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ИНСТИТУТ ЯДЕРНОЙ ФИЗИКИ
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A b s t r a c t

Many-body perturbation theory is used for relativistic calculations of energy levels and of fine-structure intervals for 20 lower states of francium. The zeroth approximation is obtained by the relativistic Hartree-Fock method. The second order correlation corrections and Lamb-shifts are calculated. The accuracy for the s,p and f energy levels is not worse than 0.5%.

As far as we know, until now the position of the energy levels of Fr has not been measured. (Only the wavelength of transition $7s\text{-}7p_{3/2}$ is known /1/). On the other hand, there is the possibility of relatively exact calculation of the position of these levels with the help of many-body perturbation theory. We have made such a calculation for Cs /2/. The position of the s,p and f levels and the fine structure (FS) of the p and f levels has proved to be reproduced with an accuracy of 0.1÷0.4% and with an accuracy of 1÷2%, respectively. Exception is the d-states for which the correlation corrections are very large. For example, the zeroth approximation (relativistic Hartree--Fock (RHF) method) gives the wrong sign of the FS. Taking into account the second order correlation correction makes the situation much better, but the contribution of the higher orders, which is not taken into account, turns out to be rather large ($5d$: 3% for energy and 35% for the FS, $6d$: 0.1% for energy and 12% for the FS). Because the Fr atom is an analog of Cs, the accuracy of determination of the position of s,p and f levels can be expected to be not worse than 0.5% as well. And the position of d-levels can be corrected by extrapolating the higher-order correlation corrections from Cs.

We are interested in the energy levels of external electron, which are counted from the boundary of continuous spectrum, i.e. from the energy of ion Fr^+. Therefore, it is convenient to use the wave functions of an ion Fr^+, found by RHF method as the zeroth approximation for the wave functions of the core of Fr. The wave functions of the states of external electron (for discret and continuum spectrum) are then calculated in the field of the frozen core (approximation V^{N-1}). In this case, the correlation correction are calculated according to the formulas presented in /2/. The magnetic interaction and retardation for the external electron in heavy atom may be neglected /2,3/. The radiative correction (Lamb-shift) could be significant in heavy atoms because it increases fastly ($\sim Z^2$) as Z grows. There is no difficulty in evaluating it.
The Lamb-shift for a highly-excited level of electron in the Coulomb field is proportional to the density of wave function at $r \to 0$ (to be precise, at $r \leq a_B/Z$). For the external electron in a heavy atom the Lamb-shift is also deter-

mined by the region $r \lesssim a_B/Z$, because the contribution from the region $r \sim a_B$ does not increases with Z. In the region $r \lesssim a_B/Z$ the Coulomb field is not shielded and the wave function of electron differs only by normalization from the Coulomb one /4/:

$$\frac{|\psi(r\to 0)|^2}{|\psi_{coul}(r\to 0)|^2} = \frac{n^3}{\nu^3 Z^2}\left(1 - \frac{ds}{dn}\right) \qquad (1)$$

where $s = n - \nu$, n is the principal quantum number, ν is the effective principal quantum number ($E = -Ry/\nu^2$). The Lamb-shift of Coulomb levels $S_{1/2}$ and $P_{1/2}$ from Z = 10 to Z = 100 has been calculated in Ref. /5/. Using its results, one obtains:

$$\Delta E_{LAMB} = \frac{2\alpha}{\pi}\frac{(Z\alpha)^2}{\nu^3}\left(1 - \frac{ds}{dn}\right) F(Z\alpha)\cdot Ry \qquad (2)$$

where $F(Z\alpha)$ is the function which is weakly Z-dependent (and is tabulated in /5/). At Z = 87 $F(Z\alpha)$ = 2.13 for $S_{1/2}$ and $F(Z\alpha)$ = 0.26 for $P_{1/2}$. Unfortunately, we don't know $F(Z\alpha)$ for the other orbitals. However, the estimates according to the nonrelativistic formulas, show that it is small. For example, the contribution to fine structure is given by a formula

$$\Delta E_{LAMB} = \frac{\alpha}{\pi}\Delta E_{LS} \qquad (3)$$

ΔE_{LS} - spin-orbit splitting. The contributions from the zeroth approximation (RHF) and the correlation corrections to the lower energy levels and to the FS intervals of Fr are presented in Tables 1 and 2. In addition, Table 1 also presents the Lamb-shift of s-levels. Tables 3 and 4 give the same contributions for Cs. For convenience in the comparison with the results for Fr, the contributions to the FS of CS are multiplied by the factor $\left(Z(Fr)/Z(Cs)\right)^2$. It is seen that both the value of energy and the correlation correction in n+1 - level of Fr prove to be close to those in n-level of Cs.

The calculated value of the wavelength of transition $7s\text{-}7p_{3/2}$ in Fr (λ = 714 nm) has turned out to be 0.6% less than the experimental one (λ = 717.97±0.01 nm /1/). It corresponds to the error $\Delta E/E$ = 0.25% in the position of 7s -level. Proceeding from the known value of the wavelength of transition $7s - 7p_{3/2}$ and from the higher order correlation corrections in

Cs (remind that both the zeroth and second approximation in Cs and Fr have proven to be fairly close), we have made an attempt to refine the position of energy levels of Fr. The final results for the states with $\nu < 5$ are given in Table 5. The levels 10s, 5d, and 6f have been obtained by extrapolating the correlation correction (it behaves like $1/\nu^3$ at large ν). The levels with $\nu > 5$, not presented in the Table, are given, within good accuracy, by the Rydberg formula. Calculation of the position of 7s, 7p, 8p levels has been previously made in Ref. /6/. In that paper the energy levels of Fr have been first calculated in the Hartree-Slater approximation (without taking into account the correlation corrections) and then corrected, proceeding from the calculated and experimental data on Cs, Ba^+, and Ra^+. Our results on the 7s, 7p, 8p levels coincide, practically, with the results from /6/.

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Table 1

The values of energy levels of Fr, obtained by the RHF method, correlation corrections to them and the Lamb-shifts (cm^{-1}). We don't present energies of $j = \ell - 1/2$ -levels, since $|E(j=\ell-1/2)| = |E(j=\ell+1/2)| + \Delta E(FS)$; $\Delta E(FS)$ see in Table 2.

	RHF	Correlations	Lamb-shift	Sum
7s	-28704	-4297	77	-32924
8s	-12261	-935	19	-13177
9s	-6851	-365	7	-7209
$7p_{3/2}$	-17651	-1259	-	-18910
$8p_{3/2}$	-8810	-395	-	-9205
$9p_{3/2}$	-5318	-187	-	-5505
$6d_{5/2}$	-13927	-2027	-	-15954
$7d_{5/2}$	-7748	-777	-	-8525
$5f_{7/2}$	-6867	-86	-	-6953

Table 2

Fine structure intervals of Fr, obtained by the RHF method, and the correlation corrections to them (cm^{-1})

	RHF	Correlations	Sum
7p	1203	457	1660
8p	430	116	546
9p	203	47	250
6d	-98.0	182.9	84.9
7d	-21.4	115.3	93.9
5f	-0.920	-0.024	-0.944

Table 3

The values of energy levels of Cs, obtained by the RHF method, correlation corrections to them and Lamb-shifts (cm^{-1})

	RHF	Correlatinns	Lamb-shift	Sum	$E_{exp}-E_{theor}$
6s	-27926	-3514	28	-31412	-5
7s	-12104	-820	7	-12917	-45
8s	-6790	-326	3	-7113	-23
$6p_{3/2}$	-18388	-1279	-	-19667	8
$7p_{3/2}$	-9079	-399	-	-9478	-18
$5d_{5/2}$	-14168	-2150	-	-16318	492
$6d_{5/2}$	-7924	-856	-	-8780	-5
$4f_{7/2}$	-6865	-61	-	-6916	9

Table 4

Fine structure intervals of Fr, multiplied by the factor $\left[Z(Fr)/Z(Cs) \right]^2 = 2.502$ (cm^{-1})

	RHF	Correlations	Sum	$E_{exp} - E_{theor}$
6p	1011	380	1391	-5
7p	378	85	463	-10
5d	-55	213	158	86.6
6d	0.07	120	120	-12.5
4f	-0.543	0.093	-0.450	-0.003

Table 5

The corrected energy levels of Fr

		Interval			Interval
7s	-32841		9s	-7182	
$7p_{1/2}$	-20568	1655	$5f_{5/2}$	-6952	-0.944
$7p_{3/2}$	-18913		$5f_{7/2}$	-6953	
$6d_{3/2}$	-16596	~150	$9p_{1/2}$	-5754	249
$6d_{5/2}$	-16446		$9p_{3/2}$	-5505	
8s	-13136		$8d_{3/2}$	-5280	~ 50
$8p_{1/2}$	-9745	540	$8d_{5/2}$	-5230	
$8p_{3/2}$	-9205		10s	-4540	
$7d_{3/2}$	-8614	90	6f	-4439	
$7d_{5/2}$	-8524		5g	-4400	
			limit	0	

References

1. S.Liberman, J.Pinard, H.T.Duong, P.Juncar, P.Pillet, J.-L.Vialle, P.Jacquinot, F.Touchard, S.Büttgenbach, C.Thibault, M. de Saint-Simon. R.Klapisch, A.Pesnelle, G.Huber, Phys. Rev. 22A (1980) 2732.
2. V.A.Dzuba, V.V.Flambaum, O.P.Sushkov, Preprint IYF 85-82 (1982), J. Phys. B, in press.
3. N.C.Pyper and P. Marketos, J. Phys., 14B (1981) 4469.
4. I.I.Gol'dman, V.D.Krivchenko, Problems in Quantum Mechanics (GITTL, Moscow, 1957; Addison-Wesley, 1961).
5. P.J.Mohr, Phys. Rev. Lett. 34 (1975) 1050.
6. H.Lundberg, A.Rosen, Z. Phys. 286A (1978). 329.