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Effects of $3d$ subshells on resonance oscillator strengths for the zinc isoelectronic sequence

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Theoretical values of the oscillator strengths of the resonance transition of atoms of the zinc isoelectronic sequence are in satisfactory agreement with each other, but differ substantially from the measured values. Recent relativistic random-phase-approximation calculations on this sequence treated the inner-shell electrons as a frozen core. We investigate here the effect of relaxing the core by taking account of the perturbations of the $3d$ electrons and compare the results with the measured values. Inclusion of the $3d$-subshell correlation effects somewhat improves agreement with experiment, but a significant difference remains.

I. INTRODUCTION

The relativistic random-phase approximation (RRPA) has been applied to the calculation of excitation energies and oscillator strengths of several isoelectronic sequences.[1-4] The complete RRPA was applied to the helium sequence.[1] When applied to the calculation of the excitations of the L-shell electrons of the beryllium isoelectronic sequence,[2] a substantial simplification resulted from neglecting the perturbing effects of the K-shell electrons. This truncated RRPA yielded oscillator strengths f which differed when the alternative length (L) and velocity (V) forms of the transition matrix element were employed. Inclusion of the intershell correlation removed the discrepancy, most of the change occurring in f_V.

In the calculations on the zinc isoelectronic sequence,[4] the 24 pairs of coupled integro-differential equations were reduced to two pairs by adopting a frozen-core description of the inner-shell electrons. Neglect of intershell correlation was based on consideration of the results of the earlier RRPA studies of the beryllium isoelectronic sequence[2] where f_L was affected only slightly by the inclusion of intershell coupling, and of the magnesium isoelectronic sequence[3] for which the oscillator strengths, calculated neglecting the intershell coupling, were in good agreement with experimental values.

In this paper the RRPA is used to investigate the effect of relaxing the frozen-core restriction on the $3d$-subshell electrons for the $4s^2\,{}^1S_0$-$4snp\,{}^1P_1$ transitions, with $n=4$, 5, 6, of atoms of the zinc isoelectronic sequence.

II. THEORY

The details of the derivation of the equations of the RRPA as well as a method for their numerical solution have been given in previous papers.[1-4] We present here a summary of those features which are of relevance to the present work.

An external field of the form $A_+e^{-i\omega t}+A_-e^{i\omega t}$ induces perturbations $w_{i\pm}$ in the ground-state Dirac-Hartree-Fock (DHF) orbitals u_i of an N-electron atom, which then take the form

$$u_i(\vec{\mathbf{r}})+w_{i+}(\vec{\mathbf{r}})e^{-i\omega t}+w_{i-}(\vec{\mathbf{r}})e^{i\omega t}\,.$$

In order that the perturbed orbitals remain normalized to first order in the external field, we require that

$$\langle u_i|w_{j+}\rangle+\langle w_{i-}|u_j\rangle=0,\quad i,j\leq F \tag{1}$$

where F denotes the Fermi surface.

The perturbations are given by the RRPA equations

$$(h_0+V-\epsilon_i\mp\omega)w_{i\pm}=(A_\pm-V_\pm^{(1)})u_i,\quad i=1,2,\ldots,N \tag{2}$$

where h_0 is the one-electron Dirac operator, V is the DHF potential, ϵ_i is the DHF orbital eigenvalue, and $V_\pm^{(1)}$, given explicitly in natural units by

$$V_\pm^{(1)}u_i=\sum_{j=1}^{N}e^2\int\frac{d\vec{\mathbf{r}}'}{|\vec{\mathbf{r}}-\vec{\mathbf{r}}'|}\,[(u_j^*w_{j\pm})'u_i+(w_{j\mp}^*u_j)'u_i-(w_{j\mp}^*u_i)'u_j-(u_j^*u_i)'w_{j\pm}]\,, \tag{3}$$

represents the correlation effects included in the RRPA.

By writing the orbitals and perturbations in a spherical basis, the RRPA equations are reduced to coupled equations for the radial factors. We denote these radial terms by $S_i^\pm$. The number of pairs of radial equations corresponds to the possible virtual electric dipole transitions of each ground-state electron, listed for the zinc isoelectric sequence in Table I. The radial equations are solved by a combination of Green's function and iterative methods.

TABLE I. Electric dipole virtual excitation channels for atoms of the zinc isoelectronic sequence.

Electric dipole channels			Channel index
$1s_{1/2}\rightarrow np_{1/2}$	$1s_{1/2}\rightarrow np_{3/2}$		1, 2
$2s_{1/2}\rightarrow np_{1/2}$	$2s_{1/2}\rightarrow np_{3/2}$		3, 4
$2p_{1/2}\rightarrow ns_{1/2}$	$2p_{1/2}\rightarrow nd_{3/2}$		5, 6
$2p_{3/2}\rightarrow ns_{1/2}$	$2p_{3/2}\rightarrow nd_{3/2}$	$2p_{3/2}\rightarrow nd_{5/2}$	7, 8, 9
$3s_{1/2}\rightarrow np_{1/2}$	$3s_{1/2}\rightarrow np_{3/2}$		10, 11
$3p_{1/2}\rightarrow ns_{1/2}$	$3p_{1/2}\rightarrow nd_{3/2}$		12, 13
$3p_{3/2}\rightarrow ns_{1/2}$	$3p_{3/2}\rightarrow nd_{3/2}$	$3p_{3/2}\rightarrow nd_{5/2}$	14, 15, 16
$3d_{3/2}\rightarrow np_{1/2}$	$3d_{3/2}\rightarrow np_{3/2}$	$3d_{3/2}\rightarrow nf_{5/2}$	17, 18, 19
$3d_{5/2}\rightarrow np_{3/2}$	$3d_{5/2}\rightarrow nf_{5/2}$	$3d_{5/2}\rightarrow nf_{7/2}$	20, 21, 22
$4s_{1/2}\rightarrow np_{1/2}$	$4s_{1/2}\rightarrow np_{3/2}$		23, 24

III. CALCULATIONS

In this section we summarize the formulation of the radial RRPA equations and the approximations we have employed in solving them.

A. Complete RRPA

If no approximation is made to the RRPA equations, there are, for the Zn isoelectronic sequence, 24 pairs of coupled equations for the radial factors $S_i^{\pm}$ of the form

$$[L_i-(\epsilon_i\pm\omega)]S_i^{\pm}=E_i(S_i^{\pm})+\sum_{j=1}^{24}V_i^{\pm}(S_j^{+},S_j^{-}),\qquad i=1,2,\ldots,24 \quad (4)$$

where L_i is the DHF operator for an excited electron in the field of $N-1$ electrons, E_i is an exchange term, and $V_i^{\pm}$ is the radial counterpart of $V_{\pm}^{(1)}$ in Eqs. (3). The term $V_i^{\pm}$ couples together each of Eqs. (4) and makes a complete RRPA calculation computationally prohibitive for many-electron elements. Specific expressions for L_i, E_i, and $V_i^{\pm}$ are given for the Be isoelectronic sequence in Ref. 2. The symbolic expressions above suffice for the purposes of this discussion.

B. Truncated or frozen-core RRPA

If intershell correlation is neglected, the truncated RRPA formulation results. To implement it, we neglect all virtual perturbations of DHF orbitals which are not in the shell of interest. By freezing all but the $n=4$ shell perturbations, we obtain

$$[L_i-(\epsilon_i\pm\omega)]S_i^{\pm}=E_i(S_i^{\pm})+\sum_{j=23}^{24}V_i^{\pm}(S_j^{+},S_j^{-}),\quad i=23,24. \quad (5)$$

$S_{i=23}^{\pm}$ and $S_{i=24}^{\pm}$ may now be obtained by solving four coupled equations in place of the original 48.

If the RRPA equations are solved exactly, the orthogonality requirement of Eq. (1) is satisfied for all i,j. In the truncated approximation in which the first F_0 orbitals (in the case considered here $F_0=22$) are set equal to zero, the orthogonality condition becomes

$$\langle u_i|w_{j+}\rangle+\langle w_{i-}|u_j\rangle=0,\quad F_0<i,j\le F, \quad (6a)$$

$$\langle u_i|w_{j+}\rangle=\langle w_{j-}|u_i\rangle=0,\quad i\le F_0,\ F_0<j\le F\ . \quad (6b)$$

Since solution of the truncated equations does not guarantee the satisfaction of Eqs. (6), Lagrange multipliers λ are incorporated into Eqs. (5) which then become

$$[L_i-(\epsilon_i\pm\omega)]S_i^{\pm}=E_i(S_i^{\pm})+\sum_{j=23}^{24}V_i^{\pm}(S_j^{+},S_j^{-})-\sum_{k\in\kappa_i}\Big(\sum_{j=23}^{24}\lambda_{ik}^{\pm}(S_j^{+},S_j^{-})F_k\Big),\quad i=23,24 \quad (7)$$

where F_k is the radial part of an occupied-state DHF wave function and the sum over k includes all occupied orbitals with the same κ quantum number as the perturbation $S_i^{\pm}$.

C. RRPA with perturbative treatment of intershell correlation

A less demanding approximation assumes that the perturbations of nearby inner-shell orbitals are small compared to the perturbations of the outer shells. Only the most deeply lying shells are completely frozen. Relaxing the fixed-core assumption for the $3d$ subshells results in the equations

$$[L_i-(\epsilon_i\pm\omega)]S_i^{\pm}=E_i(S_i^{\pm})+\sum_{j=17}^{24}V_i^{\pm}(S_j^{+},S_j^{-})-\sum_{k\in\kappa_i}\Big(\sum_{j=17}^{24}\lambda_{ik}^{\pm}(S_j^{+},S_j^{-})F_k\Big),\quad i=23,24 \quad (8a)$$

$$[L_i - (\epsilon_i \pm \omega)]S_i^{\pm} = E_i(S_i^{\pm}) + \sum_{j=17}^{24} V_i^{\pm}(S_j^{+}, S_j^{-}) - \sum_{k \in K_i} \left(\sum_{j=17}^{24} \lambda_{ik}^{\pm}(S_j^{+}, S_j^{-}) F_k \right), \quad i = 17, 18, \ldots, 22. \quad (8b)$$

Assuming, in Eqs. (8), that the contributions to $V_i^{\pm}$ and $\lambda_{ik}^{\pm}$ from $S_{17 \le i \le 22}^{\pm}$ may be neglected compared to those from $S_{i=23,24}^{\pm}$, we can solve Eqs. (8a) as in the truncated approximation. The solutions for ω and $S_{i=23,24}^{\pm}$ may then be inserted into Eqs. (8b). If the exchange term is neglected, Eqs. (8b) can be solved directly, by application of the Green's-function method. Inclusion of the exchange term requires an iteration scheme; however, because the d-subshell equations are uncoupled from each other, the further complications are not serious.

D. RRPA with self-consistent perturbative treatment of intershell correlation

The previous approach can be carried to self-consistency by inserting the calculated $S_{17 \le i \le 22}^{\pm}$ into the right-hand sides of Eqs. (8), solving Eqs. (8a) again for ω and $S_{i=23,24}^{\pm}$ and repeating the procedure until self-consistent solutions are obtained. The effects of the perturbations of the $3d$ subshells are thereby fully treated, except for the neglect of the coupling with the remaining inner subshells.

IV. RESULTS AND DISCUSSION

Table II presents the excitation energies and oscillator strengths for the resonance transition of ions belonging to the zinc isoelectronic sequence. The DHF intermediate-coupling results have been taken from Ref. 4. The inclusion of Lagrange multipliers to enforce the constraints of Eqs. (6) leaves the RRPA length results of Ref. 4 virtually unaffected while bringing the velocity values into closer agreement with the length values.

TABLE II. Resonance excitation energies, in a.u., and oscillator strengths of ions of the zinc isoelectronic sequence.

Ion		DHF [a]	RRPA (λ) [b]	RRPA($3d+\lambda$) [c]	Other theory	Expt.
Ga^{+1}	ΔE	0.2984	0.3076		0.3017 [d]	0.3221 [e]
	f_L	2.303	1.971	1.683	2.26 [f]	1.39 [g]
	f_V	2.010	1.954	1.729		
Br^{+5}	ΔE	0.6693	0.6882		0.681 [h]	0.6893 [e]
	f_L	2.133	1.838	1.605	1.91 [h]	0.82 [i,j]
	f_V	2.214	1.817	1.635		
Mo^{+12}	ΔE	1.3268	1.3440		1.32 [h]	1.3365 [k]
	f_L	1.769	1.537	1.386	1.57 [h]	
	f_V	1.933	1.532	1.415		
W^{+44}	ΔE	7.5154	7.5285		7.57 [h]	
	f_L	1.230	1.151	1.092	1.16 [h]	
	f_V	1.316	1.150	1.102		
U^{+62}	ΔE	17.6087	17.6283			
	f_L	1.414	1.365	1.307		
	f_V	1.471	1.357	1.309		

[a] Dirac-Hartree-Fock intermediate coupling from Ref. 4.
[b] Truncated RRPA with Lagrange multipliers; see Eqs. (7).
[c] RRPA with $3d$-subshell effects included pertubatively; see Eqs. (8), omitting the term E_i. ΔE for RRPA ($3d+\lambda$) is identical to ΔE for RRPA (λ).
[d] Zilitis, Ref. 5.
[e] Moore, Ref. 6.
[f] Warner, Ref. 7.
[g] Sørensen, Ref. 8.
[h] Cowan, Ref. 9.
[i] Pinnington, Kernahan, and Donnelly, Ref. 10.
[j] Knystautas and Drouin, Ref. 11.
[k] Reader and Acquista, Ref. 12.

TABLE III. $4s^2\,{}^1S_0$-$4s5p\,{}^1P_1$ and $4s^2\,{}^1S_0$-$4s6p\,{}^1P_1$ excitation energies, in a.u. and oscillator strengths of ions of the zinc isoelectronic sequence. $A(B)$ denotes $A\times10^B$.

		$4s^2\,{}^1S_0$-$4s5p\,{}^1P_1$			$4s^2\,{}^1S_0$-$4s6p\,{}^1P_1$		
Ion		DHF [a]	RRPA (λ) [b]	RRPA ($3d+\lambda$) [c]	DHF [a]	RRPA (λ) [b]	RRPA ($3d+\lambda$) [c]
Ga^{+1}	ΔE	0.5045	0.5070		0.5863	0.5874	
	f_L	7.80(−2)	3.47(−2)	1.43(−2)	1.86(−2)	4.07(−3)	3.69(−4)
	f_V	5.67(−2)	3.39(−2)	1.69(−2)	1.20(−2)	3.93(−3)	6.83(−4)
Br^{+5}	ΔE	1.8296	1.8353		2.3328	2.3356	
	f_L	2.27(−4)	3.34(−2)	5.82(−2)	1.86(−3)	1.90(−2)	3.17(−2)
	f_V	3.54(−3)	3.38(−2)	5.49(−2)	4.86(−3)	1.90(−2)	3.02(−2)
Mo^{+12}	ΔE	5.1546	5.1616		6.9454	6.9489	
	f_L	5.82(−2)	1.37(−1)	1.72(−1)	2.68(−2)	5.13(−2)	6.65(−2)
	f_V	7.71(−2)	1.36(−1)	1.67(−1)	3.34(−2)	5.07(−2)	6.43(−2)
W^{+44}	ΔE	38.4362	38.4445		54.1667	54.1707	
	f_L	1.42(−1)	1.84(−1)	2.06(−1)	5.38(−2)	6.53(−2)	7.66(−2)
	f_V	1.54(−1)	1.83(−1)	2.04(−1)	5.73(−2)	6.48(−2)	7.54(−2)
U^{+62}	ΔE	74.7705	74.7796		104.2819	104.2864	
	f_L	8.28(−2)	1.06(−1)	1.22(−1)	3.62(−2)	4.35(−2)	5.33(−2)
	f_V	8.97(−2)	1.06(−1)	1.21(−1)	3.85(−2)	4.33(−2)	5.27(−2)

[a] Dirac-Hartree-Fock intermediate coupling from Ref. 4.
[b] Truncated RRPA with Lagrange multipliers; see Eqs. (7).
[c] RRPA with 3d-subshell effects included perturbatively; see Eqs. (8), omitting the term E_i.
ΔE for RRPA ($3d+\lambda$) is identical to ΔE for RRPA (λ).

Table III presents the $4s^2\,{}^1S_0$-$4s5p\,{}^1P_1$ and $4s^2\,{}^1S_0$-$4s6p\,{}^1P_1$ excitation energies and oscillator strengths. The oscillator strengths for these transitions are considerably smaller than those for the resonance transition. Near the neutral end of the isoelectronic sequence extensive cancellation occurs in the transition integral, and the computed oscillator strengths are sensitive to the approximations used in solving the RRPA equations. Inclusion of Lagrange multipliers in the truncated equations changes the oscillator strength by only a small amount from the values obtained when they are not included, but generally improves the agreement between the length and velocity forms. In contrast, the approximate incorporation of perturbations of the 3d subshells, as described in Sec. III C, neglecting the 3d exchange terms and denoted by RRPA ($3d+\lambda$) in the tables, substantially alters the oscillator strengths, see Fig. 1, and produces large differences between f_L and f_V for the moderately ionized elements. These differences are in large part attributable to the approximate nature of the solution of the 3d channel equations and to the neglect of the other M-shell channels. The variation in oscillator strength for Ga^{+1}, in a direction opposite to that for the other ions, is consistent with the minimum which occurs

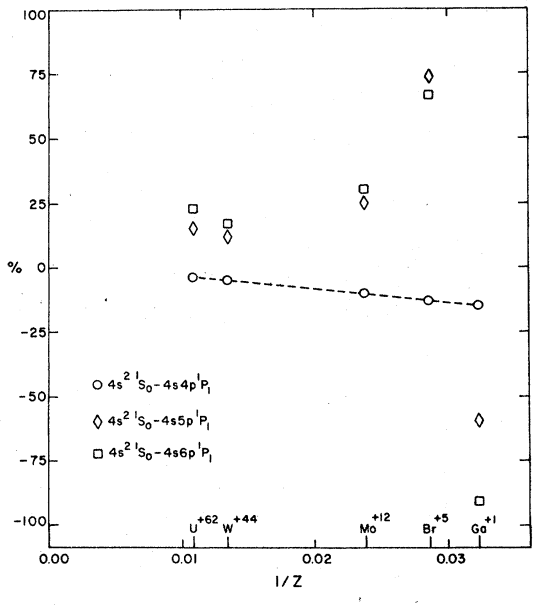

FIG. 1. Percent change in f_L from the frozen-core values when the effects of the 3d subshells are included perturbatively.

TABLE IV. RRPA excitation energies, in a.u., and oscillator strengths calculated including the full effects of the $3d$-subshells, compared with those obtained allowing only for a partial relaxation of the $3d$ subshells with the $3s$ and $3p$ subshells remaining frozen. Oscillator strengths obtained allowing for the partial relaxation of the $3s$ and $3p$ subshells are also given. $A(B)$ denotes $A\times10^{B}$.

		RRPA ($3d+\lambda$) [a]			RRPA (full $3d+\lambda$)			RRPA ($3s+3p+$full $3d+\lambda$) [b]	
Ion	Transition	ΔE	f_L	f_V	ΔE	f_L	f_V	f_L	f_V
Ga^{+1}	$4s^2\,{}^1S_0$-$4s4p\,{}^1P_1$	0.3076	1.683	1.729	0.2954	1.701	1.697	1.691	1.749
	$4s^2\,{}^1S_0$-$4s5p\,{}^1P_1$	0.5070	1.43(−2)	1.69(−2)	0.5043	7.14(−3)	6.99(−3)	6.83(−3)	6.96(−3)
Br^{+5}	$4s^2\,{}^1S_0$-$4s4p\,{}^1P_1$	0.6882	1.605	1.635	0.6678	1.618	1.625	1.604	1.613
	$4s^2\,{}^1S_0$-$4s5p\,{}^1P_1$	1.8353	5.82(−2)	5.49(−2)	1.8320	5.97(−2)	5.89(−2)	6.12(−2)	6.08(−2)
Mo^{+12}	$4s^2\,{}^1S_0$-$4s4p\,{}^1P_1$	1.3440	1.386	1.415	1.3177	1.394	1.413	1.378	1.389

[a] Values from Tables II and III.
[b] ΔE is identical to ΔE for RRPA (full $3d+\lambda$).

in the f vs $1/Z$ curve in Fig. 4 of Ref. 4 near Ge^{+2} as a result of a change in the sign of the transition matrix. The large numerical changes near the minimum correspond to a small shift of the curve.

The large disparity between experiment[8,10,11] and the RRPA, Hartree-Fock,[5] scaled Thomas-Fermi-Dirac,[7] and HFR[9] values for the resonance transition has been discussed.[4] The agreement between length and velocity oscillator strengths which are sensitive to different portions of the wave function, the increase of the discrepancy between theory and experiment with increasing nuclear charge (Z), and the reasonable agreement for Zn I between the truncated RRPA results of Chu and Johnson[13] ($f=1.59$), the RPA calculation of Amusia *et al.*[14] which included some M-shell correlation effects ($f=1.50$), and experiment[15,16] ($f=1.45; 1.35$) suggest that the discrepancy is not due to the neglect of the $3d$ subshells. However, these factors are not conclusive. For example, Froese Fischer[17] has shown that the importance of correlation effects can, in some cases, initially increase along an isoelectronic sequence, before the predicted asymptotic $1/Z$ decrease of inter-electron correlation becomes manifest.

The approximate incorporation of perturbations of the $3d$ subshells decreases the oscillator strengths by amounts ranging from 15% for Ga^{+1} to 4% for U^{+62}. For Ga^{+1} the discrepancy between theory and experiment is reduced by one-half and for Br^{+5} by one-fourth. The influence of the $3d$ electrons on the resonance transition decreases with increasing nuclear charge (see Fig. 1), contrary to the behavior of the discrepancy. The slight deterioration in agreement between length and velocity results that occurs when the $3d$ subshells are included may, as for the 4s-5p transitions, be attributed to the approximations made when solving the M-shell channel equations. For Mo^{+12}, inclusion of the exchange term in the d-subshell equations reduces f_L and f_V by less than 1% and slightly improves the agreement between them.

Since the partial inclusion of $3d$-subshell correlation improves agreement between theory and experiment only to a limited extent, we have investigated whether a full treatment of the effects of the $3d$ electrons, as described in Sec. III D, would further improve agreement. This more detailed treatment was applied to Ga^{+1} and to Br^{+5} because of the large discrepancy between the calculated and measured values, and to Mo^{+12} because of its importance in the study of tokamak plasmas. Table IV presents the results of these calculations. The oscillator strengths for the resonance transition remain virtually unaltered from those of the perturbative treatment of the $3d$ subshells, the principal change being an improvement in the agreement between length and velocity results. Even for the $4s^2\,{}^1S_0$-$4s5p\,{}^1P_1$ transition of Br^{+5} where the $3d$ electrons have a major influence on the oscillator strength, the results of the full inclusion of the $3d$ subshells differ by less than 10% from those of the perturbative approach, although the change for Ga^{+1} is greater because of extensive cancellation in the transition matrix. Table IV also presents the results of calculations which allow for the partial relaxation of the $3s$ and $3p$ subshells in addition to the full relaxation of the $3d$ subshells. The perturbations of the $3s$ and $3p$ electrons have a minor effect on the oscillator strength.

In conclusion, taking into account the influence of the $3d$ subshells within the framework of the

RRPA reduces the discrepancy between theoretical resonance oscillator strengths and experimentally determined values for elements of the zinc isoelectronic sequence, but still leaves a sizable difference, especially for the moderately charged ions such as Br^{+5}.

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