Uzhhorod University Scientific Herald. Series Physics. Issue 8. Part 2. – 2000

ACCURATE QED PERTURBATION THEORY CALCULATION OF THE STRUCTURE OF HEAVY AND SUPERHEAVY ELEMENT ATOMS AND MULTICHARGED IONS WITH THE ACCOUNT OF NUCLEAR SIZE EFFECT AND QED CORRECTIONS

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A consistent theoretical approach, based on the quantum electrodynamics (QED) perturbation theory, is developed for the calculation of spectroscopic characteristics of heavy and superheavy atomic systems, multicharged and negative ions. The zeroth approximation is generated by the effective *ab initio* model functional, constructed on the basis of the gauge invariance principle. The wave function zeroth basis is found from the Dirac equation with the potential, which includes the core *ab initio* potential, the electric and polarization potentials of a spherically symmetric nucleus (the Gaussian form of charge distribution in the nucleus and the uniformly charged sphere are considered). The magnetic inter-electron interaction is taken into account in the lowest (over α^2 parameter) approximation, the Lamb shift polarization part – in the Ueling-Serber approximation. The self-energy part of the Lamb shift is effectively taken into account with the use of the 'exact' calculation for H-like ions with point nuclei. The nuclear size effect is taken into account in the electric and polarization potentials. The method is applied for the calculation for the following systems: (1).1*s*(2)2*lj*,3*lj*,4*lj* energy levels for Li-like ions in the nuclear charge interval *Z*=20-100; (2) energy levels, hyperfine structure intervals, E1-,M1-transitions amplitudes, electron affinity energies for heavy atoms of Cs, Sn, Pb;

1. An accurate description of the energy and spectroscopic characteristics for heavy and superheavy atomic systems and multicharged ions is of a great importance for solution of many problems of modern atomic physics [1-14]. In heavy atomic systems the quantum electrodynamics (QED) and nuclear effects, in particular, the nucleus volume and multi-particle QED effects or the effects of mutual screening of electrons play a considerable role. Another very important problem is the problem of correct description of the properties of superheavy elements. It is well known that in the region of *Z*=114 there is the hypothetical "island of stability" of the superheavy elements. Search for these elements is intensely carried out during the recent decades, but no positive results have been obtained. At present time in atomic physics there is a great number of different methods for calculation of properties of atomic and molecular systems. They have certain advantages and disadvantages and, as a rule, each method has its own best "field" of application. As the universal method is absent hitherto, new unified, consistent methods, based fully on QED, are to be developed. Namely on the QED basis it is possible to reach the spectroscopic accuracy in description of the characteristics of heavy and superheavy atomic systems, highly charged ionized atoms and molecules. Besides, such a fundamental problem as the atomic parity non-conservation also requires the special preise calculation procedures. Our purpose is to develop a consistent QED approach, providing an exact correct solution of the problem of calculation of spectra and other characteristics of the above systems with the adequate account of relativistic,

QED, nuclear effects. The developed method is compared with those of [1–7].

2. A consistent theoretical approach, based on the QED perturbation theory, is developed for the calculation of heavy and superheavy atomic systems, multicharged and negative ions [12, 13]. The zeroth approximation is generated by an effective *ab initio* model functional, constructed on the basis of the gauge-invariance principle [3–5]. The wave function zeroth basis is found from the Dirac equation with the potential, including the core *ab initio* potential, the electric and polarization potentials of a spherically symmetric nucleus. We approximate the charge distribution in the nucleus by the Gaussian function. With regard to normalization, one can write:

$$\rho(r \mid R) = (4\gamma^{3/2}/\pi^{1/2})\exp(-\gamma r^2) \quad ,$$

where $\gamma=4/\pi R^2$ and R is the effective nucleus radius. On the basis of this definition the Coulomb potential for the spherically symmetric density can be trivially written. Regarding the polarization potential it should be noted that the current calculations of the polarization are restricted by the first term of the expansion over the parameter α. This value is presented as a matrix element of some potential. It includes the well-known Ueling-Serber potential. In our calculational scheme we use this potential in the square form which is approximated by a simple analytical function with high precision. The general scheme of our method is based on the construction of the QED perturbation theory series. The basis of the zeroth order wave functions is generated by the relativistic Dirac equation with the quoted special potentials. A special attention shuld be paid to the accurate account of the high-order corrections. In our approach the correlation corrections of high orders are taken into account within the Green functions method (with the use of the Feynman diagrams technique). We have taken into accounted all second-order correlation corrections and the predominant classes of the higher-order diagrams (electron screening, particle-hole interaction, mass operator iterations). The magnetic inter-electron interaction is taken into account in the lowest (over α^2 parameter) approximation. The Lamb shift polarization part is taken into account by means of the Ueling-Serber approximation. The self-energy part of the Lamb shift is effectively accounted with the use of the 'exact' calculation for H-like ions with point nuclei [1–3].

Table 1. Results of the different calculations of 2s1/2-2p1/2 transition energies (in cm^{-1}) in Li-like ions
A – multi-configuration Hartree-Fock-Dirac method; B – relativistic perturbation theory of the total inter-electron interaction; C –expansion over the $1/Z$ parameter; D –semi-empirical calculation; E- – calculation within the relativistic perturbation theory with model zeroth approximation; F – our data.

Z	A	B	C	D	E	F	Exp. data
20	291226	289786	289970	290057	291610	290670	290023
22	324759	323209	323392	323530	324470	324120	323468
24	358782	357124	357286	357505	358650	357690	357359
26	393349	391582	391699	392034	392960	392490	392003
28	428432	426635	426680	427179	427890	427453	426985
30	464248		462277	462994	463450	463085	
36	576276		573251	575137	574550	574290	574380
41	675717				672100	671890	
59	1099427				1094670	1094230	
69	1396756				1389200	138820	
79	1751903				1740100	1739875	
92	2279524				2263600	2263490	

Table 2. Results of the different calculations of 2p1/2-2p3/2 splitting energies (in cm^{-1}) in Li-like ions: A – multi-configuration Hartree-Fock-Dirac method; B – relativistic perturbation theory of the total inter-electron interaction; C –expansion over the $1/Z$ parameter; D –semi-empirical calculation; E- – calculation within the relativistic perturbation theory with model zeroth approximation; F – our data.

Z	A	B	C	D	E	F	Exp. Data
20	40706	40797	41034	40844	40860	40870	40884
22	61965	62093	62343	62145	62140	62190	62275
24	90686	90863	91158	90915	90900	90960	91071
26	128482	128722	129027	128768	128740	128750	128722
28	177143	177462	177757	177495	177400	177492	177537
30	238648	239062	239317	239078	238920	238970	
36	522969	523827	523685	523712	523400	523461	523315
41	914259	915728			914650	914720	
59	4416072	4423638			4414000	4414920	
69	8832958	8849877			8825000	8825900	
79	16345446	16382500			16323100	16329350	
92	33692315	33800872			33621800	33622902	

3. We have applied our method in the following calculations of the 1s(2)2lj,3lj,4lj energy levels for Li-like ions (nuclear charge Z=20–100) and the energy levels, electron affinity energies for Cs, Sn, Pb atoms. We have also carried out the calculation of the energy spectra of superheavy element atoms with Z=110, 112, 114.

In Tables 1 and 2 we present the results of our calculation for the energies of 2s1/2-2p1/2 transitions and 2p1/2-2p3/2 splitting in Li-like ions. For comparison we also present the available experimental data and the results of the other calculations. In the region of Z<36 all results differ from each other by the way of the inter-electron interaction being taken into account. It should be noted that for highly charged ions of the Li isoelectronic sequence the account of the relativistic, radiative , nuclear and QED corrections is of a principal importance. For the ions with $Z > 36$ the experimental data are not available and the role of the accurate theoretical calculation significantly increases. In Table 3 we present some results of the calculation of electron affinity energies (EA) for some complex atoms (Si, Ge, Sn, Pb).

Table 3. Electron affinity energies (EA; in eV) of some complex atoms: A – compilation-based values, recommended in refs. [9, 11]; B – values, calculated in this work

Ion	Configuration	Term	A (eV)	B (eV)
Pb	$6p^3$	^4S	0,37	0,401
Si	$3p^3$	^4S	1,39	1,393
Si	$3p^3$	^2D	0,53	0,527
Si	$3p^3$	^2P	0,34	0,327
Ge	$4p^3$	^4S	1,20	1,161
Sn	$5p^3$	^4S	1,20	1,128

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РОЗРАХУНОК СТРУКТУРИ АТОМІВ ВАЖКИХ ТА СУПЕРВАЖКИХ ЕЛЕМЕНТІВ, БАГАТОЗАРЯДНИХ ІОНІВ З УРАХУВАННЯМ ЕФЕКТУ ЯДЕРНОГО РОЗМІРУ ТА КЕД ПОПРАВОК НА ПІДСТАВІ КЕД ТЕОРІЇ ЗБУРЕНЬ

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Розвинуто послідовний теоретичний підхід, який грунтується на квантово-електродинамічній теорії збурень, для розрахунку спектроскопічних характеристик важких та суперважких атомних систем і багатозарядних іонів. Нульове наближення генерується ефективним модельним функціоналом *ab initio*, який сконструювано на основі принципу калібровочної інваріантності. Нульовий базис хвильових функцій знайдено на підставі розв'язку рівняння Дірака з потенціалом, який складається з *ab initio* потенціалу атомного остову, електричного та поляризаційного потенціалів сферично симетричного ядра (розглянуто гаусову форму розподілу заряду в ядрі та однорідно заряджену сферу). Магнітну міжелектронну взаємодію враховано у нижчому (за параметром α^2) наближенні, поляризаційну частину лембівського зміщення – у наближенні Улінга-Сербера, власно-енергетичну частину лембівського зміщення ефективно враховано з використанням точних розрахунків для H-подібних іонів з точковим ядром. Ефект ядерного розміру враховано в електричному та поляризаційному потенціалах. Метод використано в розрахунках 1)1s(2)2lj,3lj,4lj енергетичних рівнів Li-подібних іонів з зарядом ядра Z=20–100; 2) енергетичних рівнів, інтервалів надтонкої структури, амплітуд E1-,M1- переходів, енергій електроної спорідненості для важких атомів Cs, Sn, Pb.