Volume 9, Number 10
1009-1963/2000/09(10)/0742-07
CHINESE PHYSICS
October, 2000
© 2000 Chin. Phys. Soc.

CALCULATION OF THE RELATIVISTIC CORRECTION ENERGIES OF Ne-LIKE IONS WITH ORBITAL POLARIZATION CORRECTION*

Li Xiang-dong (李向东), Tan Ming-liang (谭明亮),
Yi You-gen (易有根), Sheng Yong (盛 勇),
Jiang Gang (蒋 刚), Zhang Zhi-hong(张志红)†, and Zhu Zheng-he(朱正和)
Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, *China*
Zhao Yong-kuan (赵永宽) and Tang Yong-jian (唐永健)
Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, Chengdu 610003, *China*

(Received 10 July 1999; revised manuscript received 26 June 2000)

This paper reports the theoretical calculation of Breit, self-energy, and vacuum polarization corrections in the Ne-like system using multi-configuration Dirac-Fock method with the orbital polarization. The relations of these corrections with the atomic number and the orbital symmetries are shown and the calculated correction energies are compared with other calculated results. Our Breit correction energies are all smaller by 1eV as maximum than the other theoretical Breit correction energies and the differences reveal systematical relation with atomic number. It is found that the configuration interactions have great effect on Breit corrections while the orbital polarization has much smaller effect on Breit corrections. The self-energy and vacuum polarization obtained by our calculation are much different from that in previous literatures for some transitions.

Keywords: Ne-like, relativistic correction energy, orbital polarization
PACC: 3130, 3130J, 3120T, 3000, 3320

I. INTRODUCTION

Calculation of structure and properties of atoms with medium or higher atomic number requires more careful consideration of relativistic effects than that with low atomic numbers. This has been achieved using multi-configuration Dirac-Fock (MCDF) equation.[1,2] All such results have been based on an approximate relativistic many-electron Hamiltonian, H, in which interelectronic interaction is purely Coulombic. This kind of Hamiltonian is known not to be good enough for precise calculation of quantities such as binding energies of inner-shell electrons and transition energies in heavy atoms.[3] The results can be improved by including the Breit interaction[4−6] along with the self-energy (SE) and vacuum polarization (VP). In the non-relativistic limit, the Breit interaction yields the familiar Breit-Pauli Hamiltonain containing terms described as spin-other-orbital, spin-spin and orbital-orbital interactions whose effects are well known. Theoretical efforts based on MCDF or the relativistic many-body perturbation theory (RMBPT) methods have obtained relativistic transition energies including high-order electron-correlation effects, Breit interaction and quantum electrodynamics (QED) correction.[7−13] Unfortunately, due to the difficulties of calculation of QED effects, the accuracy of QED effects are not satisfactory so far. So the QED effects attracted much interest. Recently there is considerable interest in transition energies of Ne-like systems. So the study of relativistic correction energies of Ne-like system are popular. But much of the work just provided relativistic correction energies of Ne-like system for a specific transition.[8,10,12] In this paper we provide detailed calculation of the correction energies for Ne-like ions using MCDF methods with the orbital polarization and compared our results with the results from the literatures.

Due to its complication, the properties of the correction energy cannot be seen directly from the initial formulas of these corrections. It is clear that the properties of these correction energies depend on the elements, symmetry of orbital occupied by the electron and the type of level, even the coupling schemes. So the calculation of the correction energies for a specific element and the comparison of the corrections among different elements in the same isoelectronic sequence are important for the understanding of the properties

*Project supported by the Foundation of China Academy of Engineering Physics (Grant No. 98020207).
†Department of Physics, Yantai Teachers Collage, Yantai 264000, China.

of correction energy itself and the relations of the correction energy with the other physics quantities.

Ⅱ. THEORITICAL ATOMIC CORRECTION ENERGIES

A. Magnetic and retardation contributions

The dynamic correction to the electrostatic Coulomb interaction, which accounts the exchange of a single transverse photon, can be included through the transverse operator or the Breit operator in first order perturbation theory. The general form of the Breit interaction operators[14] is

$$\begin{aligned} B_\omega(\boldsymbol{r}_1,\boldsymbol{r}_2) =& -\alpha_1\cdot\alpha_2\frac{\cos(\omega R)}{R} \\ &+(\alpha_1\cdot\nabla)(\alpha_2\cdot\nabla)\frac{\cos(\omega R)-1}{\omega^2 R} \\ =& -\alpha_1\cdot\alpha_2\frac{\cos(\omega R)}{R} \\ &-(\alpha_1\cdot\nabla)(\alpha_2\cdot\nabla)\frac{\cos(\omega R)-1}{\omega^2 R} \\ =& -\alpha_1\cdot\alpha_2\frac{1}{R}-\frac{1}{2}(\alpha_1\cdot\nabla_1)(\alpha_2\cdot\nabla_2)R \\ &+O(\omega^2 R), \end{aligned} \tag{1}$$

where $\boldsymbol{r}_1$, $\boldsymbol{r}_1$ are particle position vectors; $\boldsymbol{R}=\boldsymbol{r}_1-\boldsymbol{r}_2$; ∇_1,∇_2,∇ are gradient operators corresponding to $\boldsymbol{r}_1,\boldsymbol{r}_2$ and $\boldsymbol{R}$, respectively. The symbol ω is the energy of the exchanged virtual photon divided by the velocity of light, c, both in atomic units. The symbol α_1 and α_2 are the usual Dirac matrices. In the low energy limit $\omega\to 0$, Eq.(1) reduces to a rather simple form.[14] In second quantised form, the transverse interaction may be written as[15]

$$\begin{aligned} H^{\mathrm{T}} =& \frac{1}{2}\sum_{\mathrm{pqrs}} N(b_{\mathrm{p}}^{+}b_q^{+}b_r b_{\mathrm{s}}) \\ &\left\langle \mathrm{pq}\left|\frac{1}{2}\left(B\left(\frac{\omega_{\mathrm{ps}}}{c},R\right)+B\left(\frac{\omega_{qr}}{c},R\right)\right)\right|\mathrm{sr}\right\rangle, \end{aligned} \tag{2}$$

where $b_{\mathrm{p}}^{+}(b_{\mathrm{p}})$ are anticommuting creation (destruction) operators for orbital p having one-electron energy ε_{p}(a.u.), $\omega_{\mathrm{ps}}=\varepsilon_{\mathrm{p}}-\varepsilon_{\mathrm{s}}$. Detailed derivations of the matrix of the Breit and generalized Breit interactions have been provided by Grant[1,2] and by Mann and Johnson[3] in terms of a sum products of angular factors and radial integrals.

B. Radiative corrections

There are two main radiative corrections to atomic electron energies: the self-energy and vacuum polarization. The self-energy arises from the electron's interaction with the radiation field, which leads to mean-square fluctuations in the electron position. The self-energy shift can be expressed, in atomic units, as[16]

$$\Delta E=\frac{1}{\alpha\pi}\frac{(\alpha Z)^4}{n^3}F(\alpha Z), \tag{3}$$

where Z is the atomic number, α the fine-structure constant, and n the principal quantum number. Tabulations of $F(\alpha Z)$ for 1s, 2s, 2p-, 2p are given by Mohr,[16] and the $F(\alpha Z)$ for orbitals $n\geq 3$ is estimated with Eqs.(1) and (2) in Ref.[17].

The second important radiative correction is the vacuum polarization (VP), which arises because the effective potential seen by the electron is modified by the polarized vacuum charge distribution due to the virtual electron-positron pairs. Expressions for the second- and fourth-order perturbation potentials that take finite nuclear size into account have been given as follows.[18]

(i) The second-order vacuum polarization potential

$$V_2(r)=-\frac{3}{2}\frac{Z\alpha e^2}{\pi r}K_1\left(\frac{2r}{\lambda\!\!\!^{-}_{\mathrm{e}}}\right), \tag{4}$$

where

$$K_1(x)=\int_1^\infty \mathrm{d}t\mathrm{e}^{-xt}\left(\frac{1}{t^2}+\frac{1}{2t^4}\right)(t^2-1)^{1/2}. \tag{5}$$

(ii) The fourth-order vacuum polarization potential

$$V_4(\boldsymbol{r})=-\frac{e^2\alpha^2}{\pi^2}\int \mathrm{d}^3\boldsymbol{r}'\frac{\rho(\boldsymbol{r}')}{\boldsymbol{r}-\boldsymbol{r}'}L_1\left(\frac{2}{\lambda\!\!\!^{-}_{\mathrm{e}}}|\boldsymbol{r}-\boldsymbol{r}'|\right), \tag{6}$$

where

$$\begin{aligned} L_1(x)=&\int_1^\infty \mathrm{d}t\mathrm{e}^{-xt}\left\{\left(-\frac{13}{54t^2}-\frac{7}{108t^4}-\frac{2}{9t^6}\right)(t^2-1)^{1/2}\right. \\ &+\left(\frac{44}{9t}-\frac{2}{3t^2}-\frac{5}{4t^5}-\frac{2}{9t^7}\right)\ln(t+(t^2-1)^{1/2}) \\ &+\left(-\frac{4}{3t^2}-\frac{2}{3t^4}\right)(t^2-1)^{1/2}\ln(8t(t^2-1)) \\ &+\left(\frac{8}{3t}-\frac{2}{3t^5}\right)\int_t^\infty \mathrm{d}y\left[\frac{3y^2-1}{y(y^2-1)}\right. \\ &\cdot\ln(y+(y^2-1)^{1/2}) \\ &\left.\left.-\frac{1}{(y^2-1)^{1/2}}\ln(8y(y^2-1))\right]\right\}. \end{aligned} \tag{7}$$

In our calculation the fourth-order vacuum polarization potential is used.

Ⅲ. RESULTS AND DISCUSSION

1. In order to test our calculated correction energies, we first calculate the transition energies for Yb^{60+}(Z=70) Ne-like ion state, since we can obtain its experimental self energy for the transition 3A $(1s^22s_{1/2}2p^63p_{3/2})_{J=1} \rightarrow (1s^22s^22p^6)$. We list our results against the results from Ref.[8] in Table 1.

Table 1. Comparison of the transition energy (in eV) for line 3A $(1s^22s_{1/2}2p^63p_{3/2})_{J=1} \rightarrow (1s^22s^22p^6)$ of Ne-like Yb^{60+}(Z=70).

	Transition energy	$E_{\rm Breit}$	$E_{\rm VP}$	$E_{\rm SE}$
Experiment	9341.86	/	/	–18.37
Results from Ref.[8]	9344.80	–15.40	+3.09	–16.49[a)]
				–19.91[b)]
Our results	9341.42	–16.40	+3.19	–17.61

a) Self-energy calculated using the effective-charge approach.[8]

b) Self-energy calculated assuming hydrogenic wave function and bare ytterbium nucleus.[8]

Table 1 shows that our calculated transition energy for 3A of Ne-like Yb^{60+} is almost the same as the experimental value while the results from Ref.[8] have 2.94 eV differences from the experiment. The discrepancies between our calculations and Ref [8] mainly come from the estimation of the Breit and self-energy(SE) correction energy. The cause for this kind of difference will be discussed below. Although the fourth-order vacuum polarization(VP) potential is used in our calculations while the second-order vacuum polarization(VP) potential is used in Ref.[8], the differences between $E_{\rm VP}$ are small. The self-energy in our calculation is more close to the experimental self-energy than that from Ref.[8]. This confirms that our calculation, which considers the orbital polarization, is relatively reliable. In Table 2 we compare the Breit and QED corrections calculated with different methods from Ref.[10].

Table 2. Comparison of Breit and QED corrections (in Hartree) to the transition $(2s_0^2 2p_0^{-2} 2p_{3/2}^3 3s_{1/2})_{J=2} \rightarrow$gs(M2) with the different calculation methods.

Theoretical results	Method	Ag^{37+}	Xe^{44+}	La^{47+}	Nd^{50+}	Eu^{53+}
$E_{\rm Breit}$	MBPT[a)]	–0.154	–0.244	–0.291	–0.343	–0.399
	$MCDF_1$[a)]	–0.161	–0.253	–0.300	–0.352	–0.410
	MCDF[b)]	–0.176	–0.273	–0.322	–0.377	–0.436
$E_{\rm QED}$	MBPT[a)]	0.024	0.038	0.045	0.053	0.061
	$MCDF_1$[a)]	0.025	0.040	0.049	0.057	0.067
	MCDF[b)]	0.023	0.036	0.042	0.050	0.058

a) Theoretical results from Ref.[10]. $MCDF_1$ is the same method as we used in this paper except the calculation of VP and choice of the configurations.

b) Our calculated results.

Table 2 shows that all of our Breit corrections are smaller than both MBPT and $MCDF_1$ and the differences can affect the atomic fine structure. We have compared our calculated transition energies of M2 with both MBPT and $MCDF_1$ and found that our results for M2 have only 0.2 eV difference from experimental values.[19,20] On the other hand, since the M2 transition does not involve in hole-state, the ground-state correlation and Coster-Kronig fluctuation for M2 should be small so that they are ignored in M2. Obviously our results for M2 transition are reliable, although we do not estimate the residual electron correlation. For the transitions involving inner-shell electron, the residual electron correlation can be made up by polarization potential.[19] So our calculation of correction energies should be relatively reliable.

2. In order to study the regularity of correction energies in Ne-like ions, we calculated the Breit, VP and SE correction energy contributions for each orbital involving n=3 and n=2 shells. We give all the results in Figs.1–3.

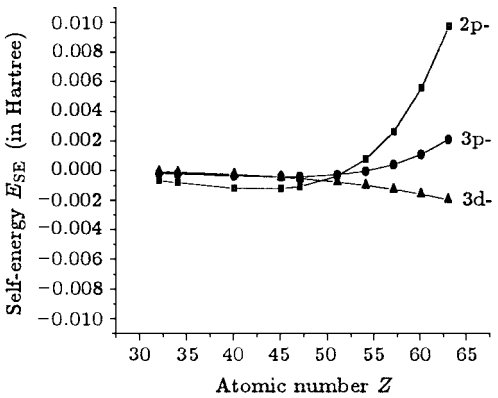


Fig.1. The self-energy of orbitals vs atomic number curve.

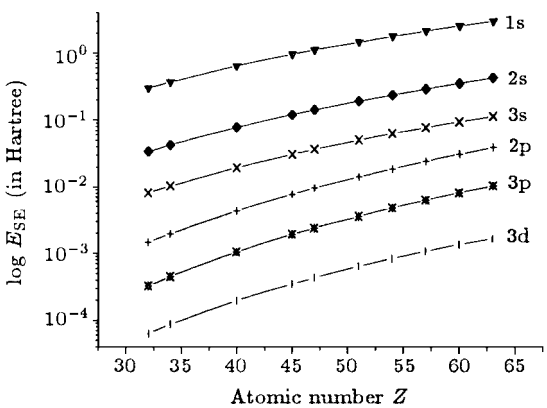


Fig.2. The self-energy of orbitals vs atomic number curve.

Figures 1 and 2 show the change of self-energy of each orbital with the atomic number. In our calculation we used the relativistic orbital notations. All the orbitals involving n=3 and n=2 shells can be expressed as 1s, 2s, 2p-, 2p, 3s, 3p- 3p, 3d- and 3d. Firstly, the absolute contributions of self-energy to all of the orbitals increase with the atomic number. The self-energy of 1s, 2s, 2p, 3p and 3d show the same tendency with the change of atomic number. The tendency, in certain extent, almost has no relationship with the orbital symmetries. The only difference among these orbitals is the different contributions to the self-energy. All of the self-energy of these orbitals are positive. The orbitals with the symmetry s provide the biggest self-energy contributions. Table 3 lists the VP and SE contributions to each orbital for Ne-like Eu^{53+}. These are the biggest contributions to each orbital in the elemental range $32 \leq Z \leq 63$ of recent interest. It can be seen that VP<SE and VP decrease more rapidly with the reduction of orbital symmetry than SE does. Figure 3 also shows that the absolute values of VP increase with atomic number and when the principal quantum number n is increased the tendency become smooth. So the SE and VP contributions to heavy atoms become more important in calculating the atomic fine structure.

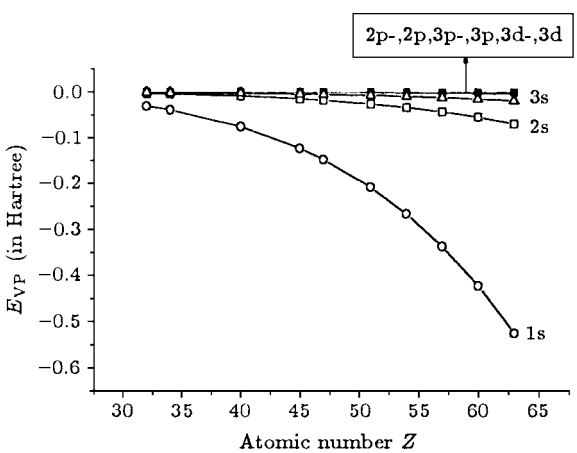


Fig.3. The energy of VP vs atomic number curve.

Table 3. VP and SE contributions (in Hartree) to each orbital for Ne-like Eu^{53+}.

	1s	2s	2p-	2p	3s	3p-	3p	3d-	3d
SE	3.096	4.38(−1)	9.84(−3)	4.05(−2)	1.17(−1)	2.20(−3)	1.06(−2)	−1.84(−3)	1.72(−3)
VP	−5.25(−1)	−6.90(−2)	−4.30(−3)	−4.04(−4)	−1.85(−2)	−1.33(−3)	−1.30(−4)	−1.22(−6)	−2.77(−7)

Figure 1 shows the relations of the self-energy in orbitals 2p-, 3p- and 3d- with atomic number. It can be seen that the self-energy changes smoothly with the atomic number when the orbital symmetry reduces or the orbital principal quantum number increases. The dominant contribution to self-energy for these three orbitals is from the orbital 2p- of Ne-like Eu^{53+}(Z=63) and it is about −0.27eV. So the self-energy contributions of 2p-, 3p- and 3d- have small effects on the calculation. Thus in single electron transition the SE contributions of these three orbitals can be neglected. Figures 1 and 2 reveal that the self-energies have close relations with symmetries of orbital, principal quantum number n and atomic number: (a) The

self-energy first decreases rapidly with the reduction of the orbital symmetry. Then the self-energy decreases with the increase of principal quantum number n. When n=3 (M shell) in Ne-like ions the contributions to self-energy can be ignored. (b) The absolute values of self-energy for all of the orbitals increase with the atomic number.

Figure 3 illustrates the dependence of VP on the atomic number for all orbitals. The electrons in s orbital give the dominant contributions to VP energy and the VP energy also decreases with the increase of the principal quantum number n. In this case the VP contributions are almost zero for 2p-, 2p, 3p-, 3p, 3d-, 3d in the Ne-like ions. Therefore, the effects of VP contributions mainly relate to s orbital for Ne-like systems.

3. For a specific configuration state function (CSF) the QED contributions are the sum of self-energy and VP energies of all electrons which construct the CSF. For a transition the QED contributions are the subtraction between the QED corrections of the upper and the lower levels. Table 4 lists the comparison of our calculated correction energies for the transitions from n=3 to n=2 Ne-like systems with other theoretical results.

Table 4. Comparison of our calculated correction energies for the transitions from n=3 to n=2 Ne-like systems with other theoretical results. The transition energies are arranged in an increasing order from upper row to lower row for the same element. All quantities are in units of eV.

Elements	Transition	$E^{1}_{\rm Breit}$ [a]	$E^{2}_{\rm Breit}$ [a]	$E^{2}_{\rm Breit}-E^{1}_{\rm Breit}$	$E^{1}_{\rm VP}$ [a]	$E^{2}_{\rm VP}$ [a]	$E^{1}_{\rm SE}$ [a]	$E^{2}_{\rm SE}$ [a]
Ag	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3s_{1/2})_{J=2} \rightarrow$gs(M2)	–4.39	–4.80	–0.41	–0.14	–0.12	+0.83	+0.74
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3s_{1/2})_{J=1} \rightarrow$gs(3G)	–4.30	–4.71	–0.41	–0.14	–0.12	+0.83	+0.74
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3p\text{-}_{1/2})_{J=2} \rightarrow$gs(E2L)	–3.62	–4.05	–0.43	–0.02	–0.002	–0.09	–0.27
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3p_{3/2})_{J=2} \rightarrow$gs(E2M)	–4.12	–4.55	–0.43	–0.02	+0.001	–0.02	–0.19
	$(2s^2_0 2p\text{-}_{1/2} 2p^4_{1/2} 3s_{1/2})_{J=1} \rightarrow$gs(3F)	–7.29	–7.71	–0.42	–0.12	–0.11	+1.11	+1.02
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3d_{5/2})_{J=1} \rightarrow$gs(3D)	–5.21	–5.64	–0.43	–0.02	+0.0017	–0.07	–0.25
	$(2s^2_0 2p\text{-}_{1/2} 2p^4_{1/2} 3p_{3/2})_{J=2} \rightarrow$gs(E2U)	–7.33	–7.76	–0.43	–0.00	+0.014	+0.27	+0.09
	$(2s^2_0 2p\text{-}_{1/2} 2p^4_{1/2} 3d\text{-}_{3/2})_{J=1} \rightarrow$gs(3C)	–7.95	–8.37	–0.42	–0.00	+0.017	+0.19	–0.011
	$(2s_{1/2} 2p\text{-}^2_{1/2} 2p^4_{1/2} 3p\text{-}_{1/2})_{J=1} \rightarrow$gs(3B)	–2.98	–3.42	–0.44	+0.44	+0.467	–3.52	–3.87
	$(2s_{1/2} 2p\text{-}^2_{1/2} 2p^4_{1/2} 3p_{3/2})_{J=1} \rightarrow$gs(3A)	–3.73	–4.17	–0.44	+0.45	+0.473	–3.47	–3.81
Xe	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3s_{1/2})_{J=2} \rightarrow$gs(M2)	–6.88	–7.43	–0.55	–0.26	–0.23	+1.36	+1.21
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3s_{1/2})_{J=1} \rightarrow$gs(3G)	–6.74	–7.28	–0.54	–0.26	–0.23	+1.36	+1.21
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3p\text{-}_{1/2})_{J=2} \rightarrow$gs(E2L)	–5.61	–6.18	–0.57	–0.04	–0.0072	–0.23	–0.52
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3p_{3/2})_{J=2} \rightarrow$gs(E2M)	–6.49	–7.06	–0.57	–0.03	–0.0030	–0.11	–0.38
	$(2s^2_0 2p\text{-}_{1/2} 2p^4_{1/2} 3s_{1/2})_{J=1} \rightarrow$gs(3F)	–11.29	–11.85	–0.56	–0.18	–0.16	+1.39	+1.36
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3d_{5/2})_{J=1} \rightarrow$gs(3D)	–8.79	–9.35	–0.56	–0.07	–0.027	+0.23	–0.15
	$(2s^2_0 2p\text{-}_{1/2} 2p^4_{1/2} 3p_{3/2})_{J=2} \rightarrow$gs(E2U)	–11.91	–12.48	–0.57	+0.01	+0.038	+0.39	+0.11
	$(2s^2_0 2p\text{-}_{1/2} 2p^4_{1/2} 3d\text{-}_{3/2})_{J=1} \rightarrow$gs(3C)	–12.81	–13.36	–0.55	+0.02	+0.047	+0.2	–0.11
	$(2s_{1/2} 2p\text{-}^2_{1/2} 2p^4_{1/2} 3p\text{-}_{1/2})_{J=1} \rightarrow$gs(3B)	–4.84	–5.42	–0.58	+0.84	+0.88	–5.98	–6.488
	$(2s_{1/2} 2p\text{-}^2_{1/2} 2p^4_{1/2} 3p_{3/2})_{J=1} \rightarrow$gs(3A)	–6.09	–6.67	–0.58	+0.86	+0.89	–5.92	–6.416
	$(2s_{1/2} 2p\text{-}^2_{1/2} 2p^4_{1/2} 3d_{5/2})_{J=2} \rightarrow$gs(E2S)	–6.95	–7.52	–0.57	+0.86	+0.89	–6.05	–6.537
La	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3s_{1/2})_{J=2} \rightarrow$gs(M2)	–8.17	–8.779	–0.61	–0.33	–0.300	+1.65	+1.452
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3s_{1/2})_{J=1} \rightarrow$gs(3G)	–7.99	–8.602	–0.61	–0.33	–0.300	+1.65	+1.452
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3p\text{-}_{1/2})_{J=2} \rightarrow$gs(E2L)	–6.33	–7.265	–0.94	–0.05	–0.011	–0.32	–0.663
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3d_{5/2})_{J=1} \rightarrow$gs(3D)	–10.06	–10.69	–0.63	–0.04	–0.003	–0.26	–0.546
	$(2s^2_0 2p\text{-}_{1/2} 2p^4_{1/2} 3s_{1/2})_{J=1} \rightarrow$gs(3F)	–14.04	–14.67	–0.63	–0.27	–0.239	+2.17	+1.943
	$(2s^2_0 2p\text{-}_{1/2} 2p^4_{1/2} 3p_{3/2})_{J=2} \rightarrow$gs(E2U)	–14.39	–15.05	–0.66	+0.02	+0.055	+0.43	+0.097
	$(2s_{1/2} 2p\text{-}^2_{1/2} 2p^4_{1/2} 3p_{3/2})_{J=1} \rightarrow$gs(3A)	–7.37	–8.028	–0.66	+1.11	+1.155	–7.29	–7.873
	$(2s_{1/2} 2p\text{-}^2_{1/2} 2p^4_{1/2} 3d_{5/2})_{J=2} \rightarrow$gs(E2S)	–8.39	–9.032	–0.64	+1.11	+1.158	–7.47	–8.030
Nd	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3s_{1/2})_{J=2} \rightarrow$gs(M2)	–9.59	–10.27	–0.68	–0.42	–0.386	+1.97	+1.752
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3s_{1/2})_{J=1} \rightarrow$gs(3G)	–9.38	–10.06	–0.68	–0.42	–0.386	+1.97	+1.752
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3d_{5/2})_{J=1} \rightarrow$gs(3D)	–11.66	–12.36	–0.70	–0.04	+0.007	–0.45	–0.810
	$(2s^2_0 2p\text{-}_{1/2} 2p^4_{1/2} 3s_{1/2})_{J=1} \rightarrow$gs(3F)	–16.99	–17.69	–0.70	–0.35	–0.309	+2.67	+2.434
Eu	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3s_{1/2})_{J=2} \rightarrow$gs(M2)	–11.15	–11.89	–0.74	–0.54	–0.492	+2.35	+2.081
	$(2s^2_0 2p\text{-}^2_0 2p^3_{3/2} 3s_{1/2})_{J=1} \rightarrow$gs(3G)	–10.90	–11.64	–0.74	–0.54	–0.492	+2.35	+2.081

[a] The quantities with the upper label 1 are the theoretical results from Ref.[12] and those with the upper label 2 are our calculated results.

In Table 4 all of our calculations of Breit correction energies are smaller than the theoretical Breit corrections in Ref.[12]. The discrepancies increase only with the atomic number. We believe these discrepancies partly come from the choice of orbital polarization in our calculation and partly from the choice of electron configurations, e.g., from the estimation of configuration interactions. Our calculation show that the effects of orbital polarization on Breit contributions are small, for instance, they are within 0.15 eV for Eu^{53+} and within 0.02 eV for Ge^{22+}. It is so small that the orbital polarization almost has no effect on Breit contribution to transition energy. On the other hand, the choice of different set of configurations has great effects as high as 1 eV (in the atomic range $32 \leq Z \leq 70$) on the Breit energy. It is obvious that the differences between our calculations and those from Ref [12] for Breit contributions come from different choices of configurations. The Breit contributions to the transition energies are the principal corrections in calculation of the atomic transition energy (see Table 4).

The VP energy correction and self-energy correction (QED effects) are relatively smaller than the Breit correction. For a certain type of transitions, such as 3G, M2, 3A and 3B, which involve the transition of s electron, however, the VP and self-energy contributions are large enough to affect the fine structure. From our calculations of VP and self-energy contributions to each orbital, we deduced that the transitions involving the s electron, especially the s electron with low principal quantum number, are greatly affected by the QED effects. In our calculations we used fourth-order VP potential while Ref.[12] used second-order VP potential. Theoretically our results should be more accurate. Table 4 shows that all of our VP contributions to transition energies are smaller than the values in Ref [12]. The differences between SEs may come from the relativistic orbitals. Our calculation shows that there are little effects on either VP or SE due to the configuration interaction and orbital polarization.

4. Our calculation contains twelve elements in the range from Z=32 to Z=70. The transitions from n=3 to n=2 for Ne-like sequences involving 35 CSFs. The change of Breit, VP and SE contributions of these 35 CSFs with atomic number are shown in Figs.4–6.

Figures 4–6 contain all of the 35 CSFs involved in n=3 and n=2 Ne-like ions. They show that SE is the main part of the QED contributions to the different type of CSF. Our calculations show that the SE contributions to QED are as large as about 7–10 times VP contribution to QED in Ne-like systems in the atomic range $32 \leq Z \leq 63$. In Figs.4–6 the curves are divided into two groups. The first group contains eight CSFs related to 2s hole states and the second group contains the remain twenty-seven CSFs. Although the curves in the first and the second groups are almost overlapped, the differences in the first group or in the

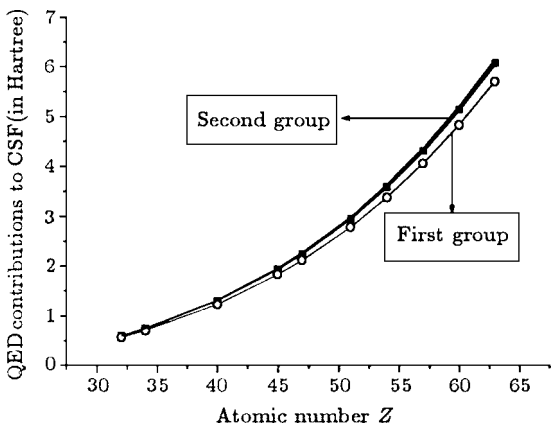


Fig.4. QED contributions to CSF vs atomic number.

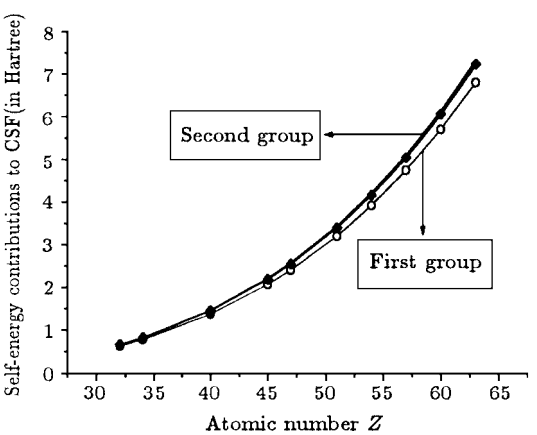


Fig.5. The self-energy contributions to CSF vs atomic nubmer.

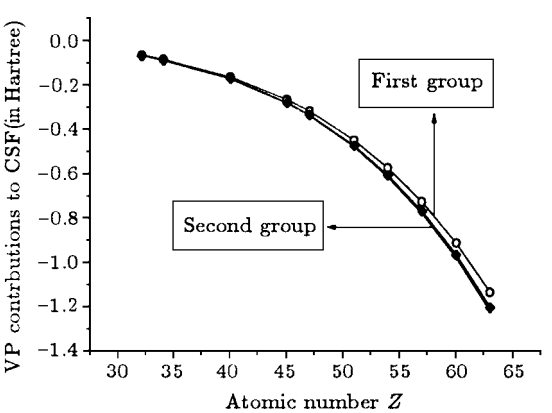


Fig.6. VP contributions to CSF vs atomic number.

second group still exist. As a special case for the QED, the biggest discrepancy of QED contributions is 0.3379 eV for the first group and 3.676 eV for the second group. So in Ne-like system the QED contributions to CSFs, which involved in 2s hole states, can be taken as a constant for a given atom. For example, the QED contributions to 2s hole states of Ag^{37+} are about 57.3748 eV.

IV. CONCLUSION

This paper reports a detailed calculation and discussion on Breit and QED corrections for Ne-like ions. It is shown that the Breit corrections are greatly affected by the configuration interactions. Since the Breit correction is the main part of all corrections, so the paper demonstrates the importance of the proper choice of configurations in the atomic structure calculation. Breit, VP and SE are all independent of the oribital polarization, and VP and SE are little affected by the configuration interactions. It is also shown that the identification of relativistic symmetries nl and nl_- is also important for transition energies. A full collection of the results can be obtained on request.

REFERENCES

[1] I. P. Grant, *Adv. Phys.,* **19**(1970), 747; *Comp. Phys. Commun.,* **5**(1973),263; *J. Phys.,* **B3**(1974),1571.

[2] I. P. Grant, D. F. Mayers, N. C. Pyper, *J. Phys.,* **B9** (1976),2777.

[3] J. B. Mann, W. R. Johnson, *Phys. Rev.,* **A4**(1971),383.

[4] G. Breit, *Phys. Rev.,* **34**(1929),553; *Phys. Rev.,* **36**(1930), 383; *Phys. Rev.,* **39**(1932),616.

[5] E. E. Salpeter, *Phys. Rev.,* **A6**(1952),2395.

[6] J. C. Slater, Quantum Theory of Atomic Structure, Vol.**2**(1974),p.189.

[7] T. J. Scholl, R. Cameron, S. D. Rosner, L. Zhang, R. A. Holt, Craig J. Sansonetti, *Phys. Rev. Lett.,* **71** (1993),2188.

[8] P. Beiersdorfer, M. H. Cheng, R. E. Marrs, M. A. Levine, *Phys. Rev.,* **A41**(1990),3453.

[9] A. Simionouici, D. D. Dietrich, R. Keville, T. Cowan, P. Beiersdorfer, *Phys. Rev.,* **A48**(1993),3056.

[10] E. Avgoustoglou, W. R. Johson, Z. W. Liu, J. Sapirstein, *Phys. Rev.,* **A51**(1995),1196.

[11] J. E. Rice, K. B. Fournier, J. L. Terry, M. A. Graf, M. Finkenthal, *Phys. Rev.,* **A53**(1996),3953.

[12] P. Beiersdorfer, S. Von Goeler, M. Bitter, E. Hinnov, R. Bell, M. H. Cheng, *Phys. Rev.,* **A37**(1988),4153.

[13] J. F. Seely, R. A. Wagner, *Phys. Rev.,* **A41**(1990),5246.

[14] I. P. Grant, N. C. Pyper, *J. Phys.,* **B9**(1976),761.

[15] I. P. Grant, B. J. Mckenzie, *J. Phys.,* **B13**(1980),2671.

[16] P. J. Mohr, *Phys. Rev. Lett.,* **34**(1975),1050; *Phys. Rev.,* **A26**(1982),2338.

[17] S. Klarsfeld, A. Maquet, *Phys. Lett.,* **43B**(1973),201.

[18] L. W. Fullerton, G. A. Rinker, *Phys. Rev.,* **A13** (1976),1283.

[19] X. D. Li, M. L. Tan, Y. G. Yi, Z. H. Zhu, *Chinese Physics,* **9**(2000),13.

[20] X. D. Li, M. L. Tan, Y. G. Yi, Z. H. Zhu, *Chinese Physics,* **9**(2000),100.