# Relativistic many-body calculations of transition amplitudes for berylliumlike ions

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(Received 30 December 1999; revised manuscript received 11 May 2000; published 14 September 2000)

Transition amplitudes for allowed transitions in Be-like ions are determined to second order within the framework of relativistic many-body perturbation theory. The calculations start with a $V^{(N-2)}$ Dirac-Fock potential and include correlation corrections systematically. Multiconfiguration reference states are employed to account for the valence-valence correlations within the valence shell and perturbation theory is applied to systematically improve upon the wave functions. The transition amplitudes obtained in different gauges are in close agreement. The theoretical transition amplitudes agree well with experiment for all ions except for the neutral Be atom.

PACS number(s): 32.70.Cs, 31.15.Md, 31.25.−v, 31.30.Jv

## I. INTRODUCTION

In this paper, we present a systematic study of transition amplitudes for allowed transitions in the Be-like ions. The Be-like ions are the simplest atomic systems in which both valence-valence and core-valence correlations are important. Energies and transition amplitudes for transitions in the Be-like ions have been the subject of many theoretical and experimental investigations. Numerous experimental data for the transition amplitudes in the Be-like ions can be found in the literature [1–19]. The calculation of transition amplitudes for transitions in highly charged ions is one of the most fascinating problems in atomic physics. Both correlation and relativistic effects are important in highly charged ions. The transition amplitudes provide a quite sensitive measure of the reliability of approximate solutions to the many-body problem. Relativistic effects become more and more important with increasing $Z$ along the isoelectronic sequence, so that the usual perturbative treatment of relativistic effects is not adequate. Many calculations have been carried out for transition amplitudes in the Be-like ions. Among others, several approaches are Hartree-Fock (HF) calculations [20], configuration interaction (CI) calculations [21,22], variational CI techniques [23], non-closed-shell many-electron theory [20], $Z$-expansion methods [24], multiconfiguration Hartree-Fock (MCHF) calculations [21,25,26], multiconfiguration Dirac-Fock (MCDF) calculations [9,27,28], superposition-of-configuration calculations [29], and the multiconfiguration relativistic random-phase approximation (MCRRPA) calculations [30,31]. We proposed a relativistic many-body perturbation theory (MBPT) approach to calculate the transition rates for Be-like ions [32–36]. Recently, Safronova *et al.* [37] applied the relativistic MBPT to calculate the transition rate for Be-like ions. Large discrepancies existed between the relativistic MBPT results and experiment for ions of low ionicities where correlation effects play an important role; notably, the relativistic MBPT results differ significantly from other theoretical calculations.

In this paper, we perform relativistic MBPT calculations up to second order to study transition amplitudes for allowed transitions in the Be-like ions. In the present calculations, the reference states are described by multiconfiguration wave functions that account for the valence-valence correlations. The core-valence and core-core correlations are treated by perturbation. It is possible in this way to take into account strongly interacting configurations to all orders and treat the weakly interacting ones by means of low-order perturbation. Transition amplitudes for allowed transitions in the Be-like ions are determined to second order in both length and velocity gauges. In Sec. II, we derive the second-order relativistic MBPT formulas for energies and transition amplitudes of atoms with two valence electrons. In Sec. III, we carry out the angular reduction of the second-order formulas. Results and discussions are given in Sec. IV.

## II. SECOND-ORDER MBPT FORMULAS

The atomic systems satisfy the Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle. \tag{2.1}$$

Here, $H$ is the ''no-pair'' Hamiltonian given by

$$H = H_0 + V_I. \tag{2.2}$$

In second-quantized form,

$$H_0 = \sum_i \epsilon_i a_i^\dagger a_i, \tag{2.3}$$

and

$$V_I = 1/2 \sum_{ijkl} g_{ijkl} a_i^\dagger a_j^\dagger a_l a_k - \sum_{ij} U_{ij} a_i^\dagger a_j. \tag{2.4}$$

In Eq. (2.3), $\epsilon_i$ is the eigenvalue of the one-electron Dirac equation

$$h(\vec{r}) u_i(\vec{r}) = \epsilon_i u_i(\vec{r}), \tag{2.5}$$

where the Dirac Hamiltonian $h(\vec{r})$ is given by

$$h(\vec{r}) = c\vec{\alpha}\cdot\vec{p} + \beta c^2 + V_{NUC}(r) + U(r). \tag{2.6}$$

Atomic units (a.u.) are employed in this paper. The nuclear Coulomb potential, $V_{NUC}(r)$, in general includes the effect of the finite size of the nucleus. The model potential $U(r)$ accounts approximately for the effect of the electron-electron

 

interactions. In Eq. (2.4), the quantity $U_{ij}$ is a one-electron matrix element of the model potential $U(r)$,

$$U_{ij}=\int u_i^\dagger(\vec{r})U(r)u_j(\vec{r}), \tag{2.7}$$

and $g_{ijkl}$ is the Coulomb integral

$$g_{ijkl}=\int d^3r d^3r' \frac{1}{|\vec{r}-\vec{r}'|}u_i^\dagger(\vec{r})u_k(\vec{r})u_j^\dagger(\vec{r}')u_l(\vec{r}'). \tag{2.8}$$

We now specialize the discussion to atoms with two valence electrons outside a closed core. A zeroth-order wave function describing an atomic state with angular momentum $JM$ may be written as

$$|\Psi_{JM}^{(0)}\rangle=\sum_{(vw)\in P} C_{vw}|\Phi_{vw}^{(0)}\rangle, \tag{2.9}$$

where the quantity $C_{vw}$ are configuration weight coefficients and where the configuration wave functions $|\Phi_{vw}^{(0)}\rangle$ are defined by

$$|\Phi_{vw}^{(0)}\rangle=\eta_{vw}\sum_{m_v m_w}\langle j_v m_v j_w m_w|JM\rangle a_v^\dagger a_w^\dagger|0\rangle, \tag{2.10}$$

with

$$\eta_{vw}=\begin{cases}1 & \text{for } v\neq w\\ 1/\sqrt{2} & \text{for } v=w.\end{cases} \tag{2.11}$$

In Eq. (2.10), $|0\rangle$ designates the core wave function. The indices $v$ and $w$ stand for valence orbitals. The configurations included in the zeroth-order wave function span the model space $P$. In the present calculations, we include all possible configurations within the complex in the model space. In the following paragraph, the letters $a,b,c,d,\ldots$ denote occupied core orbitals, the letters $m,n,r,s,\ldots$ denote excited orbitals outside the core (including the valence orbitals), whereas $i,j,k,l,\ldots$ represent either excited or core orbitals. With this notation, we may write

$$V_I=\frac{1}{2}\sum_{ijkl} g_{ijlk}N[a_i^\dagger a_j^\dagger a_k a_l]+\sum_{ij}\Delta_{ij}N[a_i^\dagger a_j] + \sum_a (\tfrac{1}{2}V_{HF}-U)_{aa}, \tag{2.12}$$

where $N[\cdots]$ designates the normal product, and $\Delta_{ij}=(V_{HF}-U)_{ij}$. Here, $V_{HF}$ is the Hartree-Fock potential

$$(V_{HF})_{ij}=\sum_a [g_{iaja}-g_{iaaj}]. \tag{2.13}$$

We introduce the wave operators $\Omega_{vw}$ that map the zeroth-order wave function onto the exact wave function

$$|\Psi_{JM}\rangle=\sum_{(vw)\in P} C_{vw}\Omega_{vw}|\Phi_{vw}^{(0)}\rangle. \tag{2.14}$$

Substituting Eq. (2.14) into Eq. (2.1) yields

$$\sum_{(vw)\in P} C_{vw}H\Omega_{vw}|\Phi_{vw}^{(0)}\rangle=E\sum_{(vw)\in P} C_{vw}\Omega_{vw}|\Phi_{vw}^{(0)}\rangle. \tag{2.15}$$

Projection of Eq. (2.15) on the left with $\langle\Phi_{v'w'}^{(0)}|$ leads to an eigenvalue equation

$$\sum_{(vw)\in P} C_{vw}(H_{eff})_{v'w'vw}=EC_{v'w'}, \tag{2.16}$$

where the effective Hamiltonian is given by

$$(H_{eff})_{v'w'vw}=\langle\Phi_{v'w'}^{(0)}|H\Omega_{vw}|\Phi_{vw}^{(0)}\rangle. \tag{2.17}$$

In arriving at Eq. (2.16), we have used $\langle\Phi_{v'w'}^{(0)}|\Omega_{vw}|\Phi_{vw}^{(0)}\rangle=\delta_{v'v}\delta_{w'w}$. It follows from Eq. (2.16) that the eigenvectors of the effective Hamiltonian contain the configuration weight coefficients and the eigenvalues are the exact energies of the corresponding exact states.

Multiplication with $\Sigma_{(v'w')\in P}\Omega_{v'w'}|\Phi_{v'w'}^{(0)}\rangle\langle\Phi_{v'w'}^{(0)}|$ on the left of Eq. (2.15) yields

$$\sum_{(vw),(v'w')\in P} C_{vw}\Omega_{v'w'}|\Phi_{v'w'}^{(0)}\rangle\langle\Phi_{v'w'}^{(0)}|H\Omega_{vw}|\Phi_{vw}^{(0)}\rangle = E\sum_{(vw)\in P} C_{vw}\Omega_{vw}|\Phi_{vw}^{(0)}\rangle. \tag{2.18}$$

A comparison of Eq. (2.15) and Eq. (2.18) shows that

$$H\Omega_{vw}|\Phi_{vw}^{(0)}\rangle=\sum_{(v'w')\in P}\Omega_{v'w'}|\Phi_{v'w'}^{(0)}\rangle\langle\Phi_{v'w'}^{(0)}|H\Omega_{vw}|\Phi_{vw}^{(0)}\rangle, \tag{2.19}$$

which leads to

$$[\Omega_{vw},H_0]|\Phi_{vw}^{(0)}\rangle = V_I\Omega_{vw}|\Phi_{vw}^{(0)}\rangle - \sum_{(v'w')\in P}\Omega_{v'w'}|\Phi_{v'w'}^{(0)}\rangle\langle\Phi_{v'w'}^{(0)}|V_I\Omega_{vw}|\Phi_{vw}^{(0)}\rangle. \tag{2.20}$$

Equation (2.20) is the generalized form of the Bloch equation.

It is convenient to introduce correlation operators $\chi_{vw}$ defined by

$$\Omega_{vw}=1+\chi_{vw}. \tag{2.21}$$

It follows from Eqs. (2.9), (2.14), and (2.21) that

$$|\Psi_{JM}\rangle=|\Psi_{JM}^{(0)}\rangle+\sum_{(vw)\in P} C_{vw}\chi_{vw}|\Phi_{vw}^{(0)}\rangle. \tag{2.22}$$

Operating on the zeroth-order wave functions, the correlation operators generate the higher-order corrections. Substituting Eq. (2.21) into Eq. (2.17) leads to

$$(H_{eff})_{v'w'vw}=\langle\Phi_{v'w'}^{(0)}|H(1+\chi_{vw})|\Phi_{vw}^{(0)}\rangle. \tag{2.23}$$

In the present calculations, we are interested in the second-order transition amplitudes. It suffices to diagonalize the first-order effective Hamiltonian that is given by

$$(H_{eff}^{(1)})_{v'w'vw}=\langle\Phi_{v'w'}^{(0)}|H|\Phi_{vw}^{(0)}\rangle$$
$$=\eta_{v'w'}\eta_{vw}\sum_{\substack{m_v m_{v'}\\ m_w m_{w'}}}\langle j_{v'}m_{v'}j_{w'}m_{w'}|J'M'\rangle$$
$$\times\langle j_v m_v j_w m_w|JM\rangle\times[(\delta_{v'v}\delta_{w'w}-\delta_{v'w}\delta_{w'v})$$
$$\times(\epsilon_v+\epsilon_w)+\delta_{w'w}\Delta_{v'v}+\delta_{v'v}\Delta_{w'w}$$
$$-\delta_{v'w}\Delta_{w'v}-\delta_{w'v}\Delta_{v'w}+\tilde{g}_{v'w'vw}], \quad (2.24)$$

where $\tilde{g}_{ijkl}=g_{ijkl}-g_{ijlk}$. It is evident that

$$[\Omega_{vw},H_0]=[\chi_{vw},H_0]. \quad (2.25)$$

Therefore, we can replace $\Omega_{vw}$ by $\chi_{vw}$ for the commutators in Eq. (2.20).

We assume that the correlation operators $\chi_{vw}$ can be expanded in powers of $V_I$ as

$$\chi_{vw}=\chi_{vw}^{(1)}+\chi_{vw}^{(2)}+\cdots. \quad (2.26)$$

It follows from Eqs. (2.22) and (2.26) that

$$|\Psi_{JM}\rangle=|\Psi_{JM}^{(0)}\rangle+|\Psi_{JM}^{(1)}\rangle+\cdots, \quad (2.27)$$

where

$$|\Psi_{JM}^{(n)}\rangle=\sum_{(vw)\in P}C_{vw}|\Phi_{vw}^{(n)}\rangle. \quad (2.28)$$

The $n$th-order configuration wave functions $|\Phi_{vw}^{(n)}\rangle$ are given by

$$|\Phi_{vw}^{(n)}\rangle=\chi_{vw}^{(n)}|\Phi_{vw}^{(0)}\rangle. \quad (2.29)$$

The energy can be correspondingly expanded as

$$E=E^{(0)}+E^{(1)}+\cdots. \quad (2.30)$$

Substituting Eqs. (2.27) and (2.30) into Eq. (2.1) yields

$$(H_0-E^{(0)})|\Psi_{JM}^{(0)}\rangle=0 \quad (2.31)$$

and

$$(H_0-E^{(0)})|\Psi_{JM}^{(1)}\rangle=(E^{(1)}-V_I)|\Psi_{JM}^{(0)}\rangle. \quad (2.32)$$

The wave function $|\Psi_{JM}\rangle$ is normalized using the intermediate normalization condition

$$\langle\Psi_{JM}^{(0)}|\Psi_{JM}\rangle=1. \quad (2.33)$$

In addition, we assume that the zeroth-order wave function is normalized to unity,

$$\langle\Psi_{JM}^{(0)}|\Psi_{JM}^{(0)}\rangle=1, \quad (2.34)$$

which leads to

$$\sum_{(vw)\in P}C_{vw}^2=1 \quad (2.35)$$

and

$$\langle\Phi_{v'w'}^{(0)}|\Phi_{vw}^{(0)}\rangle=\delta_{v'v}\delta_{w'w}. \quad (2.36)$$

It follows from Eqs. (2.33) and (2.34) that

$$\langle\Phi_{v'w'}^{(0)}|\Phi_{vw}^{(n)}\rangle=0. \quad (2.37)$$

This choice leads to unnormalized wave functions, with

$$\langle\Psi_{JM}|\Psi_{JM}\rangle=N^{-2}, \quad (2.38)$$

where to second order

$$N=1-1/2\sum_{(vw),(v'w')\in P}C_{v'w'}C_{vw}\langle\Phi_{v'w'}^{(1)}|\Phi_{vw}^{(1)}\rangle. \quad (2.39)$$

From Eqs. (2.31), (2.34), and (2.36), we see that

$$E^{(0)}=\langle\Psi_{JM}^{(0)}|H_0|\Psi_{JM}^{(0)}\rangle=E_{core}^{(0)}+E_{val}^{(0)}, \quad (2.40)$$

where

$$E_{core}^{(0)}=\sum_a\epsilon_a, \quad (2.41)$$

$$E_{val}^{(0)}=\sum_{(vw)\in P}C_{vw}^2\epsilon_{vw}. \quad (2.42)$$

In Eq. (2.42), $\epsilon_{vw}=\epsilon_v+\epsilon_w$. Projection of Eq. (2.32) on the left with $\langle\Psi_{JM}^{(0)}|$ yields

$$E^{(1)}=E_{core}^{(1)}+E_{val}^{(1)}, \quad (2.43)$$

where

$$E_{core}^{(1)}=\sum_a(\tfrac{1}{2}V_{HF}-U)_{aa}, \quad (2.44)$$

$$E_{val}^{(1)}=\sum_{(vw)\in P}C_{vw}^2[\Delta_{vv}+\Delta_{ww}]+1/2\sum_{(vw),(v'w')\in P}C_{v'w'}C_{vw}\eta_{v'w'}\eta_{vw}\sum_{\substack{m_v m_{v'}\\ m_w m_{w'}}}\langle j_{v'}m_{v'}j_{w'}m_{w'}|JM\rangle\langle j_v m_v j_w m_w|JM\rangle$$
$$\times(\tilde{g}_{w'v'wv}+\tilde{g}_{v'w'vw}). \quad (2.45)$$

We are now in a position to obtain the first-order correction for the wave functions. From Eqs. (2.20), (2.21), (2.25), (2.26), and (2.29), we see that

$$\left(H_0-\sum_a \epsilon_a-\epsilon_{vw}\right)|\Phi_{vw}^{(1)}\rangle = -V_I|\Phi_{vw}^{(0)}\rangle+\sum_{(v'w')\in P}|\Phi_{v'w'}^{(0)}\rangle\langle\Phi_{v'w'}^{(0)}|V_I|\Phi_{vw}^{(0)}\rangle. \tag{2.46}$$

The solution to Eq. (2.46), which is automatically orthogonal to the zeroth-order wave function $|\Psi_{JM}^{(0)}\rangle$, is

$$|\Phi_{vw}^{(1)}\rangle=|D_{1vw}\rangle+|D_{2vw}\rangle+|D_{3vw}\rangle+|T_{1vw}\rangle+|T_{2vw}\rangle+|T_{3vw}\rangle+|Q_{vw}\rangle, \tag{2.47}$$

where the double ($D$), triple ($T$), and quadrupole ($Q$) excitations are given by

$$|D_{1vw}\rangle=-\eta_{vw}\sum_{m_vm_w}\langle j_vm_vj_wm_w|JM\rangle\times\sum_{(vm)\notin P}\frac{\Delta_{mw}}{\epsilon_m-\epsilon_w}a_v^\dagger a_m^\dagger|0\rangle, \tag{2.48}$$

$$|D_{2vw}\rangle=-\eta_{vw}\sum_{m_vm_w}\langle j_vm_vj_wm_w|JM\rangle\times\sum_{(mw)\notin P}\frac{\Delta_{mv}}{\epsilon_m-\epsilon_v}a_m^\dagger a_w^\dagger|0\rangle, \tag{2.49}$$

$$|D_{3vw}\rangle=-\eta_{vw}\sum_{m_vm_w}\langle j_vm_vj_wm_w|JM\rangle\times\sum_{(mn)\notin P}\frac{g_{mnvw}}{\epsilon_{mn}-\epsilon_{vw}}a_m^\dagger a_n^\dagger|0\rangle, \tag{2.50}$$

$$|T_{1vw}\rangle=-\eta_{vw}\sum_{m_vm_w}\langle j_vm_vj_wm_w|JM\rangle\times\sum_{mb}\frac{\Delta_{mb}}{\epsilon_m-\epsilon_b}a_m^\dagger a_b a_v^\dagger a_w^\dagger|0\rangle, \tag{2.51}$$

$$|T_{2vw}\rangle=-\eta_{vw}\sum_{m_vm_w}\langle j_vm_vj_wm_w|JM\rangle\times\sum_{mnb}\frac{g_{mnbw}}{\epsilon_{mn}-\epsilon_{bw}}a_m^\dagger a_n^\dagger a_b a_v^\dagger|0\rangle, \tag{2.52}$$

$$|T_{3vw}\rangle=-\eta_{vw}\sum_{m_vm_w}\langle j_vm_vj_wm_w|JM\rangle\times\sum_{mnc}\frac{g_{mnvc}}{\epsilon_{mn}-\epsilon_{vc}}a_m^\dagger a_n^\dagger a_c a_w^\dagger|0\rangle, \tag{2.53}$$

$$|Q_{vw}\rangle=-\frac{\eta_{vw}}{2}\sum_{m_vm_w}\langle j_vm_vj_wm_w|JM\rangle\times\sum_{mnbc}\frac{g_{mnbc}}{\epsilon_{mn}-\epsilon_{bc}}a_m^\dagger a_n^\dagger a_c a_b a_v^\dagger a_w^\dagger|0\rangle. \tag{2.54}$$

We are interested in the transition matrix elements between two states induced by an external electromagnetic field. For a many-body system, the multipole-transition operators are given by

$$T_{kq}^{(\lambda)}=\sum_{ij}(t_{kq}^{(\lambda)})_{ij}a_i^\dagger a_j, \tag{2.55}$$

where $t_{kq}^{(\lambda)}$ is the multipole-transition operators for one electron [38]. The multipole-moment operators for a many-body system are defined by

$$Q_{kq}^{(\lambda)}=(c/\omega)^k(2k+1)!!T_{kq}^{(\lambda)}, \tag{2.56}$$

where $\omega$ is the photon energy. We consider a transition from a state $I$ with angular momentum $JM$ to a state $F$ with angular momentum $J'M'$. The zeroth-order energies of these states are $E_I^{(0)}$ and $E_F^{(0)}$, respectively. The energy of the absorbed photon is then, in zeroth-order, $\hbar\omega=E_F^{(0)}-E_I^{(0)}$. The first-order transition matrix elements are given by

$$\langle F|T_{kq}^{(\lambda)}|I\rangle^{(1)}=\langle\Psi_{J'M'}^{(0)}|T_{kq}^{(\lambda)}|\Psi_{JM}^{(0)}\rangle. \tag{2.57}$$

With the aid of Eqs. (2.9), (2.10), and (2.55), we obtain

$$\langle F|T_{kq}^{(\lambda)}|I\rangle^{(1)}=\sum_{\substack{(vw)\in P_I\\(v'w')\in P_F}}C_{v'w'}C_{vw}\eta_{v'w'}\eta_{vw}\sum_{\substack{m_vm_{v'}\\m_wmw'}}\langle j_{v'}m_{v'}j_{w'}m_{w'}|J'M'\rangle\langle j_vm_vj_wm_w|JM\rangle\times[\delta_{vv'}\langle w'|t_{kq}^{(\lambda)}|w\rangle-\delta_{wv'}\langle w'|t_{kq}^{(\lambda)}|v\rangle-\delta_{vw'}\langle v'|t_{kq}^{(\lambda)}|w\rangle+\delta_{ww'}\langle v'|t_{kq}^{(\lambda)}|v\rangle], \tag{2.58}$$

where $P_I$ and $P_F$ designate the model spaces for the initial and the final states, respectively. The first-order wave function may be employed to determine second-order corrections to transition matrix elements. The second-order transition matrix elements take the form

$$\langle F|T_{kq}^{(\lambda)}|I\rangle^{(2)}=\langle\Psi_{J'M'}^{(1)}|T_{kq}^{(\lambda)}|\Psi_{JM}^{(0)}\rangle+\langle\Psi_{J'M'}^{(0)}|T_{kq}^{(\lambda)}|\Psi_{JM}^{(1)}\rangle+\delta\omega^{(1)}\langle\Psi_{J'M'}^{(0)}|dT_{kq}^{(\lambda)}/d\omega|\Psi_{JM}^{(0)}\rangle, \tag{2.59}$$

where

$$\delta\omega^{(1)}=\frac{E_F^{(1)}-E_I^{(1)}}{\hbar} \tag{2.60}$$

is the first-order correction to the photon energy. The third term on the right-hand side is the derivative term. A simple interpretation can be given. When we expand $E=E^{(0)}+E^{(1)}+\cdots$ for the energies of the initial and the final states, the energy-dependent operator $T_{kq}^{(\lambda)}$ must also be expanded as $T_{kq}^{(\lambda)}(E_F-E_I)=T_{kq}^{(\lambda)}(\omega)+\delta\omega^{(1)}dT_{kq}^{(\lambda)}(\omega)/d\omega+\cdots$. Thus,

the derivative term arises naturally in the perturbation theory. It follows from Eqs. (2.56)—(2.59) that the transition matrix elements are related to the dipole-moment matrix elements by

$$\langle F|T^{(\lambda)}_{kq}|I\rangle^{(1)+(2)}=\frac{1}{(2k+1)!!c^k}[(\omega^k+\delta\omega^{(1)}k\omega^{k-1})\times\langle F|Q^{(\lambda)}_{kq}|I\rangle^{(1)}+\omega^k\langle F|Q^{(\lambda)}_{kq}|I\rangle^{(2)}] \tag{2.61}$$

in the length gauge, and

$$\langle F|T^{(\lambda)}_{kq}|I\rangle^{(1)+(2)}=\frac{1}{(2k+1)!!c^k}\omega^k\langle F|Q^{(\lambda)}_{kq}|I\rangle^{(1)+(2)} \tag{2.62}$$

in the velocity gauge. With the aid of Eqs. (2.47)—(2.55), we obtain

$$\begin{aligned}
\langle F|T^{(\lambda)}_{kq}|I\rangle^{(2)}=&\sum_{\substack{(vw)\in P_I\\(v'w')\in P_F}} C_{v'w'}C_{vw}\eta_{v'w'}\eta_{vw}\sum_{\substack{m_vm_{v'}\\m_wmw'}}\langle j_{v'}m_{v'}j_{w'}m_{w'}|J'M'\rangle\langle j_vm_vj_wm_w|JM\rangle\\
&\times\Bigg\{\sum_{(mn)\notin P_I}\frac{g_{vwmn}}{\epsilon_{vw}-\epsilon_{mn}}\sum_{rs}\langle r|t^{(\lambda)}_{kq}|s\rangle[\delta_{w'r}\delta_{v'm}\delta_{sn}+\delta_{w'n}\delta_{v'r}\delta_{sm}-\delta_{w'r}\delta_{v'n}\delta_{sm}\\
&-\delta_{w'm}\delta_{v'r}\delta_{sn}]+\sum_{(mn)\notin P_F}\frac{g_{v'w'mn}}{\epsilon_{v'w'}-\epsilon_{mn}}\sum_{rs}\langle r|t^{(\lambda)}_{kq}|s\rangle[\delta_{nr}\delta_{mv}\delta_{sw}+\delta_{nw}\delta_{mr}\delta_{sv}-\delta_{nr}\delta_{mw}\delta_{sv}-\delta_{nv}\delta_{mr}\delta_{sw}]\\
&+\sum_{mnb}\frac{g_{bwmn}}{\epsilon_{bw}-\epsilon_{mn}}\sum_{ar}\langle a|t^{(\lambda)}_{kq}|r\rangle[\delta_{w'm}\delta_{v'n}\delta_{ab}\delta_{rv}+\delta_{w'n}\delta_{v'v}\delta_{ab}\delta_{rm}+\delta_{w'v}\delta_{v'm}\delta_{ab}\delta_{rn}-\delta_{w'm}\delta_{v'v}\delta_{ab}\delta_{rn}\\
&-\delta_{w'n}\delta_{v'm}\delta_{ab}\delta_{rv}-\delta_{w'v}\delta_{v'n}\delta_{ab}\delta_{rm}]+\sum_{mnb}\frac{g_{bvmn}}{\epsilon_{bv}-\epsilon_{mn}}\sum_{ar}\langle a|t^{(\lambda)}_{kq}|r\rangle[\delta_{w'n}\delta_{v'm}\delta_{ab}\delta_{rw}+\delta_{w'm}\delta_{v'w}\delta_{ab}\delta_{rn}\\
&+\delta_{w'w}\delta_{v'n}\delta_{ab}\delta_{rm}-\delta_{w'n}\delta_{v'w}\delta_{ab}\delta_{rm}-\delta_{w'm}\delta_{v'n}\delta_{ab}\delta_{rw}-\delta_{w'w}\delta_{v'm}\delta_{ab}\delta_{rn}]+\sum_{mnb}\frac{g_{bw'mn}}{\epsilon_{bw'}-\epsilon_{mn}}\sum_{ar}\langle r|t^{(\lambda)}_{kq}|a\rangle\\
&\times[\delta_{v'r}\delta_{ab}\delta_{nv}\delta_{mw}+\delta_{v'v}\delta_{ab}\delta_{nw}\delta_{mr}+\delta_{v'w}\delta_{ab}\delta_{nr}\delta_{mv}-\delta_{v'r}\delta_{ab}\delta_{nw}\delta_{mv}-\delta_{v'v}\delta_{ab}\delta_{nr}\delta_{mw}-\delta_{v'w}\delta_{ab}\delta_{nv}\delta_{mr}]\\
&+\sum_{mnb}\frac{g_{bv'mn}}{\epsilon_{bv'}-\epsilon_{mn}}\sum_{ar}\langle r|t^{(\lambda)}_{kq}|a\rangle[\delta_{w'r}\delta_{ab}\delta_{mv}\delta_{nw}+\delta_{w'w}\delta_{ab}\delta_{mr}\delta_{nv}+\delta_{w'v}\delta_{ab}\delta_{mw}\delta_{nr}-\delta_{w'r}\delta_{ab}\delta_{mw}\delta_{nv}\\
&-\delta_{w'w}\delta_{ab}\delta_{mv}\delta_{nr}-\delta_{w'v}\delta_{ab}\delta_{mr}\delta_{nw}]+\sum_{(vm)\notin P_I}\frac{\Delta_{mw}}{\epsilon_m-\epsilon_w}\sum_{rs}\langle r|t^{(\lambda)}_{kq}|s\rangle[\delta_{w'r}\delta_{mv'}\delta_{sv}+\delta_{w'v}\delta_{v'r}\delta_{sm}\\
&-\delta_{w'r}\delta_{v'v}\delta_{sm}-\delta_{w'm}\delta_{v'r}\delta_{sv}]+\sum_{(mw)\notin P_I}\frac{\Delta_{mv}}{\epsilon_m-\epsilon_v}\sum_{rs}\langle r|t^{(\lambda)}_{kq}|s\rangle[\delta_{v'r}\delta_{mw'}\delta_{sw}+\delta_{v'w}\delta_{w'r}\delta_{sm}-\delta_{v'r}\delta_{w'w}\delta_{sm}\\
&-\delta_{v'm}\delta_{w'r}\delta_{sw}]+\sum_{(v'm)\notin P_F}\frac{\Delta_{w'm}}{\epsilon_{w'}-\epsilon_m}\sum_{rs}\langle r|t^{(\lambda)}_{kq}|s\rangle[\delta_{v'r}\delta_{mw}\delta_{sv}+\delta_{v'v}\delta_{mr}\delta_{sw}-\delta_{v'r}\delta_{mv}\delta_{sw}-\delta_{v'w}\delta_{mr}\delta_{sv}]\\
&+\sum_{(mw')\notin P_F}\frac{\Delta_{v'm}}{\epsilon_{v'}-\epsilon_m}\sum_{rs}\langle r|t^{(\lambda)}_{kq}|s\rangle[\delta_{w'r}\delta_{mv}\delta_{sw}+\delta_{w'w}\delta_{mr}\delta_{sv}-\delta_{w'r}\delta_{mw}\delta_{sv}-\delta_{w'v}\delta_{mr}\delta_{sw}]\\
&+\sum_{mb}\frac{\Delta_{mb}}{\epsilon_m-\epsilon_b}\sum_{ar}\langle a|t^{(\lambda)}_{kq}|r\rangle[\delta_{w'm}\delta_{v'v}\delta_{ab}\delta_{rw}+\delta_{w'v}\delta_{v'w}\delta_{ab}\delta_{rm}+\delta_{w'w}\delta_{v'm}\delta_{ab}\delta_{rv}-\delta_{w'm}\delta_{v'w}\delta_{ab}\delta_{rv}\\
&-\delta_{w'v}\delta_{v'm}\delta_{ab}\delta_{rw}-\delta_{w'w}\delta_{v'v}\delta_{ab}\delta_{rm}]+\sum_{mb}\frac{\Delta_{bm}}{\epsilon_b-\epsilon_m}\sum_{ar}\langle r|t^{(\lambda)}_{kq}|a\rangle[\delta_{ab}\delta_{w'r}\delta_{v'w}\delta_{mv}+\delta_{ab}\delta_{w'v}\delta_{v'r}\delta_{mw}\\
&+\delta_{ab}\delta_{w'w}\delta_{v'v}\delta_{mr}-\delta_{ab}\delta_{w'r}\delta_{v'v}\delta_{mw}-\delta_{ab}\delta_{w'v}\delta_{v'w}\delta_{mr}-\delta_{ab}\delta_{w'w}\delta_{v'r}\delta_{mv}]+\delta\omega^{(1)}[\delta_{vv'}\langle w'|dt^{(\lambda)}_{kq}/d\omega|w\rangle\\
&-\delta_{wv'}\langle w'|dt^{(\lambda)}_{kq}/d\omega|v\rangle-\delta_{vw'}\langle v'|dt^{(\lambda)}_{kq}/d\omega|w\rangle+\delta_{ww'}\langle v'|dt^{(\lambda)}_{kq}/d\omega|v\rangle]\Bigg\}.
\end{aligned} \tag{2.63}$$

### III. ANGULAR REDUCTION

The Dirac orbital takes the form

$$u_\alpha(\vec{r})=\frac{1}{r}\begin{pmatrix} ig_{n_\alpha\kappa_\alpha}\Omega_{\kappa_\alpha m_\alpha} \\ f_{n_\alpha\kappa_\alpha}\Omega_{-\kappa_\alpha m_\alpha}\end{pmatrix}. \tag{3.1}$$

We introduce the two-component radial function

$$u_\alpha \equiv u_\alpha(r)\equiv\begin{pmatrix} g_{n_\alpha\kappa_\alpha} \\ f_{n_\alpha\kappa_\alpha}\end{pmatrix}. \tag{3.2}$$

Carrying out the sum over magnetic substates in Eq. (2.24) leads to

$$(H^{(1)}_{eff})_{v'w'vw}=\delta_{vv'}\delta_{ww'}\Big(\sum_a \epsilon_a+\sum_a (\tfrac{1}{2}V_{HF}-U)_{aa}+\epsilon_v+\epsilon_w+\Delta_{vv}+\Delta_{ww}\Big)+V_{v'w'vw}, \tag{3.3}$$

where

$$V_{v'w'vw}=\eta_{v'w'}\eta_{vw}Y_J(v'w'vw). \tag{3.4}$$

Here, we have introduced the notation

$$Y_J(abcd)=\sum_k (-1)^{j_b+j_c+k+J}\begin{Bmatrix} j_a & j_b & J \\ j_d & j_c & k\end{Bmatrix}X_k(abcd)+\sum_k (-1)^{j_b+j_c+k}\begin{Bmatrix} j_a & j_b & J \\ j_c & j_d & k\end{Bmatrix}X_k(abdc), \tag{3.5}$$

where

$$X_k(abcd)=(-1)^k\langle a||C_k||c\rangle\langle b||C_k||d\rangle R_k(abcd). \tag{3.6}$$

The quantities $C_k$ are normalized spherical harmonics and $R_k(abcd)$ are Slater integrals. The first-order valence energy can be expressed in terms of radial integrals as

$$E^{(1)}_{val}=\sum_{(vw)\in P} C^2_{vw}[\Delta_{vv}+\Delta_{ww}]+\sum_{(vw),(v'w')\in P} C_{v'w'}C_{vw}V_{v'w'vw}. \tag{3.7}$$

Angular reduction of Eq. (2.58) yields the first-order transition amplitude that is defined as the reduced matrix element of the multipole-transition operator,

$$\langle F\|T^{(\lambda)}_k\|I\rangle^{(1)}=[J]^{1/2}[J']^{1/2}(-1)^k\sum_{\substack{(vw)\in P_I\\(v'w')\in P_F}}\eta_{v'w'}\eta_{vw}C_{v'w'}c_{vw}\times\Bigg[(-1)^{J'+j_v+j_w}\begin{Bmatrix} J' & J & k \\ j_w & j_{w'} & j_v\end{Bmatrix}\langle w'\|t^{(\lambda)}_k\|w\rangle\delta_{vv'}$$
$$+(-1)^{J+J'+1}\begin{Bmatrix} J' & J & k \\ j_v & j_{w'} & j_w\end{Bmatrix}\langle w'\|t^{(\lambda)}_k\|v\rangle\delta_{wv'}+(-1)^{j_{v'}+j_w}\begin{Bmatrix} J' & J & k \\ j_w & j_{v'} & j_v\end{Bmatrix}\langle v'\|t^{(\lambda)}_k\|w\rangle\delta_{vw'}$$
$$+(-1)^{J+j_{v'}+j_{w'}}\begin{Bmatrix} J' & J & k \\ j_v & j_{v'} & j_w\end{Bmatrix}\langle v'\|t^{(\lambda)}_k\|v\rangle\delta_{ww'}\Bigg], \tag{3.8}$$

where $[J]=2J+1$. Similarly, angular reduction of Eq. (2.63) gives

$$\langle F\|T^{(\lambda)}_k\|I\rangle^{(2)}=[J]^{1/2}[J']^{1/2}\sum_{\substack{(vw)\in P_I\\(v'w')\in P_F}}\eta_{vw}\eta_{v'w'}C_{vw}C_{v'w'}\Bigg\{(-1)^{J+J'+k}\sum_{(iv')\notin P_I}\begin{Bmatrix} J' & J & k \\ j_i & j_{w'} & j_{v'}\end{Bmatrix}\frac{\langle w'\|t^{(\lambda)}_k\|i\rangle}{\epsilon_{iv'}-\epsilon_{vw}}Y_J(iv'vw)$$
$$+(-1)^{J+J'+k}\sum_{(iw)\notin P_F}\begin{Bmatrix} J' & J & k \\ j_v & j_i & j_w\end{Bmatrix}\frac{\langle i\|t^{(\lambda)}_k\|v\rangle}{\epsilon_{iw}-\epsilon_{v'w'}}Y_{J'}(v'w'wi)+\delta_{vv'}(-1)^{j_{v'}+j_{w'}+J'}[k]^{-1}\begin{Bmatrix} J' & J & k \\ j_w & j_{w'} & j_v\end{Bmatrix}$$
$$\times\Bigg[\sum_{mb}\frac{\langle m\|t^{(\lambda)}_k\|b\rangle Z_k(wmw'b)}{\epsilon_{bw'}-\epsilon_{mw}}+\sum_{mb}\frac{Z_k(wbw'm)\langle b\|t^{(\lambda)}_k\|m\rangle}{\epsilon_{bw}-\epsilon_{mw'}}\Bigg]$$
$$+\delta_{wv'}(-1)^{j_v+j_{w'}+J+J'}[k]^{-1}\begin{Bmatrix} J' & J & k \\ j_v & j_{w'} & j_w\end{Bmatrix}$$
$$\times\Bigg[\sum_{mb}\frac{\langle m\|t^{(\lambda)}_k\|b\rangle Z_k(vmw'b)}{\epsilon_{bw'}-\epsilon_{mv}}+\sum_{mb}\frac{Z_k(vbw'm)\langle b\|t^{(\lambda)}_k\|m\rangle}{\epsilon_{bv}-\epsilon_{mw'}}\Bigg]+\delta_{vv'}(-1)^{j_v+j_w+J'+k}\begin{Bmatrix} J' & J & k \\ j_w & j_{w'} & j_v\end{Bmatrix}$$

$$\times\left[\sum_{i\neq w'}\delta_{\kappa_i\kappa_{w'}}\frac{\Delta_{w'i}\langle i\|t_k^{(\lambda)}\|w\rangle}{\epsilon_{w'}-\epsilon_i}+\sum_{i\neq w}\delta_{\kappa_i\kappa_w}\frac{\langle w'\|t_k^{(\lambda)}\|i\rangle\Delta_{iw}}{\epsilon_w-\epsilon_i}\right]+\delta_{wv'}(-1)^{J+J'+k+1}\begin{Bmatrix}J' & J & k\\ j_v & j_{w'} & j_w\end{Bmatrix}$$

$$\times\left[\sum_{i\neq w'}\delta_{\kappa_i\kappa_{w'}}\frac{\Delta_{w'i}\langle i\|t_k^{(\lambda)}\|v\rangle}{\epsilon_{w'}-\epsilon_i}+\sum_{i\neq v}\delta_{\kappa_i\kappa_v}\frac{\langle w'\|t_k^{(\lambda)}\|i\rangle\Delta_{iv}}{\epsilon_v-\epsilon_i}\right]+\delta\omega^{(1)}\left[\delta_{vv'}(-1)^{j_v+j_w+J'+k}\begin{Bmatrix}J' & J & k\\ j_w & j_{w'} & j_v\end{Bmatrix}\right.$$

$$\left.\times\langle w'\|dt_k^{(\lambda)}/d\omega\|w\rangle+\delta_{wv'}(-1)^{J+J'+k+1}\begin{Bmatrix}J' & J & k\\ j_v & j_{w'} & j_w\end{Bmatrix}\langle w'\|dt_k^{(\lambda)}/d\omega\|v\rangle\right]$$

$$\left.+(-1)^{j_v+j_w+j_{v'}+j_{w'}+J+J'}(1\leftrightarrow 2)\right\},\tag{3.9}$$

where

$$Z_k(abcd)=X_k(abcd)+\sum_{k'}[k]\begin{Bmatrix}a & c & k\\ b & d & k'\end{Bmatrix}X_{k'}(abdc).\tag{3.10}$$

In Eq. (3.9), the notation $(1\leftrightarrow 2)$ denotes all preceding terms inside the same brackets with the subscripts 1 and 2 interchanged. It is understood that the indices $v$ and $v'$ in the $\delta$ function should be interchanged with $w$ and $w'$, respectively. The first two terms in Eq. (3.9) lead to the second-order valence-valence correlation corrections to the first-order transition amplitudes, while the next four terms represent the second-order RPA corrections. The use of HF potential leads to a major simplication for Eq. (3.9). The $\Delta_{ij}$ terms vanish for the HF case.

TABLE I. Contributions to the E1 transition amplitudes for the Be-like ions. Numbers in brackets denote powers of 10.

| | $(2s2p)\ {}^1P_1^o\rightarrow(2s^2)\ {}^1S_0$ | | $(2p^2)\ {}^1S_0\rightarrow(2s2p)\ {}^1P_1^o$ | | $(2p^2)\ {}^1D_2\rightarrow(2s2p)\ {}^1P_1^o$ | |
|---|---|---|---|---|---|---|
| | I [a] | II [b] | I [a] | II [b] | I [a] | II [b] |
| $Z=4$ | | | | | | |
| T(1) | 6.7327[-4] | 1.3682[-3] | 7.9021[-4] | 2.5189[-4] | 1.4964[-3] | 1.5554[-3] |
| Val2 | 1.7188[-4] | 4.8891[-4] | 4.1492[-5] | 9.2387[-4] | -4.1417[-4] | -1.2688[-3] |
| RPA2 | -3.5759[-6] | -4.8103[-5] | -4.1970[-6] | -8.8560[-6] | -7.9477[-6] | -5.4685[-5] |
| $\delta\omega^{(1)}$ | 9.4518[-4] | 0.0000 | 4.7379[-4] | 0.0000 | -8.3027[-4] | 0.0000 |
| Total | 1.7868[-3] | 1.8090[-3] | 1.3013[-3] | 1.1669[-3] | 2.4401[-4] | 2.3197[-4] |
| $Z=30$ | | | | | | |
| T(1) | 1.5269[-3] | 2.1069[-3] | 1.3978[-3] | 8.4222[-4] | 2.2270[-3] | 2.1960[-3] |
| Val2 | 2.0625[-5] | 4.1006[-4] | -8.0161[-6] | 1.0263[-3] | -3.5668[-6] | -1.3938[-4] |
| RPA2 | -2.6785[-6] | -1.3342[-4] | -2.4461[-6] | -5.0086[-5] | -3.9001[-6] | -1.3538[-4] |
| $\delta\omega^{(1)}$ | 8.4225[-4] | 0.0000 | 4.3539[-4] | 0.0000 | -2.9812[-4] | 0.0000 |
| Total | 2.3871[-3] | 2.3836[-3] | 1.8227[-3] | 1.8184[-3] | 1.9215[-3] | 1.9212[-3] |
| $Z=60$ | | | | | | |
| T(1) | 6.4763[-3] | 6.8686[-3] | 4.9543[-3] | 4.3864[-3] | 7.5052[-3] | 7.4872[-3] |
| Val2 | 4.0380[-5] | 2.4732[-4] | -1.0768[-5] | 8.6528[-4] | -2.0803[-6] | -4.5358[-5] |
| RPA2 | -5.7204[-6] | -1.2260[-4] | -4.3551[-6] | -7.4671[-5] | -6.6082[-6] | -1.2959[-4] |
| $\delta\omega^{(1)}$ | 4.8429[-4] | 0.0000 | 2.3647[-4] | 0.0000 | -1.8707[-4] | 0.0000 |
| Total | 6.9952[-3] | 6.9933[-3] | 5.1756[-3] | 5.1770[-3] | 7.3095[-3] | 7.3122[-3] |
| $Z=90$ | | | | | | |
| T(1) | 2.2413[-2] | 2.2779[-2] | 1.6298[-2] | 1.5717[-2] | 2.5365[-2] | 2.5381[-2] |
| Val2 | 1.0180[-4] | 1.4912[-4] | -1.2129[-5] | 7.6914[-4] | -2.6236[-5] | -1.8437[-4] |
| RPA2 | -1.2402[-5] | -1.2536[-4] | -8.9840[-6] | -8.5108[-5] | -1.4000[-5] | -1.3810[-4] |
| $\delta\omega^{(1)}$ | 2.9465[-4] | 0.0000 | 1.1735[-4] | 0.0000 | -2.7631[-4] | 0.0000 |
| Total | 2.2797[-2] | 2.2802[-2] | 1.6394[-2] | 1.6401[-2] | 2.5048[-2] | 2.5058[-2] |

[a]The length results.

[b]The velocity results.

TABLE II. Transition amplitudes for the $(2s2p)\ ^1P_1^o \rightarrow (2s^2)\ ^1S_0$ transition in the Be-like ions. Numbers in parentheses denote experimental uncertainties.

| $Z$ | I[a] | II[b] | Expt. | Ref. |
|---|---|---|---|---|
| 4 | 1.7868[-3] | 1.4338[-3] | 1.52(3)[-3] | [1] |
| | | | 1.55(2)[-3] | [2] |
| 5 | 1.8833[-3] | 1.6582[-3] | 1.7(1)[-3] | [2] |
| 6 | 1.9086[-3] | 1.7326[-3] | 1.76(4)[-3] | [3] |
| 7 | 1.9163[-3] | 1.7691[-3] | 1.79(3)[-3] | [4] |
| 8 | 1.9190[-3] | 1.7918[-3] | 1.83(4)[-3] | [4] |
| 9 | 1.9206[-3] | 1.8081[-3] | 1.8(1)[-3] | [5] |
| 10 | 1.9227[-3] | 1.8217[-3] | 1.91(15)[-3] | [6] |
| 11 | 1.9258[-3] | 1.8340[-3] | | |
| 12 | 1.9302[-3] | 1.8458[-3] | 1.88(7)[-3] | [7] |
| 13 | 1.9360[-3] | 1.8579[-3] | 1.86(9)[-3] | [7] |
| 14 | 1.9436[-3] | 1.8707[-3] | 1.92(7)[-3] | [7] |
| 15 | 1.9529[-3] | 1.8844[-3] | 1.90(8)[-3] | [7] |
| 16 | 1.9640[-3] | 1.8993[-3] | 1.89(11)[-3] | [7] |
| 17 | 1.9771[-3] | 1.9157[-3] | | |
| 18 | 1.9923[-3] | 1.9338[-3] | | |
| 19 | 2.0098[-3] | 1.9537[-3] | | |
| 20 | 2.0295[-3] | 1.9755[-3] | | |
| 21 | 2.0517[-3] | 1.9996[-3] | | |
| 22 | 2.0765[-3] | 2.0259[-3] | | |
| 23 | 2.1040[-3] | 2.0547[-3] | | |
| 24 | 2.1344[-3] | 2.0864[-3] | | |
| 25 | 2.1679[-3] | 2.1210[-3] | | |
| 26 | 2.2046[-3] | 2.1583[-3] | 2.2(1)[-3] | [8] |
| 27 | 2.2446[-3] | 2.1998[-3] | | |
| 28 | 2.2883[-3] | 2.2425[-3] | | |
| 29 | 2.3357[-3] | 2.2900[-3] | | |

[a]With first-order energies.
[b]With experimental energies.

## IV. RESULTS AND DISCUSSION

We calculated the transition amplitudes for allowed electric-dipole ($E1$) transitions within the $n=2$ complex of the Be-like ions. Contributions to the $E1$ transition amplitudes of the $(2s2p)\ ^1P_1^o \rightarrow (2s^2)\ ^1S_0$, $(2p^2)\ ^1S_0 \rightarrow (2s2p)\ ^1P_1^o$, and $(2p^2)\ ^1D_2 \rightarrow (2s2p)\ ^1P_1^o$ transitions for selected ions are given in Table I. The first four rows give the first-order transition amplitude, the second-order valence-valence correction, the second-order RPA correction, and the second-order derivative terms correction. The last row gives the total second-order transition amplitude, which is the sum of all rows. In the first-order calculation, we performed a $V^{(N-2)}$ frozen-core Dirac-Hartree-Fock (DHF) calculation. Thus the $\Delta_{ij}$ terms in the second-order transition amplitude vanish. The second-order valence-valence correlation corrections and the second-order RPA corrections have greater contributions to the velocity results than to the length results. By contrast, the derivative terms are seen to contribute substantially to the length results, but have no contributions to the velocity results. The percentages of the second-order corrections to the transition amplitudes decrease with increasing nuclear charges $Z$. It is noticed that the RPA corrections always reduce the transition amplitudes. A simple physical interpretation can be given. The second-order RPA correction to the transition amplitude is the product of the zeroth-order photon energy and the matrix element of the electromagnetic dipole potential. The RPA corrections account for the core-shielding (CS) effects in atoms. The external field induces an internal field inside the atom that shields the external field. Therefore, the CS effects lead to an effective potential that weakens the electromagnetic dipole potential and reduces the dipole-moment matrix elements.

Significant differences are observed between the length results and the velocity results of the first-order transition amplitudes. Much of the difference is removed when second-order corrections are included. It is observed that the inclusion of the derivative term substantially reduces the differences between the length and the velocity results of the transition amplitudes. It has been shown [38] that the electromagnetic transition amplitudes calculated using the no-pair Hamiltonian are gauge dependent. This is a result of the restriction to positive-energy states in the no-pair Hamiltonian. The transition amplitudes obtained from Eqs. (3.8) and (3.9) are gauge independent, provided one starts from a

TABLE III. Transition amplitudes for the $(2p^2)\ {}^1S_0 \rightarrow (2s2p)\ {}^1P_1^o$ transition in the Be-like ions.

| $Z$ | I[a] | II[b] | Expt. | Ref. |
|---|---|---|---|---|
| 4 | 1.3013[-3] | 9.5833[-4] | | |
| 5 | 1.3625[-3] | 1.1515[-3] | 1.1(1)[-3] | [10] |
| 6 | 1.4010[-3] | 1.2630[-3] | 1.2(1)[-3] | [3] |
| 7 | 1.4258[-3] | 1.3150[-3] | 1.30(9)[-3] | [11] |
| 8 | 1.4433[-3] | 1.3503[-3] | 1.3(1)[-3] | [12] |
| 9 | 1.4566[-3] | 1.3765[-3] | 1.4(1)[-3] | [5] |
| 10 | 1.4676[-3] | | | |
| 11 | 1.4772[-3] | 1.4145[-3] | | |
| 12 | 1.4861[-3] | 1.4296[-3] | 1.4(1)[-3] | [7] |
| 13 | 1.4948[-3] | 1.4435[-3] | 1.5(1)[-3] | [7] |
| 14 | 1.5036[-3] | 1.4567[-3] | 1.5(1)[-3] | [13] |
| 15 | 1.5127[-3] | 1.4695[-3] | 1.5(1)[-3] | [7] |
| 16 | 1.5223[-3] | 1.4825[-3] | 1.5(1)[-3] | [7] |
| 17 | 1.5328[-3] | | | |
| 18 | 1.5442[-3] | 1.5101[-3] | | |
| 19 | 1.5566[-3] | 1.5245[-3] | | |
| 20 | 1.5704[-3] | 1.5404[-3] | | |
| 21 | 1.5857[-3] | 1.5577[-3] | | |
| 22 | 1.6026[-3] | 1.5762[-3] | | |
| 23 | 1.6215[-3] | 1.5968[-3] | | |
| 24 | 1.6423[-3] | 1.6190[-3] | | |
| 25 | 1.6655[-3] | 1.6437[-3] | | |
| 26 | 1.6911[-3] | 1.6715[-3] | 1.6(1)[-3] | [8] |
| 27 | 1.7195[-3] | 1.6998[-3] | | |
| 28 | 1.7507[-3] | 1.7326[-3] | | |
| 29 | 1.7851[-3] | 1.7697[-3] | | |

[a]With first-order energies.
[b]With experimental energies.

*local* potential and *artificially* includes contributions from negative-energy states (see the Appendix). The excellent agreement between the length and the velocity results indicates that the negative-energy states are not important to the transition amplitudes of the Be-like ions. The length-gauge transition amplitudes will be adopted for our final tabulations. It is well known that the all-order RPA transition amplitude is gauge independent. The fact that the length-gauge transition amplitudes are consistent with the velocity results suggests that the higher-order RPA corrections are not important to the transition amplitudes of the Be-like ions.

The transition amplitudes from the present calculations are present in Tables II–V. In Tables II–IV, the first column gives the second-order transition amplitudes. Discrepancies are observed between the second-order transition amplitudes and the experimental results for ions near the neutral end. Inspections of the photon energies and the dipole-moment matrix elements help us gain insight into the discrepancies. The second-order dipole-moment matrix element for the resonance transition $(2s2p)\ {}^1P_1^o \rightarrow (2s^2)\ {}^1S_0$ in the $B^{1+}$ ion is 2.0385, in agreement with the experimental result [2] 2.1(1). The energy dependence has been excluded from the dipole-moment matrix elements. The agreement between the second-order dipole-moment matrix elements and the experimental result indicates that the wave functions are reliable. On the other hand, the first-order photon energy is 4.1193[-01], which disagrees with the experimental result 3.3440[-01]. This indicates that the differences between the second-order transition amplitudes and the experimental results are due to the unreliability of the first-order photon energies. The discrepancies between the second-order transition amplitudes and the experimental results can be resolved by using the experimental energies. In Tables II–IV, the second column gives the second-order transition amplitudes with experimental energies, which are in excellent agreement with experiment for all ions except for the neutral Be atom. The second-order transition amplitudes with experimental energies for other transitions are given in Table V.

Inspections of the dipole-moment matrix elements help us gain insight into the difference between the theoretical and the experimental transition amplitudes in Be. The first-order dipole-moment matrix element for the resonance transition in Be is 2.4315. The second-order correction is 6.0781[-01], which is the quarter (note that $Z=4$ for Be) of the first-order contribution. According to the $Z$-expansion theory, the third-order contribution is expected to be 1.5195[-01], which is again the quarter of the second-order contribution. The estimated third-order dipole-moment matrix element is then 3.1913, which is in agreement with the experimental result [1] 3.22(6). This indicates that the differences between the

TABLE IV. Transition amplitudes for the $(2p^2)\ {}^1D_2 \rightarrow (2s2p)\ {}^1P_1^o$ transition in the Be-like ions.

| $Z$ | I[a] | II[b] | Expt. | Ref. |
|---|---|---|---|---|
| 4 | 2.4401[-4] | 4.6249[-4] | | |
| 5 | 7.4497[-4] | 8.2870[-4] | 8.19(19)[-4] | [14] |
| 6 | 9.6085[-4] | 1.0045[-3] | 1.0(1)[-3] | [15] |
| 7 | 1.0829[-3] | 1.1115[-3] | 1.12(3)[-3] | [16] |
| 8 | 1.1624[-3] | 1.1837[-3] | 1.1(1)[-3] | [17] |
| 9 | 1.2196[-3] | 1.2365[-3] | 1.23(3)[-3] | [18] |
| 10 | 1.2638[-3] | | | |
| 11 | 1.3002[-3] | 1.3122[-3] | | |
| 12 | 1.3320[-3] | 1.3421[-3] | 1.4(1)[-3] | [7] |
| 13 | 1.3608[-3] | 1.3695[-3] | 1.4(1)[-3] | [7] |
| 14 | 1.3881[-3] | 1.3955[-3] | 1.4(1)[-3] | [7] |
| 15 | 1.4147[-3] | 1.4210[-3] | 1.5(1)[-3] | [7] |
| 16 | 1.4410[-3] | 1.4464[-3] | 1.5(1)[-3] | [7] |
| 17 | 1.4676[-3] | 1.4720[-3] | 1.47(2)[-3] | [19] |
| 18 | 1.4944[-3] | | | |
| 19 | 1.5217[-3] | 1.5246[-3] | | |
| 20 | 1.5493[-3] | 1.5521[-3] | | |
| 21 | 1.5773[-3] | 1.5785[-3] | | |
| 22 | 1.6057[-3] | 1.6067[-3] | | |
| 23 | 1.6348[-3] | 1.6352[-3] | | |
| 24 | 1.6651[-3] | 1.6650[-3] | | |
| 25 | 1.6973[-3] | 1.6965[-3] | | |
| 26 | 1.7325[-3] | 1.7297[-3] | | |
| 27 | 1.7717[-3] | 1.7679[-3] | | |
| 28 | 1.8157[-3] | 1.8124[-3] | | |
| 29 | 1.8655[-3] | 1.8619[-3] | | |

[a]With first-order energies.
[b]With experimental energies.

theoretical and the experimental transition amplitudes are due to the omission of the higher-order corrections in the present calculations. Comparisons of the transition probabilities from the present calculations with experiment as well as with other theoretical results are given in Table VI and Table VII for selected transitions.

In summary, we perform relativistic MBPT calculations up to second order to study the transition amplitudes for allowed transitions in the Be-like ions. The transition amplitudes obtained in different gauges are in close agreement. The theoretical transition amplitudes agree well with experiment for all ions except for the neutral Be atom. The accuracy of the present calculations is expected to increase at higher $Z$ because of the rapid rate of convergence of MBPT. The discrepancies between theory and experiment for Be are a matter of concern. Further theoretical and experimental investigations are certainly needed to understand fully, and remove, the remaining discrepancies.

## ACKNOWLEDGMENTS

The author thanks Professor W. R. Johnson for providing the Hartree-Fock and the *B*-spline programs. This work was supported in part by the National Science Council of the Republic of China under Grant No. NSC88-2112-M-019-001.

## APPENDIX: GAUGE TRANSFORMATION AND TRANSITION AMPLITUDE

It is convenient to introduce an operator representing the difference between the multipole-transition operators in the length and the velocity gauges,

$$\Delta T^{(1)}_{JM} = (T^{(1)}_{JM})_l - (T^{(1)}_{JM})_v . \tag{A1}$$

The operator $\Delta T^{(1)}_{JM}$ can be written as

$$\Delta T^{(1)}_{JM} = \frac{i}{ec}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}}\Delta H_{JM}, \tag{A2}$$

where

$$\Delta H_{JM} = \sum_{ij} \langle i|(\Delta h_I)_{JM}|j\rangle a_i^\dagger a_j . \tag{A3}$$

In Eq. (A3), $h_I$ is the interaction Hamiltonian for a single electron, and $\Delta h_I$ is the change of $h_I$ under the gauge transformation. It is straightforward to show that [38]

TABLE V. Transition amplitudes for Be-like ions.

| $Z$ | I [a] | II [b] | III [c] | IV [d] | V [e] | VI [f] |
|---|---|---|---|---|---|---|
| 4 | 8.2801[-4] | 9.2570[-4] | 7.1714[-4] | 8.2812[-4] | 1.6035[-3] | 9.2589[-4] |
| 5 | 9.2411[-4] | 1.0330[-3] | 8.0048[-4] | 9.2444[-4] | 1.7898[-3] | 1.0337[-3] |
| 6 | 9.6767[-4] | 1.0814[-3] | 8.3839[-4] | 9.6844[-4] | 1.8744[-3] | 1.0831[-3] |
| 7 | 9.9153[-4] | 1.1076[-3] | 8.5940[-4] | 9.9304[-4] | 1.9830[-3] [g] | 1.1110[-3] |
| 8 | 1.0065[-3] | 1.1238[-3] | 8.7290[-4] | 1.0092[-3] | 1.9511[-3] | 1.1296[-3] |
| 9 | 1.0171[-3] | 1.1346[-3] | 8.8271[-4] | 1.0212[-3] | 1.9725[-3] | 1.1438[-3] |
| 10 | 1.0252[-3] | 1.1426[-3] | 8.9066[-4] | 1.0314[-3] | 1.9897[-3] | 1.1563[-3] |
| 11 | 1.0319[-3] | 1.1487[-3] | 8.9771[-4] | 1.0408[-3] | 2.0044[-3] | 1.1681[-3] |
| 12 | 1.0378[-3] | 1.1537[-3] | 9.0452[-4] | 1.0503[-3] | 2.0178[-3] | 1.1801[-3] |
| 13 | 1.0434[-3] | 1.1576[-3] | 9.1104[-4] | 1.0597[-3] | 2.0304[-3] | 1.1928[-3] |
| 14 | 1.0488[-3] | 1.1612[-3] | 9.1800[-4] | 1.0700[-3] | 2.0424[-3] | 1.2068[-3] |
| 15 | 1.0541[-3] | 1.1644[-3] | 9.2541[-4] | 1.0813[-3] | 2.0537[-3] | 1.2220[-3] |
| 16 | 1.0596[-3] | 1.1673[-3] | 9.3348[-4] | 1.0938[-3] | 2.0640[-3] | 1.2390[-3] |
| 17 | 1.0776[-3] [g] | 1.1826[-3] [g] | 9.5367[-4] [g] | 1.1224[-3] [g] | 2.1015[-3] [g] | 1.2769[-3] [g] |
| 18 | 1.0711[-3] | 1.1726[-3] | 9.5184[-4] | 1.1373[-3] [g] | 2.0789[-3] | 1.2783[-3] |
| 19 | 1.0769[-3] | 1.1753[-3] | 9.6248[-4] | 1.1395[-3] | 2.0818[-3] | 1.3008[-3] |
| 20 | 1.0831[-3] | 1.1776[-3] | 9.7412[-4] | 1.1583[-3] | 2.0792[-3] | 1.3252[-3] |
| 21 | 1.0894[-3] | 1.1801[-3] | 9.8691[-4] | 1.1788[-3] | 2.0715[-3] | 1.3515[-3] |
| 22 | 1.0961[-3] | 1.1825[-3] | 1.0009[-3] | 1.2014[-3] | 2.0571[-3] | 1.3799[-3] |
| 23 | 1.1032[-3] | 1.1851[-3] | 1.0164[-3] | 1.2263[-3] | 2.0363[-3] | 1.4108[-3] |
| 24 | 1.1096[-3] | 1.1871[-3] | 1.0329[-3] | 1.2533[-3] | 2.0083[-3] | 1.4441[-3] |
| 25 | 1.1172[-3] | 1.1898[-3] | 1.0514[-3] | 1.2827[-3] | 1.9755[-3] | 1.4811[-3] |
| 26 | 1.1242[-3] | 1.1924[-3] | 1.0711[-3] | 1.3150[-3] | 1.9395[-3] | 1.5219[-3] |
| 27 | 1.1307[-3] | 1.1942[-3] | 1.0921[-3] | 1.3645[-3] [g] | 1.9007[-3] | 1.5675[-3] |
| 28 | 1.1370[-3] | 1.1962[-3] | 1.1147[-3] | 1.3868[-3] | 1.8623[-3] | 1.6187[-3] |
| 29 | 1.1446[-3] | 1.1989[-3] | 1.1402[-3] | 1.4268[-3] | 1.8207[-3] | 1.6737[-3] |

[a]The $(2p^2)\ {}^3P_0 \rightarrow (2s2p)\ {}^3P_1^o$ transition
[b]The $(2p^2)\ {}^3P_1 \rightarrow (2s2p)\ {}^3P_2^o$ transition
[c]The $(2p^2)\ {}^3P_1 \rightarrow (2s2p)\ {}^3P_1^o$ transition
[d]The $(2p^2)\ {}^3P_1 \rightarrow (2s2p)\ {}^3P_0^o$ transition
[e]The $(2p^2)\ {}^3P_2 \rightarrow (2s2p)\ {}^3P_2^o$ transition
[f]The $(2p^2)\ {}^3P_2 \rightarrow (2s2p)\ {}^3P_1^o$ transition
[g]With first-order energies.

$$(\Delta h_I)_{JM} = -\frac{ie}{\hbar}\{[h,\chi_{JM}] - \hbar\omega\chi_{JM}\}, \tag{A4}$$

for *local* potential. Here, $\chi_{JM}$ is the gauge function. With the aid of Eq. (A4), Eq. (A3) can be expressed as

$$\Delta H_{JM} = -\frac{ie}{\hbar}\{[H_0,X_{JM}] - \hbar\omega X_{JM}\}, \tag{A5}$$

where

$$X_{JM} = \sum_{ij} (\chi_{JM})_{ij} a_i^\dagger a_j . \tag{A6}$$

The change in first-order amplitude under the gauge transformation is given by

$$\begin{aligned}\langle F|\Delta T_{JM}^{(1)}|I\rangle^{(1)} &= \langle \Psi_F^{(0)}|\Delta T_{JM}^{(1)}|\Psi_I^{(0)}\rangle = \frac{i}{ec}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}} \\ &\times \langle \Psi_F^{(0)}|\Delta H_{JM}|\Psi_I^{(0)}\rangle \\ &= \frac{1}{\hbar c}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}}\langle \Psi_F^{(0)}|[H_0,X_{JM}] \\ &- \hbar\omega X_{JM}|\Psi_I^{(0)}\rangle = 0.\end{aligned} \tag{A7}$$

Therefore, the first-order amplitude is gauge independent, provided we start from a *local* potential. The change in second-order amplitude is given by

$$\begin{aligned}\langle F|\Delta T_{JM}^{(1)}|I\rangle^{(2)} &= \langle \Psi_F^{(0)}|\Delta T_{JM}^{(1)}|\Psi_I^{(1)}\rangle + \langle \Psi_F^{(1)}|\Delta T_{JM}^{(1)}|\Psi_I^{(0)}\rangle \\ &+ \delta\omega^{(1)}\langle \Psi_F^{(0)}|d\Delta T_{JM}^{(1)}/d\omega|\Psi_I^{(0)}\rangle .\end{aligned} \tag{A8}$$

With the aid of Eqs. (2.32), (A2), and (A5), the first term in Eq. (A8) can be rewritten as

TABLE VI. Transition probabilities (in $\sec^{-1}$) for the $(2s2p)\ {}^1P_1^o \rightarrow (2s^2)\ {}^1S_0$ transition in the Be-like ions.

| $Z$ | MCHF [a] | MCHF [b] | CI [b] | CI [b] | MCDF [c] | MBPT [d] | This work [e] | Expt. | Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 4 | | 5.54[8] | 5.53[8] | 5.55[8] | | 3.88[8] | 4.81[8] | 5.4(2)[8] | [1] |
| | | | | | | | | 5.6(2)[8] | [2] |
| 5 | 1.20[9] | | | | | 9.43[8] | 1.11[9] | 1.2(1)[9] | [2] |
| 6 | | | | | | 1.49[9] | 1.69[9] | 1.8(1)[9] | [3] |
| 7 | | | | | 2.334[9] | 2.04[9] | 2.25[9] | 2.35(8)[9] | [4] |
| 8 | | | | | 2.885[9] | 2.58[9] | 2.80[9] | 2.92(13)[9] | [4] |
| 10 | | | | | 4.003[9] | 3.70[9] | 3.92[9] | 4.3(6)[9] | [6] |
| 12 | | | | | 5.172[9] | 4.86[9] | 5.09[9] | 5.3(4)[9] | [7] |
| 14 | | | | | 6.430[9] | 6.10[9] | 6.34[9] | 6.7(5)[9] | [7] |

[a]Reference [25].
[b]Reference [21].
[c]Reference [9].
[d]Reference [37], with experimental energies.
[e]With experimental energies.

$$\langle \Psi_F^{(0)}|\Delta T_{JM}^{(1)}|\Psi_I^{(1)}\rangle = \frac{1}{\hbar c}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}}\langle \Psi_F^{(0)}|[H_0, X_{JM}] - \hbar\omega X_{JM}|\Psi_I^{(1)}\rangle = \frac{1}{\hbar c}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}}\{(E_F^{(0)} - E_I^{(0)} - \hbar\omega)$$
$$\times\langle \Psi_F^{(0)}|X_{JM}|\Psi_I^{(1)}\rangle - \langle \Psi_F^{(0)}|X_{JM}(E_I^{(1)} - V_I)|\Psi_I^{(0)}\rangle\} = -\frac{1}{\hbar c}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}}\langle \Psi_F^{(0)}|X_{JM}(E_I^{(1)}$$
$$- V_I)|\Psi_I^{(0)}\rangle. \tag{A9}$$

The second term in (A8) can be expressed as

$$\langle \Psi_F^{(1)}|\Delta T_{JM}^{(1)}|\Psi_I^{(0)}\rangle = \frac{1}{\hbar c}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}}\langle \Psi_F^{(1)}|[H_0, X_{JM}] - \hbar\omega X_{JM}|\Psi_I^{(0)}\rangle = \frac{1}{\hbar c}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}}\{(E_F^{(0)} - E_I^{(0)} - \hbar\omega)$$
$$\times\langle \Psi_F^{(1)}|X_{JM}|\Psi_I^{(0)}\rangle + \langle \Psi_F^{(0)}|(E_F^{(1)} - V_I)X_{JM}|\Psi_I^{(0)}\rangle\} = \frac{1}{\hbar c}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}}\langle \Psi_F^{(0)}|(E_F^{(1)} - V_I)X_{JM}|\Psi_I^{(0)}\rangle. \tag{A10}$$

The third term in Eq. (A8) can be expressed as

TABLE VII. Transition probabilities (in $\sec^{-1}$) for the $(2p^2)\ {}^1D_2 \rightarrow (2s2p)\ {}^1P_1^o$ transition in the Be-like ions.

| $Z$ | HF[a] | MBPT[b] | This work[c] | Expt.[d] |
|---|---|---|---|---|
| 4 | 1.27[7] | 2.36[6] | 9.79[6] | |
| 5 | | 5.30[7] | 6.56[7] | 6.4(3)[7] |

[a]Reference [20].
[b]Reference [37], with experimental energies.
[c]With experimental energies.
[d]Reference [14].

$$\delta\omega^{(1)}\langle\Psi_F^{(0)}|\frac{d\Delta T_{JM}^{(1)}}{d\omega}|\Psi_I^{(0)}\rangle=\frac{1}{\hbar c}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}}\delta\omega^{(1)}\langle\Psi_F^{(0)}|[H_0,dX_{JM}/d\omega]\quad-\hbar\omega dX_{JM}/d\omega-\hbar X_{JM}|\Psi_I^{(0)}\rangle$$

$$=\frac{1}{\hbar c}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}}\delta\omega^{(1)}\{(E_F^{(0)}-E_I^{(0)}-\hbar\omega)\langle\Psi_F^{(0)}|dX_{JM}/d\omega|\Psi_I^{(0)}\rangle-\hbar\langle\Psi_F^{(0)}|X_{JM}|\Psi_I^{(0)}\rangle\}$$

$$=-\frac{1}{c}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}}\delta\omega^{(1)}\langle\Psi_F^{(0)}|X_{JM}|\Psi_I^{(0)}\rangle. \tag{A11}$$

The sum of Eqs. (A9), (A10), and (A11) is

$$\frac{1}{\hbar c}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}}\{(E_F^{(1)}-E_I^{(1)}-\hbar\delta\omega^{(1)})\langle\Psi_F^{(0)}|X_{JM}|\Psi_I^{(0)}\rangle+\langle\Psi_F^{(0)}|[X_{JM},V_I]|\Psi_I^{(0)}\rangle\}$$

$$=\frac{1}{\hbar c}\sqrt{\frac{4\pi J}{(J+1)(2J+1)}}\langle\Psi_F^{(0)}|[X_{JM},V_I]|\Psi_I^{(0)}\rangle. \tag{A12}$$

The commutator $[X_{JM},V_I]$ vanishes, provided we *artificially* include the contributions from negative-energy states [38]. Therefore, the second-order amplitude is gauge independent, provided we start from a *local* potential and *artificially* include the contributions from the negative-energy states.


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