Calculations of atoms with two valence electrons in the frame of CI + MBPT method

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Here we report results of the calculations for atoms with two valence electrons (Ca, Sr, Ba and Yb) with a new *ab initio* method. This method includes two stages:

1. Effective Hamiltonian for the valence electrons is formed within the second order of the many body perturbation theory (MBPT). MBPT corrections include the self-energy terms (Fig. 1 and 2) and screening of the electrostatic interaction between the valence electrons (Fig. 3 and 4).

2. Solution of the two-electron Dirac equation with the effective Hamiltonian by means of the configuration interaction (CI) method.

The detailed description of the method is given elsewhere [1]. Here we present calculations of several low-lying energy levels and ionization potentials for the most simple case of atoms with two valence electrons. Results are presented in Tables 1 — 5 in comparisson with the experiment [2].

For the ionisation potentials the accuracy of the method appear to be about

0.5% or better. Similar accuracy was obtained for levels of the ss and sp configurations. The accuracy for the sd configurations is lower. That can be caused by two reasons:

1. The accuracy of the pure CI for these states is also much lower. That can require the higher-order terms of the MBPT to be included in the effective Hamiltonian.

2. Calclulations of the diagrams Fig. 1 — 4 were made on the basis set which included s, p, d, f and g orbitals. But for d orbitals higher angular momenta could be important in the intermediate states.

It is interesting that the accuracy does not change much from Ca to Yb. It is even more surprising as Yb has shallow f shell in the core which is readily excited and gives very important contribution to the diagrams.

Summing up the results listed in the tables we conclude, that combined method provides an order of magnitude improvement of the accuracy in comparisson with the conventional CI. Another advantage of this method is that it is easy to use. When all diagrams are calculated they can be simply added to the one-electron and two-electron radial integrals which are used for the construction of the Hamiltonian for the valence electrons. After that conventional CI codes can be used.

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Table 1. Low-lying energy levels of Ca (cm^{-1}). Calculations are made with the conventional CI method and with the combined method which includes CI and MBPT. Multiplet splitting is given in parentheses.

Config.	Level	CI		CI + MBPT		Exper.[2]	
$4s^2$	$^1S_0$	0		0		0	
$4s4p$	$^3P^o_0$	13720		15230		15158	
$4s4p$	$^3P^o_1$	13769	(49)	15284	(54)	15210	(52)
$4s4p$	$^3P^o_2$	13870	(101)	15394	(110)	15316	(106)
$4s3d$	$^3D_1$	23661		21489		20335	
$4s3d$	$^3D_2$	23664	(3)	21505	(16)	20349	(14)
$4s3d$	$^3D_3$	23664	(0)	21530	(25)	20371	(22)
$4s3d$	$^1D_2$	23642		22984		21850	
$4s4p$	$^1P^o_1$	23255		23555		23652	

References

[1] V. A. Dzuba, V. V. Flambaum, M. G. Kozlov, Pis'ma v ZhETF **63**, 844 (1996) (English translation in JETP Lett.); see also the report **A4-17** at this conference

[2] C. E. Moore, *Atomic Energy Levels* Natl. Bur. Stand. (US), Circ. No. 467 (Washington) (1958)

Table 2. Low-lying energy levels of Sr (cm^{-1}).

Config.	Level	CI		CI + MBPT		Exper.[2]	
$5s^2$	$^1S_0$	0		0		0	
$5s5p$	$^3P^o_0$	12475		14242		14318	
$5s5p$	$^3P^o_1$	12648	(173)	14428	(186)	14504	(186)
$5s5p$	$^3P^o_2$	13007	(359)	14821	(393)	14899	(395)
$5s4d$	$^3D_1$	19618		18877		18159	
$5s4d$	$^3D_2$	19635	(17)	18936	(59)	18219	(50)
$5s4d$	$^3D_3$	19664	(29)	19033	(97)	18319	(100)
$5s5p$	$^1P^o_1$	20863		21444		21698	

Table 3. Low-lying energy levels of Ba (cm^{-1}).

Config.	Level	CI		CI + MBPT		Exper.[2]	
$6s^2$	$^1S_0$	0		0		0	
$6s5d$	$^3D_1$	11019		9423		9034	
$6s5d$	$^3D_2$	11104	(85)	9631	(208)	9216	(182)
$6s5d$	$^3D_3$	11281	(177)	10065	(434)	9597	(381)
$6s6p$	$^3P^o_0$	10253		12221		12266	
$6s6p$	$^3P^o_1$	10597	(344)	12583	(362)	12637	(371)
$6s6p$	$^3P^o_2$	11370	(773)	13448	(865)	13515	(878)
$6s6p$	$^1P^o_1$	17157		17740		18060	

Table 4. Low-lying energy levels of Yb (cm^{-1}).

Config.	Level	CI		CI + MBPT		Exper.[2]	
$6s^2$	$^1S_0$	0		0		0	
$6s6p$	$^3P_0^o$	14357		17075		17288	
$6s6p$	$^3P_1^o$	15022	(665)	17764	(689)	17992	(704)
$6s6p$	$^3P_2^o$	16527	(505)	19447	(683)	19710	(718)
$6s5d$	$^3D_1$	25216		25075		24489	
$6s5d$	$^3D_2$	25238	(22)	25338	(263)	24751	(262)
$6s5d$	$^3D_3$	25299	(61)	25855	(517)	25270	(519)
$6s6p$	$^1P_1^o$	24221		25306		25068	

Table 5. First two ionisation potentials (I.P.) of Ca, Sr, Ba and Yb (cm^{-1}).

	First I.P.			Second I.P.		
Atom	CI	CI + MBPT	Exper.	CI	CI + MBPT	Exper.
Ca	47806	49142	49305	91887	95626	95748
Sr	44057	45679	45926	84635	88747	88964
Ba	39881	41800	42032	76011	80421	80687
Yb	46759	50295	50444	90788	97254	98269