

Third-order many-body perturbation theory calculations for the beryllium and magnesium isoelectronic sequences

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Third-order relativistic many-body perturbation theory (MBPT) is applied to obtain energies of ions with two valence electrons in the no virtual-pair approximation (NVPA). A total of 302 third-order Goldstone diagrams are organized into 12 one-body and 23 two-body terms. Only third-order two-body terms and diagrams are presented in this paper, owing to the fact that the one-body terms are identical to the previously studied third-order terms in monovalent ions. Dominant classes of diagrams are identified. The model potential is the Dirac-Hartree-Fock potential V^{N-2} , and B -spline basis functions in a cavity of finite radius are employed in the numerical calculations. The Breit interaction is taken into account through the second order of perturbation theory, and the lowest-order Lamb shift is also evaluated. Sample calculations are performed for berylliumlike ions with $Z=4-7$, and for the magnesiumlike ion P IV. The third-order excitation energies are in excellent agreement with measurement with an accuracy at 0.2% level for the cases considered. Comparisons are made with second-order MBPT results, and with other calculations. The third-order energy correction is shown to be significant, improving the previous second-order calculations by an order of magnitude.

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I. INTRODUCTION

The development of relativistic many-body perturbation theory (MBPT) in recent decades has been motivated in part by the need for accurate theoretical amplitudes of parity non-conserving (PNC) transitions in heavy monovalent atoms such as cesium and francium. Applications of the theoretical methods developed to treat atomic PNC transitions include support of atomic clock development, tests of QED in precision spectroscopy of highly stripped ions, searches for time variation in the fine-structure constant, and provision of precise astrophysical data.

Although nonrelativistic studies [1–7] and relativistic HF calculations [8–10] for divalent atoms and ions have been done for many years, only recently have relativistic many-body calculations been reported. As examples, we note that all-order relativistic MBPT calculations for transitions in berylliumlike ions with $Z=26$ and 42 were carried out by Lindroth and Hvarfner [11], while large-scale configuration-interaction (CI) calculations for transitions in C III were performed by Chen *et al.* [12]. Relativistic many-body calculations for magnesiumlike ions include the CI calculations of

states in the $n=3$ complex by Chen and Cheng [13], and the combined CI-MBPT calculations of excitation energies in Mg I by Savukov and Johnson [14].

Second-order relativistic MBPT was applied to Be-like ions by Safronova *et al.* [15], and energies were found to be accurate at the 2% level. In this paper, we extend relativistic MBPT for divalent atoms and ions to third order. We give a detailed treatment of the two-body terms here; the one-body terms are identical to those for monovalent systems, and are discussed in detail by Blundell *et al.* [16]. The long-range goal of the present research is to extend the relativistic singles-doubles coupled-cluster (SDCC) formalism to atoms and ions with two valence electrons. The present calculations permit us to identify and evaluate those third-order terms missing from the SDCC expansion.

II. THEORETICAL METHOD

The model potential for our MBPT calculation is the Dirac-Hartree-Fock (DHF) potential V^{N-2} . The N -electron Hamiltonian is partitioned in the standard way into an unperturbed Hamiltonian H_0 and a perturbation $V(H=H_0+V)$:

$$H_0 = \sum_i \varepsilon_i a_i^\dagger a_i, \quad (1)$$

$$V = - \sum_{ij} u_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} v_{ijkl} a_i^\dagger a_j^\dagger a_l a_k, \quad (2)$$

where ε_i is the energy eigenvalue of the one-electron DHF equation, and $v_{ijkl}=g_{ijkl}+b_{ijkl}$ is the Coulomb-Breit matrix element

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$$v_{ijkl} = \int \int d\mathbf{r}_1 d\mathbf{r}_2 (1/r_{12} + b_{12}) \phi_i^\dagger(\mathbf{r}_1) \phi_j^\dagger(\mathbf{r}_2) \phi_k(\mathbf{r}_1) \phi_l(\mathbf{r}_2). \quad (3)$$

The Breit interaction is given by

$$b_{12} = -\frac{1}{2r_{12}} \left[\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 + \frac{(\boldsymbol{\alpha}_1 \cdot \mathbf{r}_{12})(\boldsymbol{\alpha}_2 \cdot \mathbf{r}_{12})}{r_{12}^2} \right]. \quad (4)$$

In the no virtual-pair approximation, the excitations are limited to positive-energy eigenstates of H [17–20].

The eigenstates of a divalent system having angular momentum (J, M) are described by the coupled states

$$|(vw)JM\rangle = \eta(vw) \sum_{m_v m_w} \langle j_v j_w, m_v m_w | JM \rangle a_v^\dagger a_w^\dagger |0\rangle, \quad (5)$$

where $|0\rangle$ represents the ground state of the ionic core, and $\eta(vw)$ is the normalization constant

$$\eta(vw) = \begin{cases} 1 & \text{for } v \neq w \\ 1/\sqrt{2} & \text{for } v = w \end{cases}. \quad (6)$$

Here v and w specify one-electron states with quantum numbers (n_v, l_v, j_v, m_v) and (n_w, l_w, j_w, m_w) . We also adopt the notation that states in parentheses are independent of magnetic quantum numbers. The model space P is defined by the set of total angular-momentum states (5); the model-space projection operator is

$$\mathbf{P} = \sum_{\substack{JM \\ (v \leq w)}} |(vw)JM\rangle \langle (vw)JM|. \quad (7)$$

The orthogonal-space operator \mathbf{Q} is simply $\mathbf{1} - \mathbf{P}$.

The wave operator Ω , which maps states in the model space onto exact eigenstates of the many-electron Hamiltonian, is found by solving the *generalized Bloch equation* [21]

$$[\Omega, H_0] \mathbf{P} = (V\Omega - \Omega \mathbf{P} V \Omega) \mathbf{P}. \quad (8)$$

The effective Hamiltonian is given in terms of the wave operator

$$H_{\text{eff}} = PH_0P + PV\Omega P. \quad (9)$$

Effective Hamiltonian

We find the configuration-weight vector by diagonalizing the first-order approximation to the effective Hamiltonian $H_{\text{eff}}^{(1)} = PH_0P + PVP$ using total angular-momentum eigenstates (5) as a basis. Higher-order energies are obtained by operating the effective Hamiltonian of the corresponding order on the configuration-weight vector. For simplicity, matrix elements of the effective Hamiltonian are given for the uncoupled states, $|vw\rangle \equiv a_v^\dagger a_w^\dagger |0\rangle$ and $|v'w'\rangle$. The multiplications of Clebsch-Gordan coefficients and the summations over magnetic quantum numbers are carried out during angular decomposition. To obtain explicit expressions for matrix elements, we make use of the Brueckner-Goldstone diagrammatic expansion given in Lindgren and Morrison [21].

In third order, each matrix element consists of 12 one-body and 23 two-body terms. They represent a total of 84 one-body and 218 two-body Goldstone diagrams. Only the two-body part of the third-order perturbation is discussed here as the one-body part and complete second-order results are already presented in Refs. [15] and [16]. We give the expression for the two-body Coulomb part of the third-order correction below:

$$Z = \sum_{abcd} \frac{g_{cdvw} g_{abcd} \tilde{g}_{w'v'ab}}{(\epsilon_{ab} - \epsilon_{v'w'}) (\epsilon_{cd} - \epsilon_{v'w'})},$$

$$S_1 = \sum_{abcm} \frac{g_{acmw} \tilde{g}_{mbac} \tilde{g}_{v'w'vb}}{(\epsilon_{bv} - \epsilon_{v'w'}) (\epsilon_{acv} - \epsilon_{mv'w'})} \times (1 + [v \leftrightarrow w, v' \leftrightarrow w']) + \text{c.c.},$$

$$S_2 = \sum_{abcm} \frac{\tilde{g}_{abwm} \tilde{g}_{mcbv} \tilde{g}_{v'w'ca}}{(\epsilon_{ac} - \epsilon_{v'w'}) (\epsilon_{abv} - \epsilon_{mv'w'})} \times (1 + [v \leftrightarrow w, v' \leftrightarrow w']) + \text{c.c.},$$

$$S_3 = \sum_{abcm} \frac{g_{abwm} \tilde{g}_{w'cab} \tilde{g}_{v'mvc}}{(\epsilon_{cv} - \epsilon_{mv'}) (\epsilon_{abv} - \epsilon_{mv'w'})} \times (1 - [v \leftrightarrow w]) (1 - [v' \leftrightarrow w']) + \text{c.c.},$$

$$S_4 = \sum_{abcm} \frac{\tilde{g}_{abwm} \tilde{g}_{v'cvb} \tilde{g}_{w'mac}}{(\epsilon_{ac} - \epsilon_{mv'}) (\epsilon_{abv} - \epsilon_{mv'w'})} \times (1 - [v \leftrightarrow w]) (1 - [v' \leftrightarrow w']),$$

$$D_1 = - \sum_{abmn} \frac{g_{abmn} \tilde{g}_{mnwb} \tilde{g}_{v'w'va}}{(\epsilon_{bw} - \epsilon_{mn}) (\epsilon_{av} - \epsilon_{v'w'})} \times (1 + [v \leftrightarrow w, v' \leftrightarrow w']) + \text{c.c.},$$

$$D_2 = \sum_{abmn} ' \frac{g_{abmn} g_{mnvw} \tilde{g}_{v'w'ab}}{(n_{abvw} - \epsilon_{mnv'})} \left[\frac{1}{(\epsilon_{vw} - \epsilon_{mn})} + \frac{1}{(\epsilon_{ab} - \epsilon_{v'w'})} \right] + \text{c.c.},$$

$$D_3 = - \sum_{abmn} ' \frac{\tilde{g}_{abmn} g_{w'nab} \tilde{g}_{v'mvw}}{(\epsilon_{abvw} - \epsilon_{mnv'})} \left[\frac{1}{(\epsilon_{ab} - \epsilon_{nw'})} + \frac{1}{(\epsilon_{vw} - \epsilon_{mv'})} \right] \times (1 + [v \leftrightarrow w, v' \leftrightarrow w']) + \text{c.c.},$$

$$D_4 = \sum_{abmn} \frac{\tilde{g}_{abmn} \tilde{g}_{w'nwb} \tilde{g}_{v'mva}}{(\epsilon_{bw} - \epsilon_{nw'}) (\epsilon_{av} - \epsilon_{mv'})} (1 - [v \leftrightarrow w]) + \text{c.c.},$$

$$D_5 = - \sum_{abmn} \frac{\tilde{g}_{w'amn} \tilde{g}_{nbaw} \tilde{g}_{v'mvb}}{(\epsilon_{avw} - \epsilon_{mnv'}) (\epsilon_{bv} - \epsilon_{mv'})} \times (1 - [v \leftrightarrow w]) (1 - [v' \leftrightarrow w']) + \text{c.c.},$$

$$\begin{aligned}
D_6 &= \sum_{abmn} \frac{\tilde{g}_{w'amn}\tilde{g}_{nbvw}\tilde{g}_{v'mab}}{(\varepsilon_{avw} - \varepsilon_{mnv'}) (\varepsilon_{ab} - \varepsilon_{mv'})} \\
&\quad \times (1 + [v \leftrightarrow w, v' \leftrightarrow w']) + \text{c.c.}, \\
D_7 &= - \sum_{abmn} \frac{\tilde{g}_{abmw}\tilde{g}_{w'mbn}\tilde{g}_{v'nva}}{(\varepsilon_{abv} - \varepsilon_{mv'w'}) (\varepsilon_{av} - \varepsilon_{nv'})} \\
&\quad \times (1 - [v \leftrightarrow w]) (1 - [v' \leftrightarrow w']) + \text{c.c.}, \\
D_8 &= \sum_{abmn} \frac{\tilde{g}_{w'bwn}\tilde{g}_{nabm}\tilde{g}_{v'mva}}{(\varepsilon_{bv} - \varepsilon_{nv'}) (\varepsilon_{av} - \varepsilon_{mv'})} \\
&\quad \times (1 - [v \leftrightarrow w]) (1 - [v' \leftrightarrow w']), \\
D_9 &= - \sum_{abmn} \frac{g_{abwm}\tilde{g}_{v'mvn}\tilde{g}_{w'nab}}{(\varepsilon_{abv} - \varepsilon_{mv'w'}) (\varepsilon_{ab} - \varepsilon_{nw'})} \\
&\quad \times (1 - [v \leftrightarrow w]) (1 - [v' \leftrightarrow w']), \\
D_{10} &= - \sum_{abmn} \frac{g_{w'bmn}\tilde{g}_{v'avb}\tilde{g}_{mnwa}}{(\varepsilon_{bv} - \varepsilon_{mnv'}) (\varepsilon_{av} - \varepsilon_{mn})} \\
&\quad \times (1 - [v \leftrightarrow w]) (1 - [v' \leftrightarrow w']), \\
T_1 &= \sum'_{amnr} \frac{g_{w'ann}\tilde{g}_{mnr}\tilde{g}_{v'rvw}}{(\varepsilon_{avw} - \varepsilon_{mnv'}) (\varepsilon_{vw} - \varepsilon_{rv'})} \\
&\quad \times (1 + [v \leftrightarrow w, v' \leftrightarrow w']) + \text{c.c.}, \\
T_2 &= \sum_{amnr} \frac{g_{w'ann}\tilde{g}_{mnwr}\tilde{g}_{v'rvw}}{(\varepsilon_{avw} - \varepsilon_{mnv'}) (\varepsilon_{av} - \varepsilon_{rv'})} \\
&\quad \times (1 - [v \leftrightarrow w]) (1 - [v' \leftrightarrow w']) + \text{c.c.}, \\
T_3 &= \sum'_{amnr} \frac{\tilde{g}_{w'avr}\tilde{g}_{v'rma}\tilde{g}_{mnvw}}{(\varepsilon_{avw} - \varepsilon_{nrv'}) (\varepsilon_{vw} - \varepsilon_{mn})} \\
&\quad \times (1 + [v \leftrightarrow w, v' \leftrightarrow w']) + \text{c.c.}, \\
T_4 &= \sum_{amnr} \frac{\tilde{g}_{w'avn}\tilde{g}_{v'num}\tilde{g}_{rmwa}}{(\varepsilon_{avw} - \varepsilon_{nrv'}) (\varepsilon_{av} - \varepsilon_{mr})} \\
&\quad \times (1 - [v \leftrightarrow w]) (1 - [v' \leftrightarrow w']), \\
Q &= \sum'_{mnr} \frac{g_{v'w'rs}g_{rsmn}\tilde{g}_{mnvw}}{(n_{vw} - \varepsilon_{rs}) (\varepsilon_{vw} - \varepsilon_{mn})}, \\
B_1 &= - \sum_{amnx} \frac{\tilde{g}_{w'amn}g_{n \max}\tilde{g}_{v'xvw}}{(\varepsilon_{avw} - \varepsilon_{mnv'}) (\varepsilon_{ax} - \varepsilon_{mn})} \\
&\quad \times (1 + [v \leftrightarrow w, v' \leftrightarrow w']),
\end{aligned}$$

$$\begin{aligned}
B_2 &= - \sum_{amxy} \frac{\tilde{g}_{v'axm}\tilde{g}_{w'mya}\tilde{g}_{xyvw}}{(\varepsilon_{avw} - \varepsilon_{mxw'}) (\varepsilon_{ay} - \varepsilon_{mw'})} \\
&\quad \times (1 + [v \leftrightarrow w, v' \leftrightarrow w']), \\
B_3 &= - \sum'_{mnxy} \frac{g_{v'w'mn}g_{mnxy}\tilde{g}_{xyvw}}{(n_{vw} - \varepsilon_{mn}) (\varepsilon_{xy} - \varepsilon_{mn})},
\end{aligned}$$

where g_{ijkl} is the Coulomb matrix element and $\tilde{g}_{ijkl} \equiv g_{ijkl} - g_{ijlk}$. The notation $\varepsilon_{ijkl} \equiv \varepsilon_i + \varepsilon_j + \varepsilon_k + \varepsilon_l$, etc., for the sum of one-electron energies has also been used. The third-order terms are arranged by the number of excited states in the sums over intermediate states. Zero, single, double, triple, quadruple excited-state terms are designated by the letters Z, S, D, T, Q . Terms associated with backwards (folded) diagrams are designated by B . Backwards diagrams are unique for open-shell systems and exist only in the third or higher order of MBPT. The summation indices (a, b, c, d) refer to core states, (m, n, r, s) refer to excited states and, in backwards diagrams, indices (x, y) refer to valence states. The states x and y are restricted to the model space. In the above equations, the notation $(1 + [v \leftrightarrow w])$ indicates that the formula to the left of the parentheses is to be evaluated twice, first as indicated in the formula, then with v and w interchanged. The resulting two terms are to be added. The notation $[v \leftrightarrow w, v' \leftrightarrow w']$ indicates that v is to be replaced by w and v' by w' . Finally, the notation $(1 - [v \leftrightarrow w]) (1 - [v' \leftrightarrow w'])$ is interpreted as $(1 - [v \leftrightarrow w]) - [v' \leftrightarrow w'] + [v \leftrightarrow w, v' \leftrightarrow w']$. The primes above the summation signs indicate many-body excited states belonging to the orthogonal space \mathcal{Q} —that is, summations over m, n, r, s are restricted in such a way that one never obtains an energy factor $(\varepsilon_{vw} - \varepsilon_{v'w'})$ in the denominator corresponding solely to a rearrangement among valence states. This restriction applies only to the term with the denominator factor $(\varepsilon_{vw} - \varepsilon_{mn})$ in D_2 , and to the term with the denominator factor $(\varepsilon_{vw} - \varepsilon_{mv'})$ in D_3 . The c.c. denotes complex conjugate. The conjugate diagrams are obtained by a reflection through a horizontal axis, with the initial and final states switched ($vw \leftrightarrow v'w'$). Direct diagrams of the two-body terms are shown in Fig. 1. Technically, there are subtle changes in energy denominators in going from the term presented to its c.c. counterpart. These changes can be deduced by redrawing the diagram upside down, and reading off the new denominators.

In D_1 and D_4 (but not in D_2 and D_3), we have combined diagrams associated with double excitations that have the same numerators, but different denominators, using the formula

$$\frac{1}{(A+B)A} + \frac{1}{(A+B)B} = \frac{1}{AB}. \quad (10)$$

Diagrams D_1 – D_4 are special in the sense that two orderings are possible. The ambiguous vertices are labeled by crosses in the diagrams. Many of the third-order terms in the two-body part have external exchanges and complex conjugates, so each diagram illustrated in Fig. 1 has from one to eight variants. The largest fraction of computer time is spent on

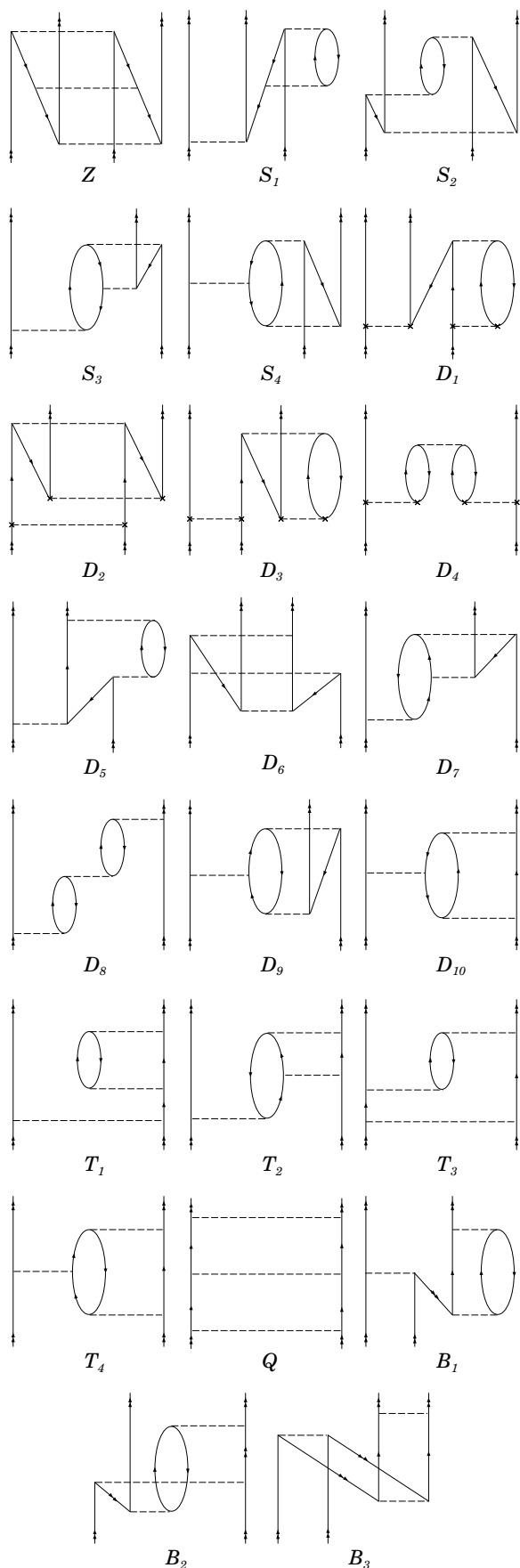


FIG. 1. Third-order Goldstone diagrams (two-body part).

TABLE I. Comparisons of third-order energies (cm^{-1}) of the triplet $(2s2p)^3P$ states of Be-like ions $Z=4-7$ with measurements are given, illustrating the rapid $(1/Z^2)$ decrease of the residual correlation corrections with increasing Z . A breakdown of contributions to the energy from Coulomb and Breit correlation corrections and the Lamb shift is given.

Z	4	5	6	7
$(2s2p)^3P_0$				
$E^{(0+1)}$	23607.9	39116.7	54204.5	69072.2
$E^{(2)}$	-3114.3	-2583.2	-2344.0	-2201.5
$B^{(2)}$	-1.7	-3.7	-6.7	-10.5
$E^{(3)}$	473.5	598.0	412.9	294.9
E_{Lamb}	-0.9	-3.3	-8.4	-17.7
E_{tot}	20964.6	37124.4	52258.4	67137.3
E_{expt}	21978.3	37336.7	52367.1	67209.2
ΔE	-1014	-212	-109	-72
$(2s2p)^3P_1$				
$E^{(0+1)}$	23607.4	39120.2	54223.4	69127.7
$E^{(2)}$	-3113.9	-2582.2	-2342.2	-2198.6
$B^{(2)}$	-0.6	-1.7	-3.3	-5.6
$E^{(3)}$	473.4	597.8	412.7	294.7
E_{Lamb}	-0.9	-3.2	-8.3	-17.5
E_{tot}	20965.5	37130.9	52282.3	67200.7
E_{expt}	21978.9	37342.4	52390.8	67272.3
ΔE	-1013	-212	-109	-72
$(2s2p)^3P_2$				
$E^{(0+1)}$	23608.2	39132.6	54272.9	69260.8
$E^{(2)}$	-3113.0	-2580.1	-2338.4	-2192.6
$B^{(2)}$	0.4	0.5	0.4	0.0
$E^{(3)}$	473.2	597.4	412.3	294.1
E_{Lamb}	-0.8	-3.2	-8.2	-17.1
E_{tot}	20968.0	37147.3	52339.1	67345.2
E_{expt}	21981.3	37358.3	52447.1	67416.3
ΔE	-1013	-211	-108	-71

evaluating the term Q , and most of the remainder is spent on repetitive evaluation of terms D_k , T_k and their variants. Angular decompositions of the direct terms are listed in the Appendix.

III. APPLICATION AND DISCUSSION

As a first illustration, we apply the theory described above to obtain energies of the ground state and excited states in the $n=2$ complex for Be-like ions. In Table I, we give a detailed breakdown of the contributions from first-, second-, and third-order perturbation theory, together with corrections from the Breit interaction and the Lamb shift, for excitation energies of $(2s2p)^3P_{0,1,2}$ states of Be-like ions. The experimental energies are taken from the NIST database for atomic spectroscopy [22]. Energies $E^{(0+1)}$ represent the lowest-order energies, including the Breit correction. Lowest-order Lamb shifts E_{Lamb} are obtained following the method described in

TABLE II. Third-order energies (cm^{-1}) of states in the $n=2$ complex of the Be-like ion N IV, including corrections for the Breit interaction and the Lamb shift.

	$^3P_0^o$	$^3P_1^o$	$^3P_2^o$	$^1P_1^o$	$^3P_0^e$	$^3P_1^e$	$^3P_2^e$	$^1D_2^e$	$^1S_0^e$
E_{tot}	67137.3	67200.7	67345.2	130764.1	175499.4	175572.8	175699.0	188899.9	235421.9
E_{expt}	67209.2	67272.3	67416.3	130693.9	175535.4	175608.1	175732.9	188882.5	235369.3
ΔE	-72	-72	-71	70	-36	-35	-34	17	53

Ref. [23]. We find that the residual differences between calculated and measured energies ΔE decrease rapidly with increasing Z . This is expected since MBPT converges better for charged ions than for neutral atoms. In fact, for highly charged ions, correlations are expected to decrease approximately as Z^{2-n} , where n is the order of perturbation theory [24]. On the other hand, QED effects (Lamb shifts) become more important along an isoelectronic sequence. The results in Table I confirm both of these trends. Theoretical excitation energies of all levels in the $n=2$ complex for Be-like N (N IV) are presented in Table II, and are seen to be in agreement with measurement to parts in 10^4 .

As a more involved example, we give a complete breakdown of contributions to energies of low-lying states in the $n=3$ complex for the Mg-like ion P IV in Table III. For both N IV and P IV, correlations are seen to account for about 5% of the total energies. For Be-like ions, the third-order correlation energies are only 15–20 % of those of the second order, which in turn are an order of magnitude smaller than the corresponding DHF energies. The Breit correction $B^{(2)}$, which is obtained by linearizing the second-order matrix elements in Breit interaction, is also small for such lightly charged ions.

Our calculations for Be-like ions are able to produce results accurate to order of ten cm^{-1} . This shows that the third-order energy correction is very important for divalent ions. By comparison, the second-order excitation energies of Saffronova *et al.* [15] for N IV agree with measurement at the level of a few hundred cm^{-1} . It should be noted that results from the CI+MBPT method [14] mentioned in the Introduction are consistently more accurate than the present third-order results. However, the CI+MBPT approach contains a free parameter in the energy denominators that is adjusted to give optimized energies. In contrast, our MBPT calculation is completely *ab initio*. For the C III ion, the large-scale CI calculations of Chen *et al.* [12] mentioned in the Introduction also give transition energies accurate to better than a hundred cm^{-1} on average. Those large-scale CI calculations are also *ab initio*, and have about the same accuracy as the present calculations for states in C III.

For the P IV ion, our results are in good agreement with experiment, the average discrepancy being several hundred cm^{-1} . Chaudhuri *et al.* [25] employed an *effective valence shell Hamiltonian* to calculate energies of Mg-like ions and obtained results for P IV having a discrepancy of about a thousand cm^{-1} , which is somewhat larger, but comparable to the accuracy of the third-order calculations.

It is worthwhile to analyze the results in terms of diagrams. The relative contributions of the third-order two-body terms for the ground-state energy of a typical member in the

Be sequence and the ion P IV are summarized in Tables IV and V. Dominant classes of diagrams are Q and B_3 . This is understandable since Q are quadruple excited-state diagrams and involve no core excitations. This class of diagrams is entirely due to valence-valence correlation effects; they are expected to be large because of the strong repulsion of the outer valence electrons. Class B_3 are backwards diagrams, which are characteristic of open-shell systems. As shown in Fig. 1, this class is also associated solely with

TABLE III. Comparison with measurement of theoretical energies (cm^{-1}) of some of the low-lying states in the $n=3$ complex of the Mg-like ion P IV, including a breakdown of contributions from Coulomb and Breit correlation corrections and the Lamb shift.

	$(3s3p)^3P_0$	$(3s3p)^3P_1$	$(3s3p)^3P_2$
$E^{(0+1)}$	67021.3	67242.9	67696.5
$E^{(2)}$	110.3	116.0	130.1
$B^{(2)}$	-0.9	0.3	1.3
$E^{(3)}$	807.4	807.6	807.6
E_{Lamb}	-21.1	-20.9	-20.5
E_{tot}	67917.1	68146.0	68615.0
E_{expt}	67918.0	68146.5	68615.2
ΔE	-0.9	-0.5	-0.2
	$(3s3p)^1P_1$	$(3p^2)^1D_2$	$(3p^2)^3P_0$
$E^{(0+1)}$	120479.5	180554.7	165971.6
$E^{(2)}$	-20906.0	-61699.8	-2027.7
$B^{(2)}$	-15.8	-8.4	-5.2
$E^{(3)}$	6470.7	48769.6	1089.6
E_{Lamb}	-20.7	-43.6	-44.0
E_{tot}	106007.7	167572.4	164984.3
E_{expt}	105190.4	166144.0	164941.4
ΔE	817	1428	43
	$(3p^2)^3P_1$	$(3p^2)^3P_2$	$(3p^2)^1S_0$
$E^{(0+1)}$	166200.8	166633.3	212201.4
$E^{(2)}$	-2013.9	-2008.1	-23060.7
$B^{(2)}$	-4.8	-2.7	-24.6
$E^{(3)}$	1087.9	1077.3	5810.7
E_{Lamb}	-43.8	-43.4	-41.3
E_{tot}	165226.1	165656.5	194885.6
E_{expt}	165185.4	165654.0	194591.8
ΔE	41	3	294

TABLE IV. Relative contributions of third-order two-body terms for C III.

Term	(%)	Term	(%)	Term	(%)	Term	(%)	Term	(%)
Z	0.1	D_1	-0.2	D_6	0.0	T_1	4.2	B_1	-0.8
S_1	0.1	D_2	0.4	D_7	0.0	T_2	-0.3	B_2	-0.1
S_2	-0.4	D_3	-1.6	D_8	0.3	T_3	-0.5	B_3	-46.1
S_3	-0.1	D_4	0.1	D_9	-0.1	T_4	2.0		
S_4	0.4	D_5	0.2	D_{10}	-1.0	Q	41.2		

valence-valence correlation. The two classes Q and B_3 tend to cancel each other as there is an extra phase of -1 associated with backwards diagrams. It is interesting to note that even after subtraction of the contributions from Q and B_3 , their difference is still larger than the contribution from any other class of diagrams for C III.

IV. CONCLUSION

The accuracy of our third-order calculations is at 0.2% level for weakly charged ions of both Be and Mg isoelectronic sequences. This level of accuracy is comparable or superior to the two *ab initio* methods mentioned in Sec. III. A complete third-order calculation is important to understand the relative importance of different contributions to energies of divalent systems. The folded diagrams as well as the quadruple excited-state diagrams are significant. The dominant role of these two classes of diagrams is attributed to the strong correlation of the two valence electrons. This conclusion is useful for workers developing mixed CI-MBPT methods which include dominant third-order diagrams. It is also helpful for researchers setting up SDCC calculations as they try to classify and account for the contributions from the third-order diagrams associated with omitted triple excitations. Although one might expect a complete fourth-order calculation for divalent systems to improve the accuracy of the present calculations still further, it is unlikely that such a complex calculation will be carried out in the near future.

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TABLE V. Relative contributions of third-order two-body terms for P IV.

Term	(%)	Term	(%)	Term	(%)	Term	(%)	Term	(%)
Z	0.1	D_1	-0.4	D_6	-0.1	T_1	9.4	B_1	-3.9
S_1	0.4	D_2	0.3	D_7	-0.3	T_2	0.1	B_2	-0.7
S_2	-0.3	D_3	-3.6	D_8	0.1	T_3	2.1	B_3	-29.2
S_3	0.2	D_4	0.6	D_9	-0.5	T_4	10.2		
S_4	1.4	D_5	-1.1	D_{10}	-5.0	Q	29.9		

APPENDIX

Angular decompositions of direct terms for the third-order two-body Coulomb part are presented:

$$\begin{aligned}
Z &= \sum_{L_1 L_2 L_3} \frac{X_{L_1}(cdwv)X_{L_2}(abcd)Z_{L_3}(w'v'ab)}{(\varepsilon_{ab} - \varepsilon_{v'w'}) (\varepsilon_{cd} - \varepsilon_{v'w'})} \\
&\quad \times (-1)^{J+L_1+L_2+L_3+j_a+j_b+j_c+j_d+j_{w'}+j_v} \\
&\quad \times \left\{ \begin{matrix} J & j_c & j_d \\ L_1 & j_v & j_w \end{matrix} \right\} \left\{ \begin{matrix} j_a & j_b & J \\ j_d & j_c & L_2 \end{matrix} \right\} \left\{ \begin{matrix} J & j_a & j_b \\ L_3 & j_{v'} & j_{w'} \end{matrix} \right\}, \\
S_1 &= \frac{1}{[w]} \sum_{LL'} \frac{X_L(acmw)Z_L(mbac)Z_{L'}(v'w'vb)}{(\varepsilon_{bv} - \varepsilon_{v'w'}) (\varepsilon_{acv} - \varepsilon_{mv'w'})} \\
&\quad \times (-1)^{J+L'+j_a+j_b+j_c+j_m+j_{w'}+j_v} \delta_{j_b j_w} \frac{1}{[L]} \left\{ \begin{matrix} J & j_{v'} & j_{w'} \\ L' & j_b & j_v \end{matrix} \right\}, \\
S_2 &= \sum_{LL'} \frac{Z_L(abwm)Z_L(mcbv)Z_{L'}(v'w'ca)}{(\varepsilon_{ac} - \varepsilon_{v'w'}) (\varepsilon_{abv} - \varepsilon_{mv'w'})} \\
&\quad \times (-1)^{1+L'+j_a+j_b+j_c+j_m+j_{w'}+j_v} \frac{1}{[L]} \left\{ \begin{matrix} J & j_a & j_c \\ L & j_v & j_w \end{matrix} \right\} \\
&\quad \times \left\{ \begin{matrix} J & j_c & j_a \\ L' & j_{w'} & j_{v'} \end{matrix} \right\},
\end{aligned}$$

$$\begin{aligned}
 S_3 &= \sum_{\substack{L_1 L_2 L_3 \\ abcm}} \frac{X_{L_1}(abwm)Z_{L_2}(w'cab)Z_{L_3}(v'mvc)}{(\epsilon_{cv} - \epsilon_{mv'}) (\epsilon_{abv} - \epsilon_{mv'w'})} \\
 &\quad \times (-1)^{J+j_v+j_w} \begin{Bmatrix} L_1 & L_2 & L_3 \\ j_c & j_m & j_b \end{Bmatrix} \\
 &\quad \times \begin{Bmatrix} j_w & j_{w'} & L_3 \\ L_2 & L_1 & j_a \end{Bmatrix} \begin{Bmatrix} J & j_{v'} & j_{w'} \\ L_3 & j_w & j_v \end{Bmatrix}, \\
 S_4 &= \sum_{\substack{L_1 L_2 L_3 \\ abcm}} \frac{Z_{L_1}(abwm)Z_{L_2}(v'cvb)Z_{L_3}(w'mac)}{(\epsilon_{ac} - \epsilon_{mw'}) (\epsilon_{abv} - \epsilon_{mv'w'})} \\
 &\quad \times (-1)^{J+L_1+L_2+L_3+j_v+j_w} \begin{Bmatrix} J & j_{v'} & j_{w'} \\ L_2 & j_w & j_v \end{Bmatrix} \\
 &\quad \times \begin{Bmatrix} j_w & j_{w'} & L_2 \\ L_3 & L_1 & j_a \end{Bmatrix} \begin{Bmatrix} L_1 & L_2 & L_3 \\ j_c & j_m & j_b \end{Bmatrix}, \\
 D_1 &= -\frac{1}{[w]} \sum_{\substack{LL' \\ abmn}} \frac{X_L(abmn)Z_L(mnwb)Z_{L'}(v'w'va)}{(\epsilon_{bw} - \epsilon_{mn}) (\epsilon_{av} - \epsilon_{v'w'})} \\
 &\quad \times (-1)^{J+L'+j_a+j_b+j_m+j_n+j_{w'}+j_v} \\
 &\quad \times \delta_{j_a j_w} \frac{1}{[L]} \begin{Bmatrix} J & j_{v'} & j_{w'} \\ L' & j_a & j_v \end{Bmatrix}, \\
 D_2 &= \sum_{\substack{L_1 L_2 L_3 \\ abmn}} \frac{X_{L_1}(abmn)X_{L_2}(mnvw)Z_{L_3}(v'w'ab)}{(\epsilon_{abvw} - \epsilon_{mnv'w'})} \\
 &\quad \times \left[\frac{1}{(\epsilon_{vw} - \epsilon_{mn})} + \frac{1}{(\epsilon_{ab} - \epsilon_{v'w'})} \right] \\
 &\quad \times (-1)^{J+L_1+L_2+L_3+j_a+j_b+j_m+j_n+j_{w'}+j_v} \\
 &\quad \times \begin{Bmatrix} j_a & j_b & J \\ j_n & j_m & L_1 \end{Bmatrix} \begin{Bmatrix} J & j_m & j_n \\ L_2 & j_w & j_v \end{Bmatrix} \begin{Bmatrix} J & j_a & j_b \\ L_3 & j_{w'} & j_{v'} \end{Bmatrix}, \\
 D_3 &= -\frac{1}{[w']} \sum_{\substack{LL' \\ abmn}} \frac{Z_L(abmn)X_L(w'nab)Z_{L'}(v'mvw)}{(\epsilon_{abvw} - \epsilon_{mnv'w'})} \\
 &\quad \times \left[\frac{1}{(\epsilon_{ab} - \epsilon_{nw'})} + \frac{1}{(\epsilon_{vw} - \epsilon_{mv'})} \right] \\
 &\quad \times (-1)^{J+L'+j_a+j_b+j_m+j_n+j_{w'}+j_v} \\
 &\quad \times \delta_{j_m j_w} \frac{1}{[L]} \begin{Bmatrix} J & j_{v'} & j_m \\ L' & j_w & j_v \end{Bmatrix},
 \end{aligned}$$

$$\begin{aligned}
 D_4 &= \sum_L \frac{Z_L(abmn)Z_L(w'nwb)Z_L(v'mva)}{(\epsilon_{bw} - \epsilon_{nw'}) (\epsilon_{av} - \epsilon_{mv'})} \\
 &\quad \times (-1)^{J+L+j_a+j_b+j_m+j_n+j_{w'}+j_v} \\
 &\quad \times \frac{1}{[L]^2} \begin{Bmatrix} J & j_{w'} & j_{v'} \\ L & j_v & j_w \end{Bmatrix}, \\
 D_5 &= -\sum_{\substack{LL' \\ abmn}} \frac{Z_L(w'amn)Z_L(nbaw)Z_{L'}(v'mvb)}{(\epsilon_{avw} - \epsilon_{mnv'}) (\epsilon_{bv} - \epsilon_{mv'})} \\
 &\quad \times (-1)^{J+1+L+j_a+j_b+j_m+j_n+j_{w'}+j_v} \\
 &\quad \times \frac{1}{[L]} \begin{Bmatrix} J & j_{v'} & j_{w'} \\ L' & j_w & j_v \end{Bmatrix} \begin{Bmatrix} j_{w'} & j_w & L' \\ j_b & j_m & L \end{Bmatrix}, \\
 D_6 &= \sum_{\substack{L_1 L_2 L_3 \\ abmn}} \frac{Z_{L_1}(w'amn)Z_{L_2}(nbvw)Z_{L_3}(v'mab)}{(\epsilon_{avw} - \epsilon_{mnv'}) (\epsilon_{ab} - \epsilon_{mv'})} \\
 &\quad \times (-1)^{1+L_1+L_2+L_3+j_v+j_w} \\
 &\quad \times \begin{Bmatrix} J & j_n & j_b \\ L_2 & j_w & j_v \end{Bmatrix} \begin{Bmatrix} J & j_n & j_b \\ j_{w'} & L_1 & j_m \\ j_{v'} & j_a & L_3 \end{Bmatrix}, \\
 D_7 &= -\sum_{\substack{L_1 L_2 L_3 \\ abmn}} \frac{Z_{L_1}(abmw)Z_{L_2}(w'mbn)Z_{L_3}(v'nva)}{(\epsilon_{abv} - \epsilon_{mv'w'}) (\epsilon_{av} - \epsilon_{nv'})} \\
 &\quad \times (-1)^{J+L_1+L_2+L_3+j_v+j_w} \begin{Bmatrix} L_1 & L_2 & L_3 \\ j_n & j_a & j_m \end{Bmatrix} \\
 &\quad \times \begin{Bmatrix} j_w & j_{w'} & L_3 \\ L_2 & L_1 & j_b \end{Bmatrix} \begin{Bmatrix} J & j_{v'} & j_{w'} \\ L_3 & j_w & j_v \end{Bmatrix}, \\
 D_8 &= \sum_L \frac{Z_L(w'bwn)Z_L(nabm)Z_L(v'mva)}{(\epsilon_{bv} - \epsilon_{nv'}) (\epsilon_{av} - \epsilon_{mv'})} \\
 &\quad \times (-1)^{J+L+j_a+j_b+j_m+j_n+j_{w'}+j_v} \\
 &\quad \times \frac{1}{[L]^2} \begin{Bmatrix} J & j_{w'} & j_{v'} \\ L & j_v & j_w \end{Bmatrix}, \\
 D_9 &= -\sum_{\substack{L_1 L_2 L_3 \\ abmn}} \frac{X_{L_1}(abwm)Z_{L_2}(v'mvn)Z_{L_3}(w'nab)}{(\epsilon_{abv} - \epsilon_{mv'w'}) (\epsilon_{ab} - \epsilon_{nw'})} \\
 &\quad \times (-1)^{J+j_v+j_w} \begin{Bmatrix} L_1 & L_2 & L_3 \\ j_n & j_b & j_m \end{Bmatrix} \\
 &\quad \times \begin{Bmatrix} j_w & j_{w'} & L_2 \\ L_3 & L_1 & j_a \end{Bmatrix} \begin{Bmatrix} J & j_{v'} & j_{w'} \\ L_2 & j_w & j_v \end{Bmatrix},
 \end{aligned}$$

$$\begin{aligned}
D_{10} = & - \sum_{\substack{L_1 L_2 L_3 \\ abmn}} \frac{X_{L_1}(w' bmn) Z_{L_2}(v' avb) Z_{L_3}(mnwa)}{(\varepsilon_{bv'w} - \varepsilon_{mnv'}) (\varepsilon_{aw} - \varepsilon_{mn})} \\
& \times (-1)^{J+j_v+j_w} \begin{Bmatrix} L_1 & L_2 & L_3 \\ j_a & j_n & j_b \end{Bmatrix} \\
& \times \begin{Bmatrix} j_{w'} & j_w & L_2 \\ L_3 & L_1 & j_m \end{Bmatrix} \begin{Bmatrix} J & j_{v'} & j_{w'} \\ L_2 & j_w & j_v \end{Bmatrix}, \\
T_1 = & \frac{1}{[w']} \sum_{LL'}' \frac{X_L(w' ann) Z_L(mnar) Z_{L'}(v' rvw)}{(\varepsilon_{avw} - \varepsilon_{mnv'}) (\varepsilon_{vw} - \varepsilon_{rv'})} \\
& \times (-1)^{J+1+L'+j_a+j_m+j_n+j_v} \times \delta_{j_j j_{w'}} \frac{1}{[L]} \begin{Bmatrix} J & j_{v'} & j_{w'} \\ L' & j_w & j_v \end{Bmatrix}, \\
T_2 = & \sum_{\substack{L_1 L_2 L_3 \\ amnr}} \frac{X_{L_1}(w' amn) Z_{L_2}(mnwr) Z_{L_3}(v' rva)}{(\varepsilon_{avw} - \varepsilon_{mnv'}) (\varepsilon_{aw} - \varepsilon_{rv'})} \\
& \times (-1)^{J+j_v+j_w} \begin{Bmatrix} L_1 & L_2 & L_3 \\ j_r & j_a & j_n \end{Bmatrix} \\
& \times \begin{Bmatrix} j_{w'} & j_w & L_3 \\ L_2 & L_1 & j_m \end{Bmatrix} \begin{Bmatrix} J & j_{v'} & j_{w'} \\ L_3 & j_w & j_v \end{Bmatrix}, \\
T_3 = & \sum_{LL'}' \frac{Z_L(w' anr) Z_L(v' rma) Z_{L'}(mnvw)}{(\varepsilon_{avw} - \varepsilon_{nrv'}) (\varepsilon_{vw} - \varepsilon_{mn})} \\
& \times (-1)^{1+L'+j_a+j_m+j_n+j_r+j_{w'}+j_v} \\
& \times \frac{1}{[L]} \begin{Bmatrix} J & j_n & j_m \\ L & j_{v'} & j_{w'} \end{Bmatrix} \begin{Bmatrix} J & j_m & j_n \\ L' & j_w & j_v \end{Bmatrix}, \\
T_4 = & \sum_{\substack{L_1 L_2 L_3 \\ amnr}} \frac{Z_{L_1}(w' arn) Z_{L_2}(v' nv'm) Z_{L_3}(rmwa)}{(\varepsilon_{avw} - \varepsilon_{nrv'}) (\varepsilon_{aw} - \varepsilon_{mr})} \\
& \times (-1)^{J+L_1+L_2+L_3+j_v+j_w} \begin{Bmatrix} L_1 & L_2 & L_3 \\ j_m & j_a & j_n \end{Bmatrix} \\
& \times \begin{Bmatrix} j_{w'} & j_w & L_2 \\ L_3 & L_1 & j_r \end{Bmatrix} \begin{Bmatrix} J & j_{v'} & j_{w'} \\ L_2 & j_w & j_v \end{Bmatrix}, \\
Q = & \sum_{\substack{L_1 L_2 L_3 \\ mnrs}} \frac{X_{L_1}(v' w' rs) X_{L_2}(rsmn) Z_{L_3}(mnvw)}{(\varepsilon_{vw} - \varepsilon_{rs}) (\varepsilon_{vw} - \varepsilon_{mn})} \\
& \times (-1)^{J+L_1+L_2+L_3+j_m+j_n+j_r+j_s+j_{w'}+j_v} \\
& \times \begin{Bmatrix} J & j_r & j_s \\ L_1 & j_{w'} & j_{v'} \end{Bmatrix} \begin{Bmatrix} j_r & j_s & J \\ j_n & j_m & L_2 \end{Bmatrix} \begin{Bmatrix} J & j_m & j_n \\ L_3 & j_w & j_v \end{Bmatrix},
\end{aligned}$$

$$\begin{aligned}
B_1 = & - \frac{1}{[w']} \sum_{\substack{LL' \\ amnx}} \frac{Z_L(w' amn) X_L(n \max) Z_{L'}(v' xvw)}{(\varepsilon_{avw} - \varepsilon_{mnv'}) (\varepsilon_{ax} - \varepsilon_{mn})} \\
& \times (-1)^{J+1+L'+j_a+j_m+j_n+j_v} \\
& \times \delta_{j_x j_{w'}} \frac{1}{[L]} \begin{Bmatrix} J & j_{v'} & j_{w'} \\ L' & j_w & j_v \end{Bmatrix}, \\
B_2 = & - \sum_{LL'}' \frac{Z_L(v' axm) Z_L(w' mya) Z_{L'}(xyvw)}{(\varepsilon_{avw} - \varepsilon_{mxw'}) (\varepsilon_{ay} - \varepsilon_{mw'})} \\
& \times (-1)^{1+L'+j_a+j_m+j_x+j_y+j_{w'}+j_v} \\
& \times \frac{1}{[L]} \begin{Bmatrix} J & j_x & j_y \\ L & j_{w'} & j_{v'} \end{Bmatrix} \begin{Bmatrix} J & j_x & j_y \\ L' & j_w & j_v \end{Bmatrix}, \\
B_3 = & - \sum_{\substack{L_1 L_2 L_3 \\ mnx}}' \frac{X_{L_1}(v' w' mn) X_{L_2}(mnxy) Z_{L_3}(xyvw)}{(\varepsilon_{vw} - \varepsilon_{mn}) (\varepsilon_{xy} - \varepsilon_{mn})} \\
& \times (-1)^{J+L_1+L_2+L_3+j_m+j_n+j_x+j_y+j_{w'}+j_v} \\
& \times \begin{Bmatrix} J & j_m & j_n \\ L_1 & j_{w'} & j_{v'} \end{Bmatrix} \begin{Bmatrix} j_m & j_n & J \\ j_y & j_x & L_2 \end{Bmatrix} \begin{Bmatrix} J & j_x & j_y \\ L_3 & j_w & j_v \end{Bmatrix}.
\end{aligned}$$

The effective interaction strength,

$$X_L(ijkl) = (-1)^L \langle i || C^L || k \rangle \langle j || C^L || l \rangle R_L(ijkl), \quad (A1)$$

is independent of magnetic quantum numbers. The reduced matrix element of the C^L tensor is

$$\langle i || C^L || k \rangle = (-1)^{i+1/2} \sqrt{[i][k]} \begin{pmatrix} j_i & j_k & L \\ -\frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} \Pi^e(l_i, l_k, L), \quad (A2)$$

where $[i] \equiv 2j_i + 1$ is the occupation number of shell i , and

$$\Pi^e(l_i, l_k, L) = \begin{cases} 1 & \text{if } l_i + l_k + L \text{ is even} \\ 0 & \text{if } l_i + l_k + L \text{ is odd.} \end{cases} \quad (A3)$$

The Slater integral $R_L(ijkl)$ is

$$\begin{aligned}
R_L(ijkl) = & \int_0^\infty \int_0^\infty dr_1 dr_2 \frac{r_1^{L-1} r_2^{L-1}}{r_1^{L+1} r_2^{L+1}} [P_i(r_1) P_k(r_1) + Q_i(r_1) Q_k(r_1)] \\
& \times [P_j(r_2) P_l(r_2) + Q_j(r_2) Q_l(r_2)]. \quad (A4)
\end{aligned}$$

The quantity $Z_L(ijkl)$ is defined by (with $[L] \equiv 2L + 1$)

$$Z_L(ijkl) \equiv X_L(ijkl) + [L] \sum_{L'} \begin{Bmatrix} j_j & j_l & L \\ j_i & j_k & L' \end{Bmatrix} X_{L'}(ijlk). \quad (A5)$$

- [1] A. Ivanova, U. Safronova, and V. Tolmachev, *Litov. Fiz. Sb.* **7**, 571 (1967).
- [2] U. I. Safronova and A. N. Ivanova, *Opt. Spektrosk.* **27**, 193 (1969) [*Opt. Spectrosc.* **27**, 103 (1969)].
- [3] E. P. Ivanova and U. I. Safronova, *J. Phys. B* **8**, 1591 (1975).
- [4] T. N. Chang, *Phys. Rev. A* **39**, 4946 (1989).
- [5] T. N. Chang, *Phys. Rev. A* **34**, 4550 (1986).
- [6] C. F. Fischer, M. Godefroid, and J. Olsen, *J. Phys. B* **30**, 1163 (1997).
- [7] F. J. Galvez, E. Buendia, and A. Sarsa, *J. Chem. Phys.* **118**, 6858 (2003).
- [8] K. T. Cheng, Y. K. Kim, and J. P. Desclaux, *At. Data Nucl. Data Tables* **24**, 111 (1979).
- [9] A. Ynnerman and C. F. Fischer, *Phys. Rev. A* **51**, 2020 (1995).
- [10] P. Jonsson and C. F. Fischer, *J. Phys. B* **30**, 5861 (1997).
- [11] E. Lindroth and J. Hvarfner, *Phys. Rev. A* **45**, 2771 (1992).
- [12] M. H. Chen, K. T. Cheng, and W. R. Johnson, *Phys. Rev. A* **64**, 042507 (2001).
- [13] M. H. Chen and K. T. Cheng, *Phys. Rev. A* **55**, 3440 (1997).
- [14] I. M. Savukov and W. R. Johnson, *Phys. Rev. A* **65**, 042503 (2002).
- [15] M. S. Safronova, W. R. Johnson, and U. I. Safronova, *Phys. Rev. A* **53**, 4036 (1996).
- [16] S. A. Blundell, W. R. Johnson, and J. Sapirstein, *Phys. Rev. A* **42**, 3751 (1990).
- [17] J. Sucher, *Phys. Rev. A* **22**, 348 (1980).
- [18] M. H. Mittleman, *Phys. Rev. A* **4**, 893 (1971).
- [19] M. H. Mittleman, *Phys. Rev. A* **5**, 2395 (1972).
- [20] M. H. Mittleman, *Phys. Rev. A* **24**, 1167 (1981).
- [21] I. Lindgren and J. Morrison, *Atomic Many-Body Theory*, 2nd ed. (Springer-Verlag, Berlin, 1986).
- [22] Technical report, National Institute of Standards and Technology, 2006, URL: <http://physics.nist.gov/PhysRefData/ASD/index.html>
- [23] K. T. Cheng, W. R. Johnson, and J. Sapirstein, *Phys. Rev. A* **47**, 1817 (1993).
- [24] J. Sapirstein, *Phys. Scr.* **46**, 52 (1993).
- [25] R. K. Chaudhuri, B. P. Das, and K. F. Freed, *J. Chem. Phys.* **108**, 2556 (1998).