

Analysis of highly charged ion states in a simplified HFD approximation

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Abstract. The analysis of calculating the total and single electron energies of a sequence of highly charged Li - and Be - like ions in Hartree-Fock-Dirac (HFD) approximation is presented. It is ascertained an unexpected order of location of some energy levels at $Z > 50$ for both the ground and the excited configurations. Possible reasons of such deviations are discussed from theoretical and computational points of view.

1. Introduction

The data on energy levels and wave functions of heavy highly charged ions is very important in different physical theoretical models and experimental applications. As an example, one could point out the processes of channeling such ions through a crystal lattice [1-3]. Due to strong Coulomb interaction with the crystal lattice periodic potential field the ion electrons could be transferred to some excited states. Post channeling, high-energy photons should be radiated due to transitions to the lower-lying states. The analysis of registered photon spectra may be helpful in revealing the essence of both the channeling process physical mechanisms and the details of multi-dipole crystalline field potential exciting ionic electrons.

2. Elements of theory

Here we do not describe the basic of well-known HFD approximation (see, e.g. [4]) but present some specific features which may be useful in the below discussion of the obtained results.

In atomic calculations, the total wave function is the determinant of single-electron wave functions. They could be found by solving the system of simultaneous integro-differential equations under the condition of minimum of total energy.

The single-electron wave function $\varphi_i(\vec{r}, \sigma)$ of a bound electron i has a form of Dirac bispinor

$$\chi_i(\vec{r}, \sigma) = \frac{1}{r} \begin{pmatrix} F_{n\kappa}(r) \Omega_{jl j_z}(\vec{n}) \\ i\alpha_0 G_{n\kappa}(r) \Omega_{j'l' j_z}(\vec{n}) \end{pmatrix}. \quad (1)$$

Here $F_{n\kappa}(r)$ is the large component and $G_{n\kappa}(r)$ is the small component of the wave function radial part, $\Omega_{jl j_z}(\vec{n})$ and $\Omega_{j'l' j_z}(\vec{n}) = -(\vec{\sigma}, \vec{n}) \Omega_{jl j_z}(\vec{n})$ present the spin-angular parts, correspondently, $\alpha_0 = 1/c$ is the fine structure constant, n is the electron principal quantum number, j and l are the total and orbital electron momenta, κ is the “effective” orbital momentum defined as follows:



$$\kappa = \begin{cases} -(j+1/2) = -(l+1) & \text{if } l = j-1/2 \\ j+1/2 & \text{if } l = j+1/2 \end{cases} \quad (2)$$

By variation procedure, the following simultaneous equations could be derived [5] (atomic units are used, $\hbar = m = e = 1$, energy in Ry) in the form

$$F_i'(r) + \frac{\kappa_i}{r} F_i(r) - [2 + \alpha_0^2 (\hat{\varepsilon}_i - U_i(r))] G_i(r) = -\frac{\alpha_0^2}{r} \sum_{k, j \neq i} D(i, j, k) \hat{Y}_{ij}^k G_j(r) \quad (3)$$

$$G_i'(r) - \frac{\kappa_i}{r} G_i(r) + (\hat{\varepsilon}_i - U_i(r)) F_i(r) = \frac{1}{r} \sum_{k, j \neq i} D(i, j, k) \hat{Y}_{ij}^k F_j(r). \quad (4)$$

Here $i = n\kappa$, $j = n'\kappa'$ run over all atomic subshells, $U_i(r)$ is the self-consistent potential in which the electrons of a subshell i move, $\hat{\varepsilon}_i = \varepsilon_{ii}$ is the single electron energy. The terms with non-diagonal parameters ε_{ij} , responsible for the wave functions orthogonality, are equal to zero for closed shells and rather small for the ground states of most atoms [5,6]. Therefore they are omitted in the above equations (3) and (4). Additional simplification done in (3) and realized in the computer codes ATOM [7] used in our calculation is the neglect of the right hand side term in (3). This term stands for correcting the single electron energies and wave functions because of so-called “exchange in small components”. Estimations show that this neglect results in inaccuracy of 0.1% for the most inner shells and of 0.01% for outer shells [8].

3. Main results and discussion

Here we present some results on the total and single-electron energies for Li-, Be-like ions in the nuclear charge range Z up to 100 calculated in HFD approximation simplified as mentioned above. Computer codes ATOM [7] have been used.

Since the single-electron wave functions of a highly charged ion are expected to be strongly localized nearby a nuclear, the radial variable r variation is restricted by a value of $R=20$ a.u. The wave functions are calculated at 600 points of r . LSJ approximation is used in calculating spin-angular coefficients in equations (1) and (2). The total and single electron energies as functions of nuclear charge Z , (increment $\Delta Z=10$) are listed in tables below.

The below presented analysis of the obtained results is intended to reveal some unexpected features, along with standard ones, which may be a subject of the discussion on simplified theoretical approximations used in the research of extra-ordinary objects such as highly charged ions.

3.1. Be-like ion configurations $1s^2 2s^2$, $1s^2 2s 2p$ and $1s^2 2p^2$

The analysis of results presented in tables 1-3 for Be-like ions of ground $1s^2 2s^2$, excited $1s^2 2s^1 2p^1$ and doubly excited $1s^2 2p^2$ configurations reveals the following:

- the relationship between the total energies of mentioned above configurations in the nuclear charge Z range up to 100 corresponds to the expected usual sequence, i.e., $E_{\text{tot}}(1s^2 2s^2) < E_{\text{tot}}(1s^2 2s 2p) < E_{\text{tot}}(1s^2 2p^2)$;
- the single electron energies ε_{1s} of the most inner sub-shell $1s$ also follows the above relationship, except for $Z=4$;
- the single electron energies ε_{2s} of $1s^2 2s^2$ and $1s^2 2s_{1/2} 2p_{1/2}$ configurations also follows the above relationship up to $Z=50$ but then changes it to the inverse one;
- the single electron energies ε_{2p} of $1s^2 2s_{1/2} 2p_{1/2}$ and $1s^2 2p^2$ configurations follows the relationship (a) for all values of Z ;
- for configurations $1s^2 2s^2$, $1s^2 2s_{1/2} 2p_{1/2}$ and $1s^2 2p^2$ the single electron energies show an expected usual relationship $\varepsilon_{2s} < \varepsilon_{2p}$ for all values of Z .

Table 1. The total E_{tot} and single electron energies ε of Be $1s^2 2s^2$ (in Ry).

Z	E_{tot}	ε_{1s}	ε_{2s}
4	-29.152	-9.467	-0.619
10	-220.509	-81.177	-15.002
20	-944.020	-362.452	-79.490
30	-2186.007	-850.315	-195.826
40	-3973.058	-1554.007	-366.575
50	-6348.905	-2488.496	-595.730
60	-9380.383	-3676.653	-889.147
70	-13166.178	-5152.791	-1255.275
80	-17850.796	-6968.754	-1706.445
90	-23649.073	-9205.204	-2261.262
93	-25651.055	-9975.930	-2451.193
100	-30894.050	-11994.819	-2949.469

Table 2. The total E_{tot} and single electron energies ε of Be $1s^2 2s 2p$ (in Ry).

Z	E_{tot}	ε_{1s}	ε_{2s}	ε_{2p}
4	-29.029	-9.489	-.789	-.483
10	-219.725	-80.740	-15.394	-14.213
20	-942.128	-361.278	-80.234	-77.587
30	-2182.934	-848.372	-196.917	-192.720
40	-3968.680	-1551.228	-368.006	-362.113
50	-6343.036	-2484.782	-597.490	-589.680
60	-9372.764	-3671.857	-891.218	-881.167
70	-13156.451	-5146.708	-1257.633	-1244.865
80	-17838.462	-6961.088	-1709.053	-1692.860
90	-23633.424	-9195.521	-2264.061	-2243.343
93	-25634.227	-9965.527	-2454.772	-2432.389
100	-30874.022	-11982.455	-2952.365	-2925.305

Table 3. The total E_{tot} and single electron energies ε of Be $1s^2 2p^2$ (in Ry).

Z	E_{tot}	ε_{1s}	ε_{2p}
4	-28.591	-9.676	-.389
10	-217.436	-80.321	-13.337
20	-936.705	-359.784	-75.376
30	-2174.269	-845.760	-189.142
40	-3956.589	-1547.422	-357.115

50	-6327.244	-2479.664	-583.184
60	-9352.865	-3665.259	-873.062
70	-13131.850	-5138.387	-1234.997
80	-17808.261	-6950.681	-1681.011
90	-23596.199	-9182.477	-2229.188
93	-25594.490	-9951.536	-2417.454
100	-30827.370	-11965.859	-2908.327

3.2. Li-like ion configurations $1s^2 2s 1s^2 2p_{1/2}$

The analysis of results presented in tables 4 and 5 for the Li-like ground $1s^2 2s$ and excited $1s^2 2p_{1/2}$ configurations show the following:

- (a) the relationship between the total energies of Li-like ions in the nuclear charge range Z up to 50 corresponds to the expected usual sequence, i.e., $E_{\text{tot}}(1s^2 2s) < E_{\text{tot}}(1s^2 2p_{1/2})$, but unexpectedly changes the relationship to the inverse one for $Z > 50$;
- (b) the single electron energies ε_{1s} of the most inner sub-shell $1s$ follows the relationship (b) for Be, except for $Z=3$;
- (c) starting from $Z > 50$ the single electron energies of configurations $1s^2 2s$ and $1s^2 2p_{1/2}$ reveal unexpected relationship $\varepsilon_{2s} > \varepsilon_{2p}$.

The latter statement (c) probably serves as one of the reasons responsible for the relationship formulated in (a).

Table 4. The total E_{tot} and single electron energies ε of Li $1s^2 2s$ (in Ry).

Z	E_{tot}	ε_{1s}	ε_{2p}
3	-14.867	-4.956	-.393
10	-205.531	-84.460	-17.565
20	-864.562	-369.787	-85.101
30	-1990.169	-861.810	-204.523
40	-3606.146	-1569.856	-378.342
50	-5751.687	-2508.995	-610.346
60	-8486.766	-3702.238	-905.911
70	-11900.010	-5184.111	-1272.538
80	-16121.245	-7006.824	-1720.790
90	-21343.487	-9251.739	-2266.009
92	-22531.726	-9761.819	-2388.553
100	-27865.795	-12053.041	-2931,715

Table 5. The total E_{tot} and single electron energies ε of Li $1s^2 2p_{1/2}$ (in Ry).

Z	E_{tot}	ε_{1s}	ε_{2p}
3	-14.748	-5.014	-.274
10	-204.838	-84.138	-16.881

20	-863.105	-369.072	-83.648
30	-1987.987	-860.673	-202.272
40	-3603.610	-1568.233	-375.357
50	-5750.060	-2506.778	-607.029
60	-8489.173	-3699.245	-903.473
70	-11912.993	-5180.015	-1273.900
80	-16157.267	-7000.978	-1732.334
90	-21425.097	-9242.708	-2301.129
92	-22626.508	-9751.837	-2431.077
100	-28033.001	-12037.293	-3018.681

4. Conclusion

Firstly, it should be mentioned that calculated in the same approximation energies of excited Li-like $1s^2 2p_{3/2}$ ion states, which are not presented here, show a usual behavior of the excited state energies with respect to corresponding ground configuration $1s^2 2s$ for all values of Z .

Secondly, it could be assumed that the mentioned unusual energy positioning of Li-like ion states for $Z > 50$ does not have any real physical reasons but mainly arises from the simplifications of HFD approximation realized in the used computer codes [7]. To obtain the highly charged ion energy levels with an accuracy closed to spectroscopic one, approximations that are more exact should be used.

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References

- [1] Babaev A, Pivovarov Yu L. 2012 *Computer Physics Communications* **183** 705
- [2] Nakano Y, Sokolik A A., Stysin A V, Nakai Y, Komaki K, Takada E, Murakami T and Azuma T 2015 *J. Phys. B: At. Mol. Opt. Phys.* **48** 144026
- [3] Sinitsyn E A, Kilin V A, Pivovarov Y L 2015 *Book of Abstracts of XI International RREPS-15 Symposium, Saint Petersburg*
- [4] Grant I P. 1970 *Adv. Phys.* **19** 747
- [5] Lindgren I, Rosen A 1974 *Case studies in Atomic Physics* **4** № 3 105
- [6] Hartree D 1960 *Calculation of atomic structures* (Moscow: Atomizdat, in Russian)
- [7] Chernysheva L V and Amusia M Ya 1983 *Automation System for Atomic Structure Researches* (Leningrad: Nauka, in Russian)
- [8] Fischer F 1970 *Computer Physics Communications* **1** 151