.6	−2480.9	−20349.3	−6514.3	−6512.9	−6509.3	−20354.4	−28589.1
$B^{(2)}$	−3.5	−1.5	0.7	−7.8	−6.5	−5.7	−0.9	−5.0	−19.2
$E_{\rm Lamb}$	−5.0	−5.0	−4.8	−4.9	−10.9	−10.8	−10.7	−10.7	−10.0
$E_{\rm tot}$	36624	36631	36648	70046	98042	98051	98066	98608	125993
$E_{\rm expt}$ [5]	37334	37340	37356	73397	98910	98919	98933	102362	127662
δE	−710	−709	−708	−3351	−868	−868	−867	−3754	−1669
$Z=6$									
$E^{(0+1)}$	54204.6	54223.4	54272.9	119482.0	143404.3	143429.2	143464.6	162582.0	207994.8
$E^{(2)}$	−2271.0	−2268.8	−2265.3	−19748.1	−6523.8	−6521.0	−6514.6	−19400.8	−27797.7
$B^{(2)}$	−6.4	−3.1	0.6	−13.0	−12.9	−11.6	−3.2	−10.6	−34.1
$E_{\rm Lamb}$	−11.6	−11.4	−11.0	−11.2	−24.7	−24.5	−24.2	−24.3	−22.6
$E_{\rm tot}$	51916	51940	51997	99710	136843	136872	136923	143146	180140
$E_{\rm expt}$ [6]	52367	52391	52447	102352	137426	137454	137502	145876	182520
δE	−451	−451	−450	−2642	−583	−582	−579	−2730	−2380
$Z=7$									
$E^{(0+1)}$	69072.2	69127.7	69260.7	147983.0	181733.3	181800.1	181904.9	205695.2	260789.0
$E^{(2)}$	−2141.0	−2137.6	−2132.0	−19407.7	−6547.4	−6542.7	−6533.3	−18866.1	−27299.6
$B^{(2)}$	−10.2	−5.3	0.2	−19.5	−21.3	−19.3	−6.5	−17.9	−52.9
$E_{\rm Lamb}$	−22.6	−22.2	−21.5	−21.8	−47.9	−47.5	−46.8	−47.2	−43.9
$E_{\rm tot}$	66898	66962	67107	128534	175117	175191	175318	186764	233393
$E_{\rm expt}$ [7]	67209	67272	67416	130694	175535	175608	175733	188882	235369
δE	−311	−310	−309	−2160	−418	−417	−415	−2118	−1976
$Z=8$									
$E^{(0+1)}$	83824.3	83950.5	84240.5	176233.8	219837.7	219983.6	220223.8	248633.1	313355.4
$E^{(2)}$	−2052.0	−2047.5	−2039.1	−19189.1	−6573.6	−6566.3	−6553.5	−18521.3	−26953.7
$B^{(2)}$	−14.9	−8.1	−0.4	−27.4	−31.8	−28.8	−10.7	−27.0	−75.7
$E_{\rm Lamb}$	−39.6	−38.9	−37.6	−38.2	−83.6	−82.9	−81.6	−82.2	−76.7
$E_{\rm tot}$	81718	81856	82164	156979	213149	213306	213578	230003	286249
$E_{\rm expt}$ [8]	81942	82079	82385	158798	213462	213618	213887	231721	287910
δE	−224	−223	−221	−1819	−313	−312	−309	−1718	−1661
$Z=9$									
$E^{(0+1)}$	98519.0	98765.4	99318.8	204414.5	257895.4	258175.2	258646.7	291614.8	365932.5
$E^{(2)}$	−1987.4	−1981.5	−1969.7	−19036.8	−6599.8	−6589.1	−6573.0	−18279.7	−26698.4
$B^{(2)}$	−20.5	−11.6	−1.2	−36.5	−44.3	−40.2	−16.0	−37.8	−102.3
$E_{\rm Lamb}$	−64.2	−63.1	−60.8	−61.9	−135.0	−133.8	−131.6	−132.6	−124.0
$E_{\rm tot}$	96447	96709	97287	185279	251116	251412	251926	273165	339008
$E_{\rm expt}$ [5]	96601	96861	97437	186841	251341	251635	252145	274597	340424
δE	−154	−152	−150	−1562	−225	−223	−219	−1432	−1416
$Z=10$									
$E^{(0+1)}$	113191.2	113625.5	114588.3	232646.9	296034.4	296525.0	297358.7	334815.4	418703.9
$E^{(2)}$	−1938.5	−1931.2	−1915.3	−18924.3	−6625.9	−6610.4	−6591.9	−18099.8	−26500.9
$B^{(2)}$	−27.0	−15.6	−2.3	−47.0	−59.0	−53.5	−22.3	−50.4	−132.8
$E_{\rm Lamb}$	−98.1	−96.3	−92.6	−94.4	−205.7	−203.7	−200.2	−201.8	−189.0
$E_{\rm tot}$	111128	111582	112578	213581	289144	289657	290544	316463	391881
$E_{\rm expt}$ [5]	111251	111705	112700	214952	289328	289839	290722		
δE	−123	−123	−122	−1371	−184	−182	−178		

TABLE IV. (*Continued*).

	$2s2p\ ^3P_0$ $2s2p^*(0)$	$2s2p\ ^3P_1$ $2s2p^*(1)$	$2s2p\ ^3P_2$ $2s2p(2)$	$2s2p\ ^1P_1$ $2s2p(1)$	$2p^2\ ^3P_0$ $2p^*2p^*(0)$	$2p^2\ ^3P_1$ $2p^*2p(1)$	$2p^2\ ^3P_2$ $2p^*2p(2)$	$2p^2\ ^1D_2$ $2p2p(2)$	$2p^2\ ^1S_0$ $2p2p(0)$
$Z=11$									
$E^{(0+1)}$	127863.3	128573.4	130137.5	261026.3	334355.3	335160.8	336526.4	378391.3	471829.6
$E^{(2)}$	−1900.4	−1891.8	−1871.0	−18837.2	−6652.1	−6629.9	−6610.9	−17958.5	−26341.8
$B^{(2)}$	−34.5	−20.3	−3.6	−58.8	−75.8	−68.7	−29.6	−64.7	−167.1
E_{Lamb}	−143.0	−140.3	−134.6	−137.3	−299.2	−296.1	−290.8	−293.0	−274.9
E_{tot}	125785	126521	128128	241993	327328	328166	329595	360075	445046
E_{expt} [9]	125880	126612	128218	243208	327476	328310	329729	361145	446136
δE	−95	−91	−90	−1215	−148	−144	−134	−1070	−1090
$Z=12$									
$E^{(0+1)}$	142551.0	143647.4	146057.8	289638.7	372946.2	374203.8	376313.0	422497.7	525465.5
$E^{(2)}$	−1869.8	−1860.4	−1833.5	−18767.1	−6679.4	−6647.8	−6631.7	−17841.5	−26208.5
$B^{(2)}$	−42.9	−25.7	−5.1	−71.9	−95.0	−85.8	−38.1	−80.6	−205.2
E_{Lamb}	−200.9	−197.0	−188.8	−192.7	−419.6	−415.0	−407.5	−410.4	−385.5
E_{tot}	140437	141564	144030	270607	365752	367055	369236	404165	498666
E_{expt} [10]	140504	141631	144091	271687	365856	367199	369330	405100	499633
δE	−67	−67	−61	−1080	−104	−144	−94	−935	−967
$Z=13$									
$E^{(0+1)}$	157265.5	158882.8	162445.1	318567.2	411885.3	413773.0	416880.9	467294.2	579770.5
$E^{(2)}$	−1844.8	−1835.2	−1800.8	−18708.3	−6709.1	−6664.1	−6656.6	−17738.2	−26091.9
$B^{(2)}$	−52.2	−31.7	−6.9	−86.3	−116.6	−104.8	−47.7	−98.2	−246.9
E_{Lamb}	−273.8	−268.4	−256.7	−262.1	−570.8	−564.1	−553.8	−557.4	−524.3
E_{tot}	155095	156748	160381	299511	404489	406440	409623	448900	552908
E_{expt} [11]	155148	156798	160429	300490	404574	406517	409690	449732	553783
δE	−53	−50	−48	−979	−85	−77	−67	−832	−875
$Z=14$									
$E^{(0+1)}$	172015.2	174313.5	179401.5	347896.5	451244.3	453989.9	458395.0	512952.2	634913.7
$E^{(2)}$	−1823.9	−1815.1	−1771.4	−18657.1	−6742.5	−6678.9	−6688.6	−17640.5	−25985.3
$B^{(2)}$	−62.5	−38.6	−9.0	−102.0	−140.8	−125.8	−58.7	−117.4	−292.0
E_{Lamb}	−363.7	−356.3	−340.2	−347.5	−756.9	−747.4	−733.6	−737.7	−694.8
E_{tot}	169765	172104	177281	328790	443604	446438	450914	494457	607942
E_{expt} [12]	169802	172144	177318	329679	443670	446494	450965	495201	608758
δE	−37	−40	−37	−889	−66	−56	−51	−744	−816
$Z=15$									
$E^{(0+1)}$	186807.0	189972.3	197037.1	377716.5	491089.1	494981.2	501022.7	559659.8	691079.5
$E^{(2)}$	−1806.1	−1799.7	−1744.4	−18610.6	−6781.6	−6692.4	−6731.9	−17540.6	−25883.2
$B^{(2)}$	−73.8	−46.1	−11.2	−118.9	−167.7	−148.8	−71.0	−138.0	−340.6
E_{Lamb}	−471.5	−462.1	−440.7	−450.1	−980.3	−967.5	−950.1	−954.1	−899.8
E_{tot}	184456	187664	194841	358537	483159	487173	493270	541027	663956
E_{expt} [13]	184478	187690	194856	359343	483195	487203	493285	541709	664685
δE	−22	−26	−15	−806	−36	−30	−15	−682	−729
$Z=16$									
$E^{(0+1)}$	201646.6	205891.3	215470.4	408123.8	531480.1	536880.7	544933.0	607626.8	748471.3
$E^{(2)}$	−1790.7	−1788.8	−1719.0	−18566.4	−6828.6	−6704.5	−6791.6	−17430.7	−25780.8
$B^{(2)}$	−86.2	−54.5	−13.7	−137.0	−197.6	−173.7	−84.9	−159.8	−392.3
E_{Lamb}	−624.4	−611.2	−580.5	−593.6	−1295.3	−1276.2	−1252.5	−1256.0	−1186.3
E_{tot}	199145	203437	213157	388827	523159	528726	536804	588780	721112
E_{expt} [14]	199181	203474	213182	389583	523237	528796	536850	589449	721825
δE	−36	−37	−25	−756	−78	−70	−46	−669	−713
$Z=17$									
$E^{(0+1)}$	216539.1	222101.0	234828.3	439223.6	572469.6	579829.2	590293.6	657088.2	807314.7
$E^{(2)}$	−1776.9	−1782.5	−1694.5	−18522.7	−6885.6	−6715.5	−6874.2	−17302.5	−25673.6
$B^{(2)}$	−99.5	−63.7	−16.4	−156.3	−230.6	−200.6	−100.6	−182.8	−447.0
E_{Lamb}	−785.8	−769.1	−728.7	−745.4	−1628.1	−1602.3	−1573.1	−1574.3	−1489.2
E_{tot}	213877	219486	232389	419799	563725	571311	581746	638029	779705
E_{expt} [2]				420493				638648	
δE				−694				−619	

TABLE IV. (*Continued*).

	$2s2p\ ^3P_0$ $2s2p^*(0)$	$2s2p\ ^3P_1$ $2s2p^*(1)$	$2s2p\ ^3P_2$ $2s2p(2)$	$2s2p\ ^1P_1$ $2s2p(1)$	$2p^2\ ^3P_0$ $2p^*2p^*(0)$	$2p^2\ ^3P_1$ $2p^*2p(1)$	$2p^2\ ^3P_2$ $2p^*2p(2)$	$2p^2\ ^1D_2$ $2p2p(2)$	$2p^2\ ^1S_0$ $2p2p(0)$
$Z=18$									
$E^{(0+1)}$	231489.4	238630.5	255247.6	471131.3	614102.3	623976.4	637268.4	708310.3	867860.9
$E^{(2)}$	−1764.5	−1781.3	−1670.6	−18477.6	−6955.2	−6725.2	−6987.0	−17147.4	−25557.7
$B^{(2)}$	−113.8	−73.8	−19.4	−176.7	−267.0	−229.5	−118.2	−206.5	−504.5
$E_{\rm Lamb}$	−961.9	−941.3	−889.4	−910.0	−1990.3	−1956.1	−1921.5	−1918.2	−1817.6
$E_{\rm tot}$	228649	235834	252668	451567	604890	615066	628242	689038	839981
$E_{\rm expt}$ [2]	228664	235860	252675	452223	605019	615098	628294		840690
δE	−15	−26	−7	−656	−129	−32	−52		−709
$Z=19$									
$E^{(0+1)}$	246502.9	255507.2	276875.3	503974.4	656414.3	669482.7	686015.4	761595.7	930390.4
$E^{(2)}$	−1753.0	−1785.7	−1646.8	−18429.5	−7039.9	−6733.8	−7137.5	−16956.6	−25429.3
$B^{(2)}$	−129.2	−84.8	−22.5	−198.2	−307.0	−260.5	−138.2	−230.7	−564.3
$E_{\rm Lamb}$	−1160.5	−1136.3	−1072.7	−1096.8	−2399.8	−2356.6	−2318.0	−2307.4	−2190.5
$E_{\rm tot}$	243460	252500	274133	484250	646668	660132	676422	742101	902206
$E_{\rm expt}$ [22]	243520	252520	274090	484856	646720	660170	676480	742650	902760
δE	−60	−20	43	−606	−52	−38	−58	−549	−554
$Z=20$									
$E^{(0+1)}$	261583.7	272754.5	299867.0	537891.6	699428.3	716515.1	736680.3	817282.9	995211.3
$E^{(2)}$	−1742.2	−1796.5	−1622.9	−18376.7	−7142.0	−6741.3	−7332.8	−16722.4	−25285.1
$B^{(2)}$	−145.6	−96.9	−25.8	−220.6	−351.1	−293.4	−160.9	−255.1	−626.4
$E_{\rm Lamb}$	−1391.7	−1363.8	−1286.4	−1314.3	−2876.5	−2822.7	−2780.7	−2759.4	−2625.0
$E_{\rm tot}$	258304	269497	296932	517980	689059	706658	726406	797546	966675
$E_{\rm expt}$ [22]	258290	269505	296950	518524	689080	706680	726450	798130	967170
δE	14	−8	−18	−544	−21	−22	−44	−584	−495
$Z=21$									
$E^{(0+1)}$	276737.8	290393.5	324390.2	573037.1	743158.6	765253.4	789400.9	875754.2	1062666.1
$E^{(2)}$	−1731.8	−1814.6	−1598.5	−18317.7	−7263.5	−6747.7	−7577.4	−16439.4	−25122.5
$B^{(2)}$	−163.1	−110.0	−29.2	−244.0	−399.3	−328.4	−186.4	−279.4	−690.3
$E_{\rm Lamb}$	−1658.0	−1626.2	−1532.9	−1564.7	−3424.9	−3358.9	−3314.3	−3278.3	−3125.5
$E_{\rm tot}$	273185	286843	321230	552911	732071	754818	778323	855757	1033728
$E_{\rm expt}$ [22]	273200	286860	321240	553440	732070	754860	778400	856160	1034250
δE	−15	−17	−10	−529	1	−42	−77	−403	−522
$Z=22$									
$E^{(0+1)}$	291971.2	308441.5	350622.9	609579.5	787607.6	815887.6	844305.9	937431.0	1133129.7
$E^{(2)}$	−1721.6	−1840.9	−1573.6	−18251.1	−7405.8	−6753.0	−7871.9	−16106.7	−24939.3
$B^{(2)}$	−181.6	−124.3	−32.8	−268.3	−452.2	−365.4	−215.1	−303.2	−755.8
$E_{\rm Lamb}$	−1965.4	−1929.7	−1818.3	−1854.0	−4057.8	−3978.0	−3932.0	−3876.8	−3704.5
$E_{\rm tot}$	288103	304547	347198	589206	775692	804791	832287	917144	1103730
$E_{\rm expt}$ [22]	288190	304600	347240	589692	775810	804890	832410	917580	1104170
δE	−87	−53	−42	−486	−118	−99	−123	−436	−440
$Z=23$									
$E^{(0+1)}$	307291.2	326911.7	378754.6	647704.1	832768.8	868619.6	901521.6	1002772.2	1207011.0
$E^{(2)}$	−1711.5	−1876.4	−1548.0	−18175.4	−7569.5	−6757.4	−8211.5	−15728.5	−24734.6
$B^{(2)}$	−201.2	−139.8	−36.5	−293.2	−509.9	−404.5	−247.1	−326.5	−822.5
$E_{\rm Lamb}$	−2316.5	−2275.9	−2140.9	−2181.4	−4778.2	−4680.2	−4632.9	−4551.9	−4360.0
$E_{\rm tot}$	303062	322620	375029	627054	819911	856778	888430	982165	1177094
$E_{\rm expt}$ [15]	303100	322600	375000	627500	820100	856900	888600	982600	1177600
δE	−38	20	29	−446	−189	−122	−170	−435	−506
$Z=24$									
$E^{(0+1)}$	322704.8	345811.7	408985.3	687611.6	878624.6	923660.7	961176.6	1072263.3	1284749.2
$E^{(2)}$	−1701.4	−1921.9	−1521.5	−18089.6	−7754.3	−6760.7	−8586.3	−15314.6	−24508.3
$B^{(2)}$	−221.9	−156.7	−40.3	−318.9	−572.6	−445.5	−282.3	−349.2	−890.3
$E_{\rm Lamb}$	−2705.2	−2660.6	−2501.1	−2545.6	−5575.9	−5459.6	−5412.9	−5302.1	−5090.8
$E_{\rm tot}$	318076	341073	404922	666658	864722	910995	946895	1051297	1254260
$E_{\rm expt}$ [16]	318030	341120	405020	667150	864730	911080	947080	1051850	1254830
δE	46	−47	−98	−492	−8	−85	−185	−553	−570

TABLE IV. (*Continued*).

	$2s2p\ ^3P_0$ $2s2p^*(0)$	$2s2p\ ^3P_1$ $2s2p^*(1)$	$2s2p\ ^3P_2$ $2s2p(2)$	$2s2p\ ^1P_1$ $2s2p(1)$	$2p^2\ ^3P_0$ $2p^*2p^*(0)$	$2p^2\ ^3P_1$ $2p^*2p(1)$	$2p^2\ ^3P_2$ $2p^*2p(2)$	$2p^2\ ^1D_2$ $2p2p(2)$	$2p^2\ ^1S_0$ $2p2p(0)$
$Z=25$									
$E^{(0+1)}$	338218.7	365143.7	441525.8	729519.1	925148.6	981231.9	1023410.8	1146408.6	1366812.3
$E^{(2)}$	−1691.3	−1978.2	−1494.1	−17992.5	−7959.1	−6763.1	−8982.1	−14878.7	−24261.2
$B^{(2)}$	−243.7	−174.9	−44.2	−345.0	−640.6	−488.7	−320.5	−371.5	−958.9
E_{Lamb}	−3140.2	−3091.0	−2901.0	−2950.1	−6465.7	−6327.0	−6281.2	−6133.5	−5903.2
E_{tot}	333144	359900	437087	708231	910083	967653	1007827	1125025	1335689
E_{expt} [17]	333350	359970	437300	708770	910360	967950	1008140	1125660	1336400
δE	−206	−70	−213	−539	−277	−297	−313	−635	−711
$Z=26$									
$E^{(0+1)}$	353844.6	384908.8	476602.4	773664.9	972318.2	1041574.0	1088394.4	1225733.5	1453705.1
$E^{(2)}$	−1681.0	−2045.8	−1465.7	−17883.5	−8181.8	−6764.6	−9383.8	−14436.0	−23995.2
$B^{(2)}$	−266.6	−194.6	−48.1	−371.7	−714.0	−533.8	−361.6	−393.7	−1028.2
E_{Lamb}	−3619.6	−3565.9	−3340.8	−3394.5	−7444.5	−7280.4	−7236.2	−7045.8	−6797.2
E_{tot}	348277	379102	471748	752015	955978	1026995	1071413	1203858	1421885
E_{expt} [18]	348180	379130	471780	752502	956100	1027200	1071700	1204200	1423000
δE	97	−28	−32	−487	−122	−205	−287	−342	−1115
$Z=27$									
$E^{(0+1)}$	369591.1	405100.1	514450.1	820300.8	1020101.2	1104932.4	1156316.7	1310764.2	1545952.2
$E^{(2)}$	−1670.6	−2125.1	−1436.2	−17762.1	−8419.8	−6765.3	−9777.1	−14000.6	−23713.0
$B^{(2)}$	−290.6	−215.8	−52.0	−398.7	−793.0	−581.0	−405.1	−415.9	−1098.1
E_{Lamb}	−4147.6	−4089.7	−3825.0	−3882.9	−8520.6	−8328.6	−8286.6	−8048.0	−7781.6
E_{tot}	363482	398669	509137	798257	1002368	1089257	1137848	1288300	1513360
E_{expt} [17]	363130	398720	509210	799040	1002040	1089190	1138140	1289000	1514350
δE	352	−51	−73	−783	328	67	−292	−700	−990
$Z=28$									
$E^{(0+1)}$	385471.2	425710.3	555319.7	869699.3	1068473.5	1171572.1	1227403.5	1402041.7	1644109.9
$E^{(2)}$	−1660.0	−2216.0	−1405.7	−17628.3	−8669.6	−6765.2	−10151.0	−13583.4	−23417.9
$B^{(2)}$	−315.7	−238.7	−55.9	−425.9	−877.4	−630.3	−450.9	−438.4	−1168.5
E_{Lamb}	−4726.9	−4664.4	−4351.6	−4414.0	−9697.6	−9471.9	−9431.9	−9136.5	−8853.6
E_{tot}	378769	418591	549506	847231	1049229	1154705	1207370	1378883	1610670
E_{expt} [3,22]	378190	418720	549500	847494	1048300	1154300	1207800	1379600	1611500
δE	579	−129	6	−263	929	405	−430	−717	−830
$Z=29$									
$E^{(0+1)}$	401490.5	446720.9	599466.5	922141.2	1117397.2	1241754.0	1301891.5	1500099.2	1748741.2
$E^{(2)}$	−1649.3	−2318.3	−1374.2	−17482.5	−8927.9	−6764.5	−10498.1	−13191.8	−23113.4
$B^{(2)}$	−341.9	−263.2	−59.8	−453.4	−967.4	−681.6	−498.6	−461.4	−1239.5
E_{Lamb}	−5363.3	−5296.9	−4931.0	−4997.3	−10989.1	−10727.3	−10689.7	−10332.4	−10033.4
E_{tot}	394136	438842	593102	899208	1096513	1223581	1280205	1476114	1714355
E_{expt} [20]	393900	438970	593290	899390	1095600	1223400	1279600	1477200	1716100
δE	236	−128	−188	−182	913	181	605	−1086	−1745
$Z=30$									
$E^{(0+1)}$	417668.2	468123.7	647171.3	977935.8	1166864.9	1315778.0	1380068.9	1605508.9	1860456.7
$E^{(2)}$	−1638.5	−2431.2	−1341.7	−17325.3	−9191.1	−6763.2	−10814.5	−12829.8	−22803.1
$B^{(2)}$	−369.3	−289.5	−63.6	−481.0	−1062.8	−734.9	−548.0	−485.0	−1311.0
E_{Lamb}	−6055.4	−5985.4	−5559.4	−5629.2	−12390.6	−12088.7	−12053.5	−11627.8	−11313.8
E_{tot}	409605	459418	640207	954500	1144220	1296191	1356653	1580566	1825029
$Z=32$									
$E^{(0+1)}$	450545.6	512034.7	754411.0	1100863.4	1267365.1	1476550.8	1548685.0	1840693.5	2107623.2
$E^{(2)}$	−1617.0	−2685.0	−1273.7	−16981.0	−9719.3	−6759.3	−11353.0	−12196.9	−22179.0
$B^{(2)}$	−427.6	−347.5	−70.9	−536.4	−1269.7	−847.7	−651.8	−534.6	−1456.1
E_{Lamb}	−7629.5	−7553.4	−6982.0	−7057.9	−15569.9	−15172.8	−15142.1	−14556.0	−14215.4
E_{tot}	440871	501449	746084	1076288	1240806	1453771	1521538	1813406	2069773
E_{expt} [21]		501600	746280	1076400					
δE		−151	−196	−112					

TABLE IV. (*Continued*).

	$2s2p\ ^3P_0$ $2s2p^*(0)$	$2s2p\ ^3P_1$ $2s2p^*(1)$	$2s2p\ ^3P_2$ $2s2p(2)$	$2s2p\ ^1P_1$ $2s2p(1)$	$2p^2\ ^3P_0$ $2p^*2p^*(0)$	$2p^2\ ^3P_1$ $2p^*2p(1)$	$2p^2\ ^3P_2$ $2p^*2p(2)$	$2p^2\ ^1D_2$ $2p2p(2)$	$2p^2\ ^1S_0$ $2p2p(0)$
$Z=36$									
$E^{(0+1)}$	518815.3	603869.7	1025134.6	1401867.2	1474646.1	1858292.3	1944426.5	2426118.1	2715626.9
$E^{(2)}$	−1576.4	−3266.2	−1128.0	−16215.1	−10717.7	−6749.7	−12107.7	−11244.9	−20988.1
$B^{(2)}$	−558.9	−485.3	−83.3	−647.5	−1745.8	−1097.9	−877.2	−642.7	−1757.0
$E_{\rm Lamb}$	−11616.6	−11534.3	−10561.0	−10643.3	−23589.0	−22935.0	−22911.5	−21902.6	−21524.8
$E_{\rm tot}$	505063	588584	1013362	1374361	1438594	1827510	1908530	2392328	2671357
$E_{\rm expt}$ [3]		588750		1374000					
δE		−166		361					
$Z=40$									
$E^{(0+1)}$	591315.8	700568.8	1389955.6	1796942.6	1691140.2	2340137.8	2438434.1	3202559.6	3514386.8
$E^{(2)}$	−1544.4	−3869.2	−973.3	−15431.3	−11582.5	−6743.9	−12571.9	−10580.1	−19945.4
$B^{(2)}$	−711.1	−652.3	−91.3	−759.2	−2302.5	−1381.3	−1125.9	−760.5	−2075.9
$E_{\rm Lamb}$	−16874.8	−16794.0	−15259.5	−15340.2	−34126.4	−33118.1	−33100.2	−31520.7	−31127.4
$E_{\rm tot}$	572186	679253	1373632	1765412	1643129	2298895	2391636	3159698	3461238
$Z=42$									
$E^{(0+1)}$	629460.6	750684.1	1615697.1	2038194.1	1803312.2	2626895.1	2730704.6	3678306.7	4001562.8
$E^{(2)}$	−1533.7	−4156.7	−894.1	−15058.5	−11964.3	−6744.7	−12737.8	−10316.1	−19486.3
$B^{(2)}$	−795.7	−746.5	−93.0	−815.7	−2611.3	−1535.7	−1259.3	−821.9	−2242.7
$E_{\rm Lamb}$	−20045.0	−19967.2	−18091.6	−18169.3	−40469.6	−39246.8	−39231.0	−37309.2	−36915.2
$E_{\rm tot}$	607086	725814	1596618	2004151	1748267	2579368	2677477	3629860	3942919
$E_{\rm expt}$ [23]		725758		2003847					
δE		56		304					
$Z=47$									
$E^{(0+1)}$	90.708	109.326	289.694	347.110	260.081	435.024	449.426	642.583	686.374
$E^{(2)}$	−0.189	−0.595	−0.086	−1.763	−1.588	−0.839	−1.617	−1.212	−2.294
$B^{(2)}$	−0.128	−0.126	−0.011	−0.119	−0.431	−0.243	−0.201	−0.121	−0.332
$E_{\rm Lamb}$	−3.692	−3.684	−3.318	−3.326	−7.430	−7.192	−7.191	−6.820	−6.773
$E_{\rm tot}$	86.698	104.921	286.279	341.901	250.632	426.750	440.417	634.429	676.975
$Z=50$									
$E^{(0+1)}$	98.966	119.632	359.258	419.876	283.341	517.353	532.561	786.546	832.706
$E^{(2)}$	−0.191	−0.637	−0.071	−1.710	−1.644	−0.842	−1.635	−1.179	−2.232
$B^{(2)}$	−0.149	−0.148	−0.010	−0.130	−0.504	−0.278	−0.230	−0.133	−0.366
$E_{\rm Lamb}$	−4.588	−4.580	−4.115	−4.122	−9.220	−8.915	−8.914	−8.443	−8.398
$E_{\rm tot}$	94.038	114.267	355.062	413.913	271.973	507.318	521.782	776.791	821.709
$Z=54$									
$E^{(0+1)}$	110.868	134.139	474.827	539.943	316.219	650.985	667.139	1024.317	1073.815
$E^{(2)}$	−0.197	−0.686	−0.051	−1.649	−1.717	−0.848	−1.656	−1.140	−2.159
$B^{(2)}$	−0.180	−0.182	−0.007	−0.145	−0.613	−0.328	−0.272	−0.148	−0.413
$E_{\rm Lamb}$	−6.010	−6.004	−5.383	−5.389	−12.061	−11.652	−11.651	−11.025	−10.984
$E_{\rm tot}$	104.482	127.267	469.386	532.759	301.829	638.157	653.561	1012.004	1060.258
$Z=60$									
$E^{(0+1)}$	130.983	157.894	708.737	781.108	370.304	914.572	931.869	1502.498	1557.416
$E^{(2)}$	−0.211	−0.750	−0.021	−1.575	−1.826	−0.864	−1.686	−1.087	−2.066
$B^{(2)}$	−0.235	−0.242	0.001	−0.168	−0.802	−0.413	−0.341	−0.167	−0.486
$E_{\rm Lamb}$	−8.702	−8.697	−7.790	−7.795	−17.441	−16.830	−16.829	−15.918	−15.882
$E_{\rm tot}$	121.834	148.205	700.926	771.569	350.236	896.465	913.013	1485.327	1538.982
$Z=63$									
$E^{(0+1)}$	142.164	170.781	858.991	935.225	399.747	1080.939	1098.678	1808.398	1866.216
$E^{(2)}$	−0.222	−0.780	−0.006	−1.544	−1.885	−0.874	−1.701	−1.061	−2.024
$B^{(2)}$	−0.267	−0.276	0.007	−0.180	−0.911	−0.459	−0.378	−0.175	−0.522
$E_{\rm Lamb}$	−10.334	−10.329	−9.256	−9.260	−20.700	−19.972	−19.971	−18.895	−18.861
$E_{\rm tot}$	131.341	159.396	849.736	924.241	376.251	1059.634	1076.628	1788.267	1844.809

TABLE IV. (*Continued*).

	$2s2p\ ^3P_0$ $2s2p^*(0)$	$2s2p\ ^3P_1$ $2s2p^*(1)$	$2s2p\ ^3P_2$ $2s2p(2)$	$2s2p\ ^1P_1$ $2s2p(1)$	$2p^2\ ^3P_0$ $2p^*2p^*(0)$	$2p^2\ ^3P_1$ $2p^*2p(1)$	$2p^2\ ^3P_2$ $2p^*2p(2)$	$2p^2\ ^1D_2$ $2p2p(2)$	$2p^2\ ^1S_0$ $2p2p(0)$
$Z=70$									
$E^{(0+1)}$	171.715	204.018	1319.595	1405.487	475.896	1583.005	1601.416	2742.835	2807.938
$E^{(2)}$	−0.258	−0.849	0.033	−1.482	−2.039	−0.906	−1.742	−1.001	−1.931
$B^{(2)}$	−0.357	−0.369	0.027	−0.205	−1.208	−0.579	−0.473	−0.184	−0.604
E_{Lamb}	−15.001	−14.997	−13.499	−13.503	−30.029	−28.996	−28.996	−27.495	−27.467
E_{tot}	156.100	187.802	1306.155	1390.298	442.620	1552.525	1570.206	2714.155	2777.937
$Z=74$									
$E^{(0+1)}$	190.984	225.201	1667.727	1759.571	524.594	1957.472	1976.023	3447.154	3516.753
$E^{(2)}$	−0.285	−0.892	0.057	−1.450	−2.143	−0.929	−1.769	−0.964	−1.878
$B^{(2)}$	−0.418	−0.432	0.044	−0.218	−1.408	−0.653	−0.531	−0.182	−0.647
E_{Lamb}	−18.281	−18.278	−16.530	−16.532	−36.587	−35.378	−35.378	−33.627	−33.602
E_{tot}	171.999	205.598	1651.298	1741.371	484.456	1920.511	1938.346	3412.380	3480.627
$Z=79$									
$E^{(0+1)}$	217.861	254.255	2212.380	2312.153	591.597	2538.101	2556.556	4547.169	4622.744
$E^{(2)}$	−0.329	−0.951	0.091	−1.412	−2.296	−0.964	−1.807	−0.915	−1.810
$B^{(2)}$	−0.509	−0.524	0.073	−0.231	−1.699	−0.755	−0.608	−0.169	−0.693
E_{Lamb}	−23.100	−23.098	−21.067	−21.069	−46.222	−44.828	−44.828	−42.795	−42.774
E_{tot}	193.923	229.682	2191.477	2289.441	541.380	2491.555	2509.313	4503.290	4577.468
$Z=80$									
$E^{(0+1)}$	223.560	260.356	2338.083	2439.512	605.727	2671.355	2689.752	4800.814	4877.633
$E^{(2)}$	−0.339	−0.964	0.098	−1.405	−2.330	−0.971	−1.816	−0.904	−1.796
$B^{(2)}$	−0.529	−0.545	0.080	−0.233	−1.763	−0.776	−0.624	−0.165	−0.701
E_{Lamb}	−24.167	−24.165	−22.084	−22.086	−48.356	−46.932	−46.932	−44.849	−44.828
E_{tot}	198.524	234.683	2316.178	2415.788	553.279	2622.676	2640.380	4754.896	4830.308
$Z=83$									
$E^{(0+1)}$	241.511	279.446	2753.611	2860.154	650.022	3110.455	3128.598	5638.813	5719.464
$E^{(2)}$	−0.373	−1.005	0.121	−1.382	−2.441	−0.996	−1.843	−0.871	−1.752
$B^{(2)}$	−0.595	−0.610	0.104	−0.238	−1.970	−0.842	−0.673	−0.147	−0.722
E_{Lamb}	−27.590	−27.589	−25.378	−25.379	−55.200	−53.710	−53.710	−51.497	−51.478
E_{tot}	212.953	250.242	2728.459	2833.154	590.411	3054.907	3072.373	5586.298	5665.512
$Z=90$									
$E^{(0+1)}$	286.289	326.388	3985.255	4104.672	760.474	4400.249	4417.300	8119.826	8210.027
$E^{(2)}$	−0.475	−1.123	0.186	−1.326	−2.764	−1.067	−1.918	−0.780	−1.637
$B^{(2)}$	−0.781	−0.794	0.180	−0.239	−2.548	−1.009	−0.795	−0.076	−0.747
E_{Lamb}	−36.961	−36.960	−34.746	−34.747	−73.939	−72.610	−72.610	−70.395	−70.378
E_{tot}	248.072	287.511	3950.874	4068.360	681.22	4325.564	4341.978	8048.575	8137.265
E_{expt} [4]				4068.47					
δE				0.11					
$Z=92$									
$E^{(0+1)}$	299.640	340.204	4417.669	4541.032	793.550	4849.872	4866.473	8990.196	9083.288
$E^{(2)}$	−0.511	−1.165	0.207	−1.308	−2.877	−1.091	−1.943	−0.750	−1.599
$B^{(2)}$	−0.845	−0.856	0.208	−0.236	−2.744	−1.060	−0.831	−0.046	−0.746
E_{Lamb}	−40.007	−40.006	−37.886	−37.887	−80.030	−78.847	−78.847	−76.726	−76.710
E_{tot}	258.276	298.177	4380.198	4501.602	707.899	4768.873	4784.852	8912.674	9004.232
E_{expt} [4]				4501.72					
δE				−0.12					
$Z=100$									
$E^{(0+1)}$	352.776	394.270	6612.724	6753.248	927.688	7113.313	7127.444	13405.319	13510.744
$E^{(2)}$	−0.706	−1.378	0.315	−1.225	−3.466	−1.212	−2.066	−0.603	−1.421
$B^{(2)}$	−1.164	−1.162	0.360	−0.196	−3.709	−1.278	−0.981	0.139	−0.687
E_{Lamb}	−54.010	−54.010	−53.141	−53.141	−108.034	−108.360	−108.360	−107.491	−107.478
E_{tot}	296.896	337.719	6560.257	6698.686	812.479	7002.462	7016.036	13297.364	13401.158

TABLE V. Comparison of the present calculations with the many-body calculations of Ref. [36]

	$Z=26$		$Z=42$	
	$^3P_1$-$^1S_0$	$^1P_1$-$^1S_0$	$^3P_1$-$^1S_0$	$^1P_1$-$^1S_0$
Present	379102	752015	725814	2004151
Ref. [36]	379118	752459	725751	2004464
Expt.	379130 [a]	752502 [a]	725758(158) [b]	2003847(1200) [b]

[a]Reference [18].
[b]Reference [23].

present calculation are lower than those from Ref. [36] by 98 and 526 cm^{-1}, respectively. Similarly, for the $2\,^1S_0$ state, we find that the energy from the present calculation is smaller than that from Ref. [36] by 55 cm^{-1}, leading to differences of about 43 and 471 cm^{-1} for the $2\,^1P_1$- $2\,^1S_0$ and $2\,^3P_1$-$2\,^1S_0$ intervals, respectively, before consideration of the QED corrections. In [36], ''screening corrections'' to the Coulomb-field QED energy shifts [41] are taken from Ref. [42], while in the present work, QED corrections are evaluated using the methods described in Ref. [40]. In both calculations, ''correlation corrections'' to the Lamb shift are taken into account using the occupation numbers for single-particle orbitals predicted from eigenvectors of $H_{\rm eff}$. Although the treatment of QED in the two calculations differs, the numerical values of the QED corrections found here are in fairly good agreement with those found in Ref. [36]. Specifically, for $Z=26$, the combined ''screening'' and ''correlation'' corrections to the Lamb shift for the $2\,^1P_1$-$2\,^1S_0$ and $2\,^3P_1$-$2\,^1S_0$ intervals found in [36] are less than the corresponding values found here by 26 cm^{-1}. Combining the correlation and QED differences, we obtain the total differences $43-26=17$ and $471-26=445$ cm^{-1}, in close agreement with the differences 16 and 444 cm^{-1} for the $2\,^1P_1$-$2\,^1S_0$ and $2\,^3P_1$-$2\,^1S_0$ intervals in Table V. The corresponding differences for the $Z=42$ case in Table V are distributed in a similar way between correlation and QED corrections.

It is also informative to compare the results of the present calculations with the high-precision calculations of Refs. [29,30] for $Z=4$–14. The accuracy of the present calculations for these low-Z ions is limited by the approximate treatment of correlation. The theoretical error for triplet states decreases rapidly from about 800 cm^{-1} for $Z=5$ to about 50 cm^{-1} for $Z=14$. As mentioned previously, the theoretical error for low Z is dominated by the omitted higher-order correlation corrections, which decrease as $1/Z$ of the second-order correlation energy. By contrast, the calculations of Ref. [29] for neutral beryllium predict levels to an accuracy of about 1 cm^{-1}, while Ref. [30] gives energies accurate to a few cm^{-1} for $Z=5$–14. Although the precision of the present calculations is lower, the fine structure separation of the $(2s2p)^3P_J$ levels, predicted in the present calculation, is found to be in good agreement with the predictions of [30] and with experiment, as shown in Table VI.

In summary, we have presented a systematic second-order MBPT study of the $n=2$ states of berylliumlike ions. These calculations are found to differ from existing experimental data for intermediate Z at the level of 50 cm^{-1} for triplet states and 500 cm^{-1} for singlet states. They provide a smooth theoretical reference database for line identification. Moreover, matrix elements from the present calculations provide basic theoretical input for calculations of energies of three-electron boronlike ions.

TABLE VI. Comparison of the $(2s2p)^3P_J$ intervals with the ''full core plus correlation'' calculations of Ref. [30]. See Table IV for references to experimental data.

	$^3P_2$-$^3P_1$	$^3P_2$-$^3P_0$
$Z=5$		
Ref. [30]	16.1	22.2
Present	16.5	23.5
Expt.	16.4	22.8
$Z=6$		
Ref. [30]	56.22	79.72
Present	57.0	81.7
Expt.	56.36	80.05
$Z=7$		
Ref. [30]	143.7	206.5
Present	145.0	209.1
Expt.	144.0	207.1
$Z=8$		
Ref. [30]	305.3	442.5
Present	307.6	445.8
Expt.	306	443
$Z=9$		
Ref. [30]	575.8	836.2
Present	578.0	840.4
Expt.	576	836
$Z=10$		
Ref. [30]	993	1446
Present	996	1450
Expt.	995	1449
$Z=12$		
Ref. [30]	2462	3586
Present	2466	3593
Expt.	2460	3587
$Z=14$		
Ref. [30]	5172	7507
Present	5177	7516
Expt.	5174	7516

ACKNOWLEDGMENTS

The work of M.S.S. and W.R.J. was supported in part by National Science Foundation Grant No. PHY-92-04089. U.I.S. acknowledges partial support from the University of Notre Dame, Department of Physics. The authors owe a debt of gratitude to J. Sapirstein for supplying values for the QED corrections in the HF case.

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