DEPENDENCE ON THE ATOMIC NUMBER Z OF APPLICABILITY CONDITIONS OF THE QUASI-CLASSICAL APPROXIMATION ON THE EXAMPLE OF IONIZATION POTENTIALS OF ATOMS AND IONS

Shpatakovskaya~G.V.

KIAM RAS, Moscow, Russia shpagalya@yandex.ru

A quasi-classical analysis and polynomial approximation of experimental and calculated data on ionization potentials in the ground state of multi-charged ions of medium [1], heavy [2] and super-heavy [3] elements, presented in the NIST tables, was carried out in works [1-3]. The approximation 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 approach is the polynomial approximation of the ionization potentials of lanthanide and actinide atoms [4]. Here the dependence of ionization potentials on atomic number is also significantly simplified for heavier homologues actinides in the case of sequential filling of outer shells.

Thus the improvement is confirmed in applicability conditions of the quasi-classical approximation predicted by the theory: a decrease in the quasi-classical parameter with an increase in the atomic number $\sim Z^{-1/3}$. That makes it possible to evaluate some atomic characteristics for super-heavy elements in the absence of measured or calculated data on them.

^{1.} Shpatakovskaya G.V. //JETP. 2022. V.135. P.179

^{2.} Shpatakovskaya G.V. //JETP Letters. 2021. V.114. P.737

^{3.} Shpatakovskaya G. V. //Plasma Physics Reports. 2023. V. 49. P. 1212

^{4.} Shpatakovskaya G.V. //JETP Letters. 2020. V.111. P.463