

DOI: 10.34854/ICPAF.51.2024.1.1.144

DEPENDENCE ON THE ATOMIC NUMBER Z OF APPLICABILITY CONDITIONS OF THE QUASI-CLASSICAL APPROXIMATION ON THE EXAMPLE OF IONIZATION POTENTIALS OF ATOMS AND IONS ^{*)}

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A quasi-classical analysis of experimental and calculated data on ionization potentials $I_N^{(Z)}$ (eV) in the ground state of multi-charged ions of medium ($18 \leq Z \leq 54$) [1], heavy ($55 \leq Z \leq 95$) [2] and super-heavy elements ($85 \leq Z \leq 110$) [3] elements, presented in the NIST tables [4], was carried out in works [1-3], based on the method proposed in [5]. The ionization potentials in isoelectronic sequences in special coordinates are shown to fall on very smooth curves, which are approximated with good accuracy by simple polynomials and reflect their main dependence on the atomic number Z . The subsequent polynomial approximation of the piecewise continuous dependence of the coefficients of these polynomials on the number of electrons N_e reproduces the data from NIST tables with an accuracy of 1-2%.

Comparison of the results for super-high atomic numbers with the results for high and medium Z shows that the general pattern becomes simpler and more transparent with increase in Z . First, the degree of interpolation polynomials in isoelectronic series decreases from 3-2 to 2-1, second, the hydrogen-like filling of the outer electron shell becomes more obvious, third, the number of tables of polynomial coefficients is reduced from five for medium to two for super-high, although the number of electrons increases.

Another example of the use of the quasi-classical approximation is the approximation of the ionization potentials of lanthanide and actinide atoms [6]. Here, also for heavier homologues, actinides, the dependence of ionization potentials on atomic number is significantly simplified in the case of sequential filling of outer shells.

This confirms the improvement in applicability conditions of the quasi-classical approximation predicted by the theory, with an increase in Z due to a decrease in the quasi-classical parameter $\sim Z^{-1/3}$.

References

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