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DEPENDENCES OF CORRELATION CORRECTIONS FOR 4f SHELL LEVELS ENERGY ON ITS OCCUPATION NUMBER

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The expressions of the averaged correlation corrections for the energy of $n_1\ell_1^{N_1}$ configurations, while considering several types of virtual configurations ($n_3\ell_3^{4\ell_3+1}\, n_2\ell_2^{4\ell_2+1}\, n_1\ell_1^{N_1+2}$, $n_1\ell_1^{N_1-2}\, n_2\ell_2\, n_3\ell_3$ and $n_3\ell_3^{4\ell_3+1}\, n_1\ell_1^{N_1}\, n_2\ell_2$), are obtained. The effective influence of these configurations for isoionic sequence of triply ionized elements of La ($4f^N$) group is investigated.

The contemporary methods, such as many-body perturbation theory, multiconfigurational approach etc., which allow one to take into account the correlation corrections, are frequently applied only for fairly light atoms and ions. While applying these modern and powerful methods for the complex spectra calculations, such as heavy ions, rare earth elements, one is confronted not only with technical problems. Nevertheless, general regularities of the correlation correction influence in the spectra of many-electron atoms and ions can be investigated by the simplified methods.

One of such methods, proposed by Rajnak and Wybourne [1], allowed to interpret the semiempirical parameters α, β, γ etc. They suggested to substitute the energy difference in the expression of the correlation correction in the second order

$$\Delta E_{\mathcal{K}\chi LS,\mathcal{K}'} = \sum_{T'} \frac{|\langle \mathcal{K}\chi LS \,|H|\, \mathcal{K}'(T')LS\rangle|^2}{E(\mathcal{K}\chi LS) - E(\mathcal{K}'(T')LS)} \quad , \tag{1}$$

by the energy, averaged by terms LS. In this case the summation in Eq. (1) over the intermediate moments of the virtual configuration $\mathcal{K}'$ may be carried out analytically. $\mathcal{K}$ denotes the configuration under investigation. The best convergence of this method over the number of virtual configurations, which must be taken into account, may be achieved by the use of the solutions of multiconfigurational Hartree-Fock-Jucys (HFJ) equations[2]. Howewer, the solution of these equations is difficult and not valid when the simplified method is used. Therefore, new transformed orbitals have been proposed [3,4]. These orbitals, obtained from

the Hartree-Fock functions of the configuration under investigation while using simple transformations

$$P(n'\ell'|r) = \mathcal{N}^{-1} r^{\Delta\ell} P(n\ell|r) \ , \ \Delta\ell = \ell' - \ell \ ;$$
$$P(n'\ell'|r) = \mathcal{N}'^{-1}(A - r^2) P(n\ell|r) \ , \ \ell' = \ell \ , \qquad (2)$$

are similar to HFJ orbitals and ensure the convergence of the method. The expressions of the correlation corrections for the $n_1\ell_1^{N_1}\, n_2\ell_2^{N_2}$ configuration under investigation are published in [3,4]. The analysis of p, d and f electron energy spectra [3-6] enables one to maintain that the method allows to take into account about 90-95% of correlation effects in comparison with a strong multiconfigurational approach. In the same way the method developed can be applied for the electron transition characteristic calculations [7], particularly for the so called "forbidden" E2 and M1 transitions.

This method allows one to investigate general regularities of correlation effects, to choose the configurations of great importance and then mix them in the strong multiconfigurational approach.

We have tried to investigate for this purpose the averaged correlation corrections of several types of configurations for the energy of configurations under investigation with one open shell $n_1\ell_1^{N_1}$. The analytical expressions of such averaged corrections have been obtained by summing up Eq. (1) over quantum numbers LS, by using some results of paper [8]. When the virtual configurations of the types $n_3\ell_3^{4\ell_3+1}\, n_2\ell_2^{4\ell_2+1}\, n_1\ell_1^{N_1+2}$ or $n_1\ell_1^{N_1-2}\, n_2\ell_2\, n_3\ell_3$ are taken into account the averaged correction has the following form :

$$\overline{\Delta\mathcal{E}}_{\mathcal{K},\mathcal{K}'} = -M\Big[\sum_k \Big(\frac{2}{2k+1} - \begin{Bmatrix} \ell_1 & k & \ell_2 \\ \ell_1 & k & \ell_3 \end{Bmatrix}\Big) \times$$
$$\times P(kk, \ell_1\ell_2\ell_1\ell_3) - \sum_{k\neq k'} \begin{Bmatrix} \ell_1 & k & \ell_2 \\ \ell_1 & k' & \ell_3 \end{Bmatrix} P(kk', \ell_1\ell_2\ell_1\ell_3)\Big] \ , \qquad (3)$$

where

$$M = \begin{cases} N_1(N_1-1)/(2\ell_1+1)(4\ell_1+1) \ , \ \mathcal{K}' \equiv n_1\ell_1^{N_1-2}\, n_2\ell_2\, n_3\ell_3 \ ; \\ (4\ell_1+2-N_1)(4\ell_1+1-N_1)/(2\ell_1+1)(4\ell_1+1) \ , \\ \qquad \mathcal{K}' \equiv n_3\ell_3^{4\ell_3+1}\, n_2\ell_2^{4\ell_2+1}\, n_1\ell_1^{N_1+2} \end{cases} \qquad (4)$$

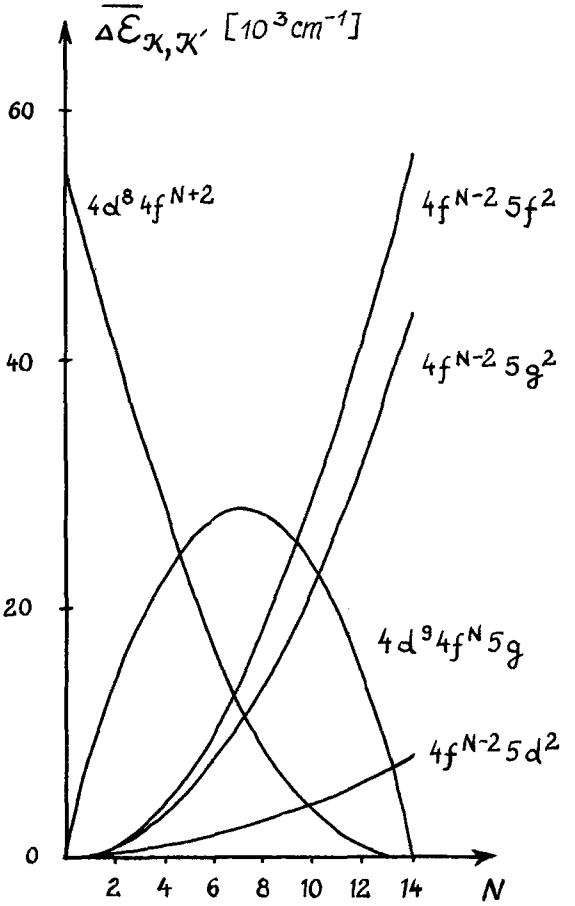

Fig. 1. Dependence of averaged correlation correction $\overline{\Delta\mathcal{E}}_{\kappa,\kappa'}$ for the energy of $4f^N$ configuration on the occupation number N of 4f shell

Respectively, for the configuration $n_3 \ell_3^{4\ell_3+1}\, n_1 \ell_1^{N_1}\, n_2 \ell_2$ we obtain

$$\overline{\Delta\mathcal{E}}_{\kappa,\kappa'} = -\frac{N_1(4\ell_1+2-N_1)}{(2\ell_1+1)(4\ell_1+1)}\left[\sum_k \frac{P(k\,k,\ell_1\ell_1\ell_2\ell_3)}{2k+1} + \right.$$

$$\left. + \sum_k \frac{P(k\,k,\ell_1\ell_2\ell_1\ell_3)}{2k+1} - \sum_{k,k'} \begin{Bmatrix} \ell_2 & \ell_3 & k \\ \ell_1 & \ell_1 & k' \end{Bmatrix} Q(k\,k',\ell_1\ell_1\ell_2\ell_3)\right], \qquad (5)$$

where the following notation is used :

$$P(kk', \ell_1\ell_2\ell_1\ell_3) = R_k(n_1\ell_1 n_2\ell_2, n_1\ell_1 n_2\ell_2)(\ell_1\|C^{(k)}\|\ell_2)(\ell_1\|C^{(k)}\|\ell_3)\times$$
$$\times R_{k'}(n_1\ell_1 n_2\ell_2, n_1\ell_1 n_3\ell_3)(\ell_1\|C^{(k')}\|\ell_2)(\ell_1\|C^{(k')}\|\ell_3)/\overline{\Delta E}(\mathcal{K},\mathcal{K}') ; \quad (6)$$

$$Q(kk', \ell_1\ell_1\ell_2\ell_3) = R_k(n_1\ell_1 n_1\ell_1, n_2\ell_2 n_3\ell_3)(\ell_1\|C^{(k)}\|\ell_1)(\ell_2\|C^{(k)}\|\ell_3)\times$$
$$\times R_{k'}(n_1\ell_1 n_2\ell_2, n_1\ell_1 n_3\ell_3)(\ell_1\|C^{(k')}\|\ell_2)(\ell_1\|C^{(k')}\|\ell_3)/\overline{\Delta E}(\mathcal{K},\mathcal{K}') . \quad (7)$$

R_k and $(\ell\|C^{(k)}\|\ell')$ are generalized Slater integrals and submatrix elements of the spherical function operator, respectively [9]. Figure 1 illustrates the dependence of averaged correlation correction on the number of electrons in the 4f shell for the case of triply ionized isoionic sequence of La group. As follows from the Figure 1 the role of different configurations, which have been taken into account, changes strongly when the number of 4f electrons increases. These dependences are parabolic, the terms in squared brackets of Eqs (3) and (5) change in magnitude only about few per cents along the sequence. Of course, when the transformed orbitals (2) are used in the correlation calculations, several types of excited configurations of the same symmetry must be taken into account, nevertheless the character of the dependences does not change. In the isoelectronic study the influence of correlation effects increases when the ionization increases, but more moderately than the spectral widths, and therefore, the relative role of correlation effects decreases.

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