Relativistic excitation energies and oscillator strengths for transitions in Zn-like ions including core-polarization effects

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Excitation energies and oscillator strengths from the $^1S_0$ ground state to the first $^3P_1^o$ and $^1P_1^o$ excited states of Zn-like ions are calculated by using the multiconfiguration relativistic random-phase approximation including excitation channels from core electrons. The disagreements among theories and experiments are much reduced but in general remain.

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I. INTRODUCTION

Accurate values of the excitation energies and oscillator strengths for the Zn-like ions are required in fusion studies because of the presence of many heavy-metal impurities in high-temperature plasmas [1]. Systematic studies of oscillator strengths in Zn-like ions have been performed by beam-foil techniques [2–10]. A Hartree-Fock (HF) calculation [11] yielded oscillator strengths for the resonance transition $(4s^2)^1S_0 \rightarrow (4s4p)^1P_1^o$ in Zn-like ions which were approximately 40% greater than the cascade-corrected experimental results. The multiconfiguration Hartree-Fock (MCHF) calculation [11] accounted for a major part of the disagreements. The inclusion of the core-polarization (CP) effects further reduced the disagreements. Because of the lacking relativistic effects, the MCHF results deviated from the experimental excitation energies [6–22] drastically for highly ionized ions. Shorer [23] performed a relativistic random-phase approximation (RRPA) calculation with the $3d$ core excitation channels for the resonance transition in Zn-like ions, and their results were more or less in line with the MCHF results for low-Z ions. Empirical lifetimes for the intercombination transition $(4s^2)^1S_0 \rightarrow (4s4p)^3P_1^o$ and the resonance transition were reported by Curtis [24],which provided a convenient exposition for sensitive comparison between experimental results and *ab initio* calculations.

The RRPA is based on a single-configuration reference state and is appropriate only for a description of excitations of a single valence electron in closed-shell systems. Double excitation effects in open-shell systems cannot be treated in the RRPA formulation. The RRPA can be improved upon by using a multiconfiguration wave function as the reference state. The electron-electron correlation effects due to the presence of "real" doubly excited configurations in the initial state are thereby included. This approach is called the multiconfiguration relativistic random-phase-approximation theory (MCRRPA) [25]. From the MCRRPA theory, we are able to perform gauge-invariant calculations including both relativistic and correlation effects in open-shell atoms. The MCRRPA approach includes the effects of certain two-particle–two-hole correlations to all orders and provides an *ab initio* method for treating the CP effects. Applications of the MCRRPA to photoexcitations of Be-, Mg-, and Pb-like ions [26–29] and to photoionization of Be, Mg, Zn, and Sr atoms [30–34] have been carried out and were in good agreement with experiment. Nevertheless, significant discrepancies existed in the $^3P_1^o$-$^1P_1^o$ separations and oscillator strengths between the MCRRPA and experimental results for the Zn-, Cd-, and Hg-like ions [27,35–37]. In recent papers [38–40], we performed large-scale MCRRPA calculations including core excitation channels for the intercombination and resonance transitions in Cd- and Hg-like ions. The inclusion of core excitation channels substantially improved the agreement between the theoretical and experimental results for the $^3P_1^o$-$^1P_1^o$ separations and oscillator strengths. In this paper, we perform a large-scale MCRRPA calculation including excitation channels from core electrons for the intercombination transition $(4s^2)^1S_0 \rightarrow (4s4p)^3P_1^o$ and the resonance transition $(4s^2)^1S_0 \rightarrow (4s4p)^1P_1^o$ in Zn-like ions. The present approach provides an *ab initio* method for treating the CP effects. In Sec. II, we give an introduction to the MCRRPA theory. Results and discussion are presented in Sec. III.

II. THE MCRRPA THEORY

The MCRRPA theory has been presented in detail in a previous paper [25]. Only a summary of the essential features will be given here. We describe the atomic system as a superposition of configuration wave functions with time-dependent weight coefficients. An external field induces perturbations for both electronic orbitals and weight coefficients. Application of the time-dependent variational principle leads to the time-dependent MCDF equations describing the response of the atom to the external field. We expand the time-dependent MCDF equations in powers of the external field. By equating to zero the terms containing neither the external field nor the perturbations, we obtain the zero-order equations, which are just the usual MCDF equations. By linearizing in the perturbations and the external field, we obtain the MCRRPA equations which describe the linear response of the atoms to the external field. If we start from a single-configuration reference state, the MCRRPA equations reduce to the usual RRPA equations. If intershell correlation is neglected, the truncated MCRRPA formulation results. To implement it, we neglect all virtual perturbations of MCDF orbitals which are not in the shell of interest.

In the MCRRPA formulation, the ground reference state of Zn-like ions is given by the multiconfiguration wave function as

$$\Psi = C_1(4s^2_{1/2})_0 + C_2(4p^2_{1/2})_0 + C_3(4p^2_{3/2})_0 , \tag{2.1}$$

where $(4l_j^2)_0$ denotes a Slater determinant constructed from the $(4l_j)$ valence orbitals and core orbitals, and the subscript 0 denotes the total angular-momentum quantum number $J=0$. The coefficients C_a $(a=1,2,3)$ in Eq. (2.1) are configuration weights. Because of numerical difficulties, we have not included the $4d^2$ configurations, but they may have non-negligible effects. The core and valence orbitals and the configuration weights are determined by solving the MCDF equations numerically. Since the MCRRPA equations include all one-particle excitations of the ground state, they automatically include, in addition to the usual RRPA correlation effects, the important final-state correlations between configurations with an excited electron and excited $4p_{1/2}$ or $4p_{3/2}$ ionic cores. These two-particle–two-hole final-state correlations were omitted in previous RRPA studies. A full solution of the MCRRPA equation for the intercombination and resonance transitions in Zn-like ions requires a solution of twenty-nine pairs of coupled equations. Previous MCRRPA calculations [27,35] neglected all virtual excitations of the core electrons, so the CP effects were completely neglected. In the present calculation, we include excitation channels from $3d$ electrons, so the CP effects of the $3d$ electrons are treated. Thirteen excitation channels are considered in the electric dipole approximation:

(i) Core excitation channels

$$\begin{aligned} &3d_{3/2} \rightarrow np_{1/2}, np_{3/2}, nf_{5/2} , \\ &3d_{5/2} \rightarrow np_{3/2}, nf_{5/2}, nf_{7/2} , \end{aligned} \tag{2.2}$$

(ii) Valence excitation channels

$$\begin{aligned} &4s_{1/2} \rightarrow np_{1/2}, np_{3/2} , \\ &4p_{1/2} \rightarrow ns_{1/2}, nd_{3/2} , \\ &4p_{3/2} \rightarrow ns_{1/2}, nd_{3/2}, nd_{5/2} . \end{aligned} \tag{2.3}$$

The first six excitation channels associated with the excitations of $3d$ orbitals electrons accounts for the polarization of these orbitals.

III. RESULTS AND DISCUSSION

Excitation energies for the intercombination transitions in Zn-like ions are presented in Table I. The CP effects reduced the intercombination excitation energies slightly from 0.1% to 0.4%. The intercombination excitation energies from the MCRRPA with CP effects are in poorer agreement with experiment than those without CP effects.

Excitation energies from the resonance transitions in Zn-like ions are presented in Table II. Because of the nonrelativistic formulation, the HF and MCHF resonance excitation energies for medium- and high-Z ions were in much poorer agreement with experiment than the RRPA results. The use of multiconfiguration wave functions as the reference state in the MCRRPA calculation increased the resonance excitation energies. The CP effects reduce the excitation energies for both transitions,

TABLE I. Excitation energies (in cm^{-1}, 1 a.u. = 219 474.6306 cm^{-1}) for the intercombination transition $(4s^2)^1S_0 \rightarrow (4s4p)^3P_1^o$ in Zn-like ions.

Ion	MCRRPA I[a]	MCRRPA II[b]	Expt.
Zn	28 483	28 358	32 501[c]
Ga^{1+}	43 998	43 886	47 816[c]
Ge^{2+}	58 793	58 683	62 496[c]
As^{3+}	73 305	73 195	76 962[c]
Br^{5+}	102 073	101 953	106 431[c]
			105 675[d]
Kr^{6+}	116 450	116 328	120 080[e]
Rb^{7+}	130 884	130 752	134 522[f]
Nb^{11+}	189 528	189 321	193 084[g]
Mo^{12+}	204 474	204 237	207 980[g]
Ag^{17+}	281 143	280 680	284 251[h]
Cd^{18+}	296 875	296 350	299 838[h]
I^{23+}	377 507	376 610	
Xe^{24+}	394 029	393 044	396 040[i]
Cs^{25+}	410 683	409 606	
Ba^{26+}	427 473	426 297	

[a]Reference [27].
[b]The present calculation including core excitation channels.
[c]Reference [13].
[d]Reference [19].
[e]Reference [6].
[f]Reference [20].
[g]Reference [17].
[h]Reference [22].
[i]Reference [21].

TABLE II. Excitation energies (in cm^{-1}) for the resonance transition $(4s^2)^1S_0 \rightarrow (4s4p)^1P_1^o$ in Zn-like ions.

Ion	HF[a]	MCHF[a]	RRPA		MCRRPA		Expt.
			I[b]	II[c]	I[d]	II[e]	
Ga^{1+}	66 084	69 244	67 532	64 833	70 168	68 017	70 700[f]
Ge^{2+}	88 141	90 160	89 831		92 254	89 388	91 873[f]
As^{3+}	108 157	109 496			113 065	109 678	112 022[f]
Br^{5+}	145 490	146 060	151 130	146 565	153 281	149 137	151 274[f]
Kr^{6+}	163 421	163 728			173 209	168 774	170 832[g]
Rb^{7+}					193 225	188 524	190 502[h]
Nb^{11+}					275 765	270 309	271 939[h,i]
Mo^{12+}	266 662	266 223	295 084	289 202	297 379	291 781	293 333[h,i]
							293 255[j]
Ag^{17+}					414 381	408 265	409 271[k]
Cd^{18+}					439 998	433 807	434 696[k]
I^{23+}					582 791	576 305	576 495[k]
Xe^{24+}	466 383	465 286	611303		614 786	608 252	607 903[j]
Cs^{25+}					648 106	641 522	641 313[k]
Ba^{26+}					682 832	676 193	675 950[l]
							675 804[k]

[a]Reference [11].
[b]Reference [23]. The calculation did not include CP effects.
[c]Reference [23]. The calculation included CP effects.
[d]Reference [27].
[e]The present calculation including core excitation channels.
[f]Reference [13].
[g]Reference [12].
[h]Reference [15].
[i]Reference [17].
[j]Reference [14].
[k]Reference [18].
[l]Reference [16].

TABLE III. The $^3P_1^o$-$^1P_1^o$ separations (in cm^{-1}) of Zn-like ions.

Ion	MCRRPA		Expt.
	I[a]	II[b]	
Ga^{1+}	26 170	24 131	22 884[c]
Ge^{2+}	33 461	30 705	29 377[c]
As^{3+}	39 760	36 483	35 060[c]
Br^{5+}	51 208	47 184	44 843[c]
			45 599[d]
Kr^{6+}	56 759	52 446	50 752[e]
Rb^{7+}	62 341	57 772	55 980[f]
Nb^{11+}	86 237	80 988	78 855[g]
Mo^{12+}	92 905	87 544	85 353[g]
			85 275[h]
Ag^{17+}	133 238	127 585	125 020[i]
Cd^{18+}	143 123	137 457	134 858[i]
I^{23+}	205 284	199 695	
Xe^{24+}	220 757	215 208	211 863[j]
Cs^{25+}	237 423	231 916	
Ba^{26+}	255 359	249 896	

[a]Reference [27].
[b]The present calculation including core excitation channels.
[c]References [13].
[d]References [13] and [19].
[e]References [12] and [6].
[f]References [15] and [20].
[g]References [15] and [17].
[h]References [14] and [17].
[i]References [18] and [22].
[j]References [14] and [21].

while the resonance excitation energies are more sensitive to the CP effects. Since the major part of the CP effects have been included in the calculation, the remaining disagreement between the MCRRPA and experimental resonance excitation energies should be due to the limited choice of configurations in our calculation of the ground reference state $^1S_0$.

To gain deeper insight into the CP effects on the excitation energies, we study the $^3P_0^o$-$^1P_1^0$ separations in the MCRRPA theory, and the results are given in Table III. A substantial part of the disagreements in $^3P_1^o$-$^1P_1^o$ separations are resolved when core excitation channels from $3d$ core electrons are taken into account. It is interesting to notice that the $^3P_1^o$-$^1P_1^o$ separations are more sensitive to the CP effects than the excitation energies.

In Table IV, oscillator strengths for the intercombination transition in Zn-like ions from the MCRRPA theory are compared with those from other theories and with experiment. For ions near the neutral end, the intercombination oscillator strengths grow rapidly with increasing nuclear charges since they increase approximately with the fifth power of effective nuclear charges [41]. The CP effects increase the intercombination oscillator strengths for ions up to Xe^{24+} and have improved the agreement with experiment. Further improvement is achieved when the experimental excitation energies are used.

The resonance oscillator strengths are presented in Table V. The CP effects in the MCRRPA calculation reduce the resonance oscillator strengths for all ions calculated, and have improved the agreement with experiment. Further improvement is also achieved when the experimental excitation energies are used. The resonance

TABLE IV. Oscillator strengths for the intercombination transition in Zn-like ions. Numbers in brackets indicate the exponent.

	MCHF[a]		MCRRPA			
Ion	I	II	I[b]	II[c]	III[c]	Expt.
Zn			9.239[−5]	1.1268[−4]	1.2914[−4]	
Ga^{1+}			3.802[−4]	4.3635[−4]	4.7543[−4]	
Ge^{2+}			8.781[−4]	9.9280[−4]	1.0573[−3]	
As^{3+}			1.617[−3]	1.8092[−3]	1.9023[−3]	
Br^{5+}			3.920[−3]	4.3218[−3]	4.5116[−3]	
Kr^{6+}			5.541[−3]	6.0650[−3]	6.2606[−3]	6.6357±1.4119[−3][d]
Rb^{7+}			7.503[−3]	8.1600[−3]	8.3953[−3]	
Nb^{11+}			1.904[−2]	2.0244[−2]	1.9849[−2]	1.87±0.12[−2][e]
Mo^{12+}	1.6[−2]	1.5[−2]	2.287[−2]	2.4176[−2]	2.4619[−2]	2.79±0.15[−2][f],2.31±0.15[−2][g]
Ag^{17+}			4.664[−2]	4.8060[−2]	4.8671[−2]	4.72±0.32[−2][g]
Cd^{18+}			5.205[−2]	5.3379[−2]	5.4007[−2]	
I^{23+}			7.958[−2]	7.9940[−2]		
Xe^{24+}	7.5[−2]	7.0[−2]	8.484[−2]	8.4934[−2]	8.5581[−2]	
Cs^{25+}			8.994[−2]	8.9741[−2]		
Ba^{26+}			9.484[−2]	9.4333[−2]		

[a]Reference [11]. Here I and II are calculations without and with CP effects, respectively.
[b]Reference [27].
[c]The present calculation including core excitation channels. Here II and III are calculations with theoretical and experimental excitation energies, respectively.
[d]Reference [6].
[e]Reference [9].
[f]Reference [10].
[g]Reference [8].

TABLE V. Oscillator strengths for the resonance transition in Zn-like ions.

		MCHF[a]		RRPA		MCRRPA			
Ion	HF[a]	I	II	I[b]	II[c]	I[d]	II[e]	III[e]	Expt.
Ga^{1+}	2.53	1.97	1.71	1.97	1.701	1.983	1.7913	1.8620	1.85±0.15[f],1.9±0.5[g]
Ge^{2+}	2.51	1.96	1.71	1.98		1.979	1.7684	1.8176	1.85±0.20[f],1.44±0.08[h]
As^{3+}	2.40	1.90	1.67			1.935	1.7263	1.7632	1.56±0.23[f],1.38±0.27[i]
Br^{5+}	2.19	1.78	1.58	1.84	1.618	1.832	1.6392	1.6627	
Kr^{6+}	2.10	1.72	1.54			1.781	1.5980	1.6175	1.53±0.15[j]
Rb^{7+}						1.733	1.5588	1.5752	
Nb^{11+}						1.564	1.4209	1.4295	
Mo^{12+}	1.69	1.42	1.30	1.54	1.394	1.527	1.3908	1.3982	
Ag^{17+}						1.374	1.2622	1.2653	
Cd^{18+}						1.348	1.2406	1.2431	
I^{23+}						1.243	1.1519	1.1523	
Xe^{24+}	1.22	1.05	0.98	1.24		1.226	1.1379	1.1372	
Cs^{25+}						1.210	1.1251	1.1247	
Ba^{26+}						1.197	1.1136	1.1131	

[a]Reference [11].
[b]Reference [23]. The calculation did not include CP effects.
[c]Reference [23]. The calculation included CP effects.
[d]Reference [27].
[e]The present calculation including core excitation channels. Here II and III are calculations with theoretical and experimental excitation energies, respectively.
[f]Reference [2].
[g]Reference [7].
[h]Reference [4].
[i]Reference [3].
[j]Reference [6].

oscillator strengths are in general more sensitive to the CP effects than the intercombination oscillator strengths.

In conclusion, we have performed a MCRRPA calculation including CP effects for the intercombination and resonance transitions in Zn-like ions. Substantial parts of the disagreements in the $^3P_1^o$-$^1P_1^o$ separations and in the oscillator strengths are resolved when the $3d$ core excitation channels are taken into account. Further improvement could be expected if additional configurations are included in the ground reference state.

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