RELATIVISTIC PERTURBATION THEORY CALCULATION OF THE Na-LIKE SPECTRA SATELLITES OF 2-3 Ne-LIKE ION TRANSITIONS

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In this paper we present the results of theoretical relativistic *ab initio* perturbation theory calculation of energy spectra (excited and ground state energies, transition probabilities) of the 3-3,3-4 electron and 2-2 vacancy transitions for the Ne-like isoelectronic sequence (Z=21-96), the autoionizing states for the Na-like ions: ClVII, ArVIII, Ti XII, FeXVI, Ge XXII, Se XXIV, Mo XXXII. Calculations were carried out on the basis of a new *ab initio* method [1-3], generalizing the known relativistic perturbation theory method with the zeroth *ab initio* and empirical effective potential approximation.

Ne-like ions are the heaviest few-electron atomic systems for which a number of high-accuracy experimental investigations were carried out during the last years [1–7]. The isoelectronic sequence of neon has been especially thoroughly investigated, but nevertheless remains of a great interest because the spectra of Ne-like ions are the source of the most important information for the solution of a wide variety of problems, which include the following [7]:

(1) Devices that would provide high precision measurements of ion wavelengths radiating in plasma need to developed. This problem is important for measurements in the X-ray region. In the last several years, experimental results have been obtained with errors of ±0.002 - 0.003 Ă. However, the differences between the experimentally observed energies in Ne-like ions obtained with various setups are often larger then these limits.

(2) Ne-like ions are efficient for diagnostics of heavy and superheavy thermonuclear plasmas. These spectra are also observed in astrophysical investigations of the solar corona.

(3) Study of the low-lying level structure of Ne-like ions is important in connection with the development of a laser for the far UV-region (cf. [5]). It has been shown that for an equilibrium plasma there exists a stationary inversion for some 3-3 transitions of Ne-like ions, and the enhancement coefficient increases with Z and reaches the value of 20-40 cm^{-1} for Z=26 (at optimum plasma parameters: electron density $n_e=5\times10^{20}$ cm^{-3}, electron temperature T_e=310 eV). Recently an enhancement coefficient of 10 cm^{-1} has been observed for the Ne-like selenium (Z=34). At present, different mechanisms of populations of the working levels are under discussion [5]. It is stated that under the plasma conditions defined in the work, the population of n=3 levels occurs though the higher levels, which are populated during dielectron recombination in F-like ions.

The main configurations of Ne-like ions is $1s^22s^22p^6$. The excited states have one vacancy in this core and one electron above the core. The presence of the vacancy in the n=2 shell leads to the relativistic and radiative effects becoming considerable even for Z>20. The spectra of Ne-like ions were discussed in a large number of theoretical studies, where the following methods were used: the perturbation theory (PT) with 1/Z [1–7], Hartree-Fock-Pauli method , Hartree-Fock-Dirac method, the relativistic version of the random-phase approximation method, the screening of the Coulomb potential and others. In the region of small Z<30, preference should be given to the PT with 1/Z method, whose advantage is the inclusion of the second and third orders of the PT for the non-relativistic part of the energy. Relativistic

corrections were taken into account using the Breit's operator. However, terms of low powers -(αZ) were evaluated incorrectly; therefore the results of the calculation for large Z cannot be considered to be satisfactory for data interpretation. Theoretical calculations and experimental data for Xe XLV coincide with the accuracy 0.001 Ă. The work of Dietrich *et al.* [7] enables one to consider problems related to Ne-like ions from a new viewpoint: using the super-HILAC installation at Berkeley, for the first time quadruple 2p-3p transitions in Ne-like ions- and F-like Xe^{44+} were studied. The forbidden lines can be also observed in laser plasma and LIVS spectra. The wavelength of some 2–3 dipole E1 transitions were also found and this enabled a conclusion to be formed about the energy intervals $\Delta n = 0$ for $2p^5 3s$, 3p, 3d states. The rates of the quadruple 2p-3p transitions were measured, their values can be compared with some dipole 3s-3p transitions.

To solve the above mentioned problems, the characteristics of the satellite spectra for resonance 2–3 transitions are of great importance. The satellite structure of spectra of Ne-like ions can be very useful for diagnostics in the range of high (up to 10 keV) plasma temperatures. Most closely located lines are the satellite ones, emitted by Ne-like ions. These lines are due to transitions between the states $2s^2 2p^5 n_1 l_1 n_2 l_2$ and $2s2p^6 n_1 l_1 n_2 l_2$ of the three-quasi-particles system. Their theoretical investigation is surely much more complicated than that for two-quasi-particles systems. However, in some cases a detailed information about the separate satellite transitions is not required, i.e., the averaged spectral characteristics of satellite formation are required. Therefore, a simplified theoretical analysis can be applied, as the averaged values are less sensitive to the approximation used. A number of experimental works have been devoted to the study of spectra of Na-like and other satellites [5]. In particular, a soft X-ray spectrum was obtained in two ways: the plasma was excited by focusing a laser beam, and by a vacuum spark. Na-like ions of iron and titanium are studied, and the lines are found which are satellites of the 2p-3s and 2p-3d transition lines of Ne-like ions. A beam-foil experiment was carried out along with the identification of some strong satellite lines of the ClVIII and ArVIII ions. The X-ray spectrum of molybdenum was probed. It was obtained by wire explosion; satellite lines were observed, but due to the insufficient accuracy they were not identified. The lines of Ne-like and Na-like ions of Ti, V, Cr, Mn, Co, Ni, and Cu were studied by means of LIVS.

Table 1. Energies (in units of 100 cm^{-1}) and probabilities (s^{-1}) of electric dipole transitions to the ground state for Ne-like Ni ion.

Level J=1	[5]	This work	[5]	This work
2p(3/2)3s(1/2)	71.280	71.261	7,6+11	8,4+11
2p(1/2)3s(1/2)	72.620	72.585	6,0+11	7,2+11
2p(3/2)3d(3/2)	78.130	78.115	1,4+11	1,6+11
2p(3/2)3d(5/2)	79.110	79.104	1,2+13	1,2+13
2p(1/2)3d(3/2)	80.520	80.518	3,2+13	3,6+13

The aim of this paper is to carry out the theoretical study of the energy spectra (excited and ground state energies, transition probabilities) of the 3-3,3-4 electron and 2-2 vacancy transitions for the Ne-like isoelectronic sequence (Z=21-96), the autoionizing states for the Na-like ions: ClVII, ArVIII, Ti XII, FeXVI, Ge XXII, Se XXIV, Mo XXXII. The calculations of spectroscopic characteristics are carried out on the basis of the new *ab initio* method [1–3], which generalizes the known relativistic perturbation theory method with the zeroth *ab initio* and empirical effective potential approximation [4–9]. The details of the calculation procedure are described in [1-11]. Here we only note the following: in order to construct the optimal PT zeroth approximation we use *ab initio* quantum electrodynamics (QED) procedure [2,8]. The lowest-order multielectron effects

contribution, in particular, the gauge-dependent radiative contribution for the certain class of the photon propagator calibrations is minimized. Such a minimization results in the construction of the optimal one-electron basis.

Table 2. The values of the energy levels for configurations 2p(5)3s,3p, 2p(5) 3p(2) in the Na-like ion of ClVII (in units of 1000 cm^{-1}: total angular moment J=3/2): columns a,b – Ref. [10]; column c – this work; column d - experimental data.

Configuration of the level	a	b	c	d
a1(p′sp′2)a2(p′sp1)a3(p′sp0)	1710	1727	1710	1710
a1(p′sp0)a2(psp1)	1726	1743	1727	1728
a1(p′sp′2)a2(p′sp1)a3(p′sp′1)	1735	1753	1739	1738
a1(psp′1)a2(psp1)a3(p′sp0)	1742	1759	1746	1744
a1(psp′2)a2(psp1)a3(p′sp′2)	1747	1765	1749	1750
a1(p′sp′1)a2(p′sp1)	1800	1812	1802	1805
a1(psp′1)a2(psp1)a3(p′sp′1)	1810	1822	1813	1814
a1(p′ss0)	1626	1643	1640	1641
a1(p′pp0)a2(p′pp′1)a3(p′p′p′0)	1863	1877	1874	
a1(p′pp′1)a2(p′pp0)a3(pp′p′2)	1874	1888	1885	
a1(p′pp′2)a2(p′p′p′0)	1875	1889	1886	
a1(ppp′1)a2(ppp′2)a3(p′pp′1)	1884	1898	1895	
a1(pp′p′2)a2(p′p′p′2)a3(p′p′p2)	1890	1904	1901	
a1(pp′p′2)a2(p′pp′2)a3(p′p′p′2)	1906	1920	1916	
a1(p′p′p′0)a2(p′pp0)a3(ppp′2)	1931	1944	1939	
a1(p′p′p′2)a2(ppp′2)a3(ppp′1)	1971	1975	1978	

Table 3. The values of the energy levels for configurations 2p(5)3s,3p, 2p(5) 3p(2) in the Na-like ion of Ar VIII (in units of 1000 cm^{-1}; total angular moment J=3/2): columns a,b – Ref. [10]; column c – this work; column d - experimental data;

Configuration of the level	a	b	c	d
a1(p′sp′2)a2(p′sp1)a3(p′sp0)	2057	2076	2059	2060
a1(p′sp0)a2(psp1)	2075	2094	2077	2080
a1(p′sp′2)a2(p′sp1)a3(p′sp′1)	2086	2105	2087	2091
a1(psp′1)a2(psp1)a3(p′sp0)	2095	2114	2096	2100
a1(psp′2)a2(psp1)a3(p′sp′2)	2101	2120	2104	2106
a1(p′sp′1)a2(p′sp1)	2157	2171	2160	2165
a1(psp′1)a2(psp1)a3(p′sp′1)	2171	2184	2175	2178
a1(p′ss0)	1961	1980	1980	1980
a1(p′pp0)a2(p′pp′1)a3(p′p′p′0)	2229	2244	2240	
a1(p′pp′1)a2(p′pp0)a3(pp′p′2)	2242	2257	2255	
a1(p′pp′2)a2(p′p′p′0)	2243	2258	2257	
a1(ppp′1)a2(ppp′2)a3(p′pp′1)	2255	2271	2268	
a1(pp′p′2)a2(p′p′p′2)a3(p′p′p2)	2261	2277	2274	
a1(pp′p′2)a2(p′pp′2)a3(p′p′p′2)	2279	2295	2291	
a1(p′p′p′0)a2(p′pp0)a3(ppp′2)	2306	2319	2316	
a1(p′p′p′2)a2(ppp′2)a3(ppp′1)	2353	2356	2356	

In Table 1 we present the values of the energies and probabilities of electric dipole transitions to the ground state for Ne-like ion of Ni. For comparison the similar data, obtained from the experiment and compilation of Grance [5], are listed.

In Tables 2 and 3 we present the theoretical values of the energy levels for $2p^5 3s3p$, $2p^5 3p^2$ configurations in Na-like ions ClVII, Ar VIII (in units of 1000 cm^{-1}; total angular moment: J=3/2) and experimental data (column d in Table 2). Due to the strong mixing of the states in the intermediate coupling scheme, the definite configurations are not indicated; we write the configurations, which give the largest contribution. In this case it is suitable to compare our data (column c in Table 2) with the calculation results, obtained within the relativistic perturbation theory with zeroth empirical model approximation (ref.[10]; columns a,b in Table 2). The analysis of the presented data enables the conclusion to be made that the applied *ab initio* relativistic perturbation theory method is quite effective in the studies of the spectral characteristics of the considered three-quasiparticles systems.

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РОЗРАХУНОК Na-ПОДІБНИХ СПЕКТРІВ САТЕЛІТІВ 2-3 ПЕРЕХОДІВ У Ne-ПОДІБНИХ ІОНАХ НА ОСНОВІ РЕЛЯТИВІСТСЬКОЇ ТЕОРІЇ ЗБУРЕНЬ

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Представлено результати розрахунків енергетичних спектрів (енергій збуджених та основного станів, імовірності переходів) 3-3, 3-4 електронних та 3-2 вакансійних переходів для Ne-подібної ізоелектронної послідовності (Z=21–96), автоіонізаційних станів Na-подібних іонів : ClVII, ArVIII, Ti XII, FeXVI, Ge XXII, Se XXIV, Mo XXXII. Розрахунки виконано на основі нового методу *ab initio*, який узагальнює відомі версії релятивістської теорії збурень з перших принципів, та нульових емпіричних наближень ефективного потенціалу.