Theoretical Investigation of Correlation, Quantum Electrodynamics, and Breit Effects on the Energy Levels of Ca-Like Tungsten

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We have investigated the electron correlation effects, the Breit interaction, and quantum electrodynamics effects on the energy levels of Ca-like tungsten (W^{54+}) using AUTOSTRUCTURE code developed by Badnell. These effects are of great importance in heavy highly charged ions. In this work, calculated results have been discussed and compared with other available results in literature.

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1. Introduction

Highly charged heavy elements and ions are of interest in atomic calculations. Atomic tungsten is a high-Z element, and of particular importance for providing tests of quantum electrodynamics (QED) in the region of a very strong Coulomb field of the nucleus [1]. In addition, the relativistic effects depend strongly on Z and are important [2, 3] besides correlation effects. Also, atomic data of tungsten ions (W, $Z = 74$) are very important in astrophysics and plasma physics.

Theoretical calculations and experimental measurements on various highly ionized Ca-like tungsten ion were reported. Theoretically, the energy levels and spectral lines of multiply ionized tungsten atoms, W^{2+} through W^{73+} including Ca-like tungsten were compiled by Kramida and Shirai [4]. Safronova and Safronova [5] tabulated wavelengths and transition probabilities for nl–$n'l'$ transitions in W^{54+} ion. Wavelengths and transition probabilities were calculated for forbidden lines of $3d^2$ ground configurations of W^{54+} ion by Quinet [6]. Electron impact excitation and polarization studies of Ca-like W^{54+} ion were presented by Dipti et al. [7]. Guo et al. [8] reported relativistic many-body calculations on energy levels, wavelengths, and transition probabilities for forbidden transitions within the ground configurations in Ca-like tungsten. Fischer et al. [9] computed energy levels of the $3d^2$ configurations for W^{54+} ion. Extensive self-consistent multi configuration Dirac–Hartree–Fock (MCDHF) calculations were performed for the $3d^2$ ground configurations of W^{54+} ion by Zhao et al. [10]. Finally, Ding et al. calculated energy levels and radiative transitions for W^{54+} ion comprehensively [11–14].

On the experimental side, Ralchenko et al. [15, 16] measured extreme ultraviolet (EUV) spectra of highly charged tungsten ions, including W^{54+} ion, using an electron-beam ion trap (EBIT). Lennartsson et al. [17] observed the $E1$ spectrum of the excited state $[\mathrm{Ne}]3s^23p^53d^3$ to the ground state $[\mathrm{Ne}]3s^23p^63d^2$ of W^{54+} ion measured between 27 and 41 Å at the Livermore EBIT-I electron-beam ion trap using a high-resolution grazing-incidence spectrometer.

In this paper, the energy levels of W^{54+} ion have been studied first using AUTOSTRUCTURE code developed by Badnell [18]. Then, the Breit interaction (magnetic interaction between the electrons and retardation effects of the electron–electron interaction) and QED (self-energy and vacuum polarization) contributions have been investigated. Two different configuration sets for calculations have been studied to investigate the impact of valence–valence correlation (VV) and core–core correlation (CC) within the framework of configuration interaction (CI) expansion: $3dnl$ (n = 3–5 and l = 0–4), $4lnl$ (n = 4–5 and l = 0–4), outside the core $1s^22s^22p^63s^23p^6$ for valence–valence correlation, and $3p^63d4l$ (l = 0–3), $3p^64l4l'$ (l = 0–1 and l' = 0–3), $3p^63d5s$, $3p^63d5p$, $3p^64d^2$, $3p^65s^2$, $3p^65s5p$, $3p^65s5d$, $3p^53d^3$, $3p^53d^24s$, $3p^53d4s4d$, $3p^54s^24p$, $3p^54s4p^2$, $3p^54p^3$, $3p^54s^24d$, $3p^53d4s4p$, $3p^43d^34s$ outside the core $1s^22s^22p^63s^2$ for core–core correlation.

2. Calculation method

AUTOSTRUCTURE code [18, 19] is a general program for the calculation of atomic and ionic energy levels, radiative, and autoionization rates and photoionization cross-sections using non-relativistic or semirelativistic wave functions. It is based on SUPERSTRUCTURE [20]. In this code, the configuration set is chosen optionally and added new configuration to improve accuracy (a configuration interaction

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expansion, CI expansion). The CI expansion is related to the choice of radial functions. Each (nl) radial function is calculated in the Thomas–Fermi or Slater-type-orbital potential model. The Hamiltonian in any coupling model (LS, IC, or ICR) is diagonalized to obtain eigenvalues and eigenvectors with which to construct the rates. This code makes use of non-relativistic or kappa-averaged relativistic wave functions and the full Breit interaction in the Pauli approximation.

Both of QED and Breit relativistic effects are added as a perturbation correction. Quantum electrodynamics contributions consist of self energy and vacuum polarization contributions to level energies. The finite-nucleus effect is taken into account by assuming an extended Fermi distribution for the nucleus. Orbitals are fixed, but the mixing coefficients are obtained by diagonalizing the modified Hamiltonian. CI method was used to account for the correlation effects.

The details of the method can be found in Refs. [18, 19, 21] and we only summarize this here briefly. For an ion with N electrons, a set of configurations

$$c = \prod_{nl} (nl)^{q_{nl}}, \quad \sum_i q_i = N \tag{1}$$

defines a trial solution $\Psi(\gamma)$ to a suitable Hamiltonian H in the multiconfigurational sum form

$$\Psi\left(\gamma|\boldsymbol{x}_1, \ldots \boldsymbol{x}_N\right) = \sum_k a_k \Phi_k \left(c_k(\gamma)|\boldsymbol{x}_1, \ldots \boldsymbol{x}_N\right), \tag{2}$$

where γ denotes configuration and coupling scheme. In intermediate coupling (IC) wave functions can be written as

$$\Psi = \Psi\left(\Gamma S L J M_J|\boldsymbol{x}_1, \ldots \boldsymbol{x}_N\right), \tag{3}$$

which are eigenvectors to the Breit–Pauli matrix $\langle k|H_{BP}|k'\rangle$ with eigenvalues E_k.

3. Results and discussion

In this study, we have presented the energy levels for W^{54+} using AUTOSTRUCTURE code developed by Badnell [18]. Also the purpose of the present work is to investigate the effects of QED, Breit, and correlations on the energy levels. Relativistic and QED effects depend strongly on Z [2, 3], and therefore it is important to include for atomic modelling in highly charged ions such as Ca-like tungsten. In addition, the electron correlation effects due to the Coulomb interaction between the electrons are also important.

We have examined the effects of valence-correlation and core-core correlation on the energy levels by choosing two different configuration sets. In calculation VV, only valence correlation is considered while core–core (CC) electron correlation contributions are considered with single and double excitations from 3p. We have focused on different VV and CC configuration sets. In the first step, we have studied minimum configurations. Then more configurations have been inserted the configuration set. Although, only the best results of them have been presented and compared. We have taken into account the configurations of $3dnl$ (n = 3–5 and l = 0–4), $4lnl$ (n = 4–5 and l = 0–4), outside the core $1s^22s^22p^63s^23p^6$ for valence–valence (VV) correlation, and $3p^63d4l$ (l = 0–3), $3p^64l4l'$ (l = 0–1 and l' = 0–3), $3p^63d5s$, $3p^63d5p$, $3p^64d^2$, $3p^65s^2$, $3p^65s5p$, $3p^65s5d$, $3p^53d^3$, $3p^53d^24s$, $3p^53d4s4d$, $3p^54s^24p$, $3p^54s4p^2$, $3p^54p^3$, $3p^54s^24d$, $3p^53d4s4p$, $3p^43d^34s$ outside the core $1s^22s^22p^63s^2$ for core–core (CC) correlation.

Table I displays the present energy levels and comparison with other available works. The AUTOSTRUCTURE energy levels are generated in cm^{-1}. But we have converted the energy values to eV in order to simplify the comparison with other works (1 eV= 8065.44 cm^{-1}). The correlation effects (valence–valence, VV, and core–core, CC) and the Breit and QED contributions on energy levels are exhibited in this table. We have omitted the core $1s^22s^22p^63s^23p^6$ in the table. We have obtained 453 energy levels from VV correlation and 1275 energy levels from CC. Here we have only listed the levels of nl (n = 3–4, l = 0–2).

In Table II, the results for the energies of the $3d^2$ states are compared with Ding et al. [14] to find out which values are better. We have obtained better results studying with CC instead of VV. Also we can see that, after considering the Breit and QED corrections, the present results are closer to the comparing values. The differences of CC+Breit+QED results are smaller than the others in all levels except $3d^2$ $^3F_2$. The differences (%) may be up to 3.360 for VV, 2.923 for VV+Breit+QED, 2.730 for CV, and 2.307 for CV+Breit+QED. We can say that the calculated results using the configuration set including electron excitations from $3p$ subshell (core–core correlation) and taking Breit and QED contributions (CC+Breit+QED) are better, in general. These CC+Breit+QED results are found to be in good agreement with other works in the literature [5, 6, 8–10, 14, 22]. It should be emphasized that electron correlation, QED and the Breit relativistic contributions should be added in the calculations to obtain accurate results. These contributions hold significance in particular for highly charged ions. We have calculated $(|E_{\rm our} - E_{\rm other}|/E_{\rm other}) \times 100$; the differences in percent, for the accuracy of our CC+Breit+QED results according to Ding et al. [14] and Fig. 1 shows the differences for all $3d^2$ and $3d^3$ levels. We note that there are small differences in the energies in comparison with results reported by Ding et al. [14]. The differences (%) are less than 2.5 for $3d^2$ levels and less than 3.5 for $3d^3$ levels.

The results obtained in this work are systematically higher than the ones available in the literature. We could not clearly explain this case. But, we think that this case occurs from the difference of used methods. We calculated present results with AUTOSTRUCTURE which uses non-relativistic or semi-relativistic wave functions. Although, comparing values are from fully relativistic methods like MCDF.

TABLE I

Energy levels, E (in eV), for Ca-like tungsten (W^{54+})

Levels		This work				Other works
		VV	VV+Breit+QED	CC	CC+Breit+QED	
$3d^2$	$^3F_2$	0.000	0.000	0.000	0.000	0.000[a,b]
$3d^2$	$^3P_0$	22.918	22.901	22.899	22.883	23.3[a], 23.123[b], 23.173[c], 23.199[d], 22.920[e], 24.322[f], 23.045[g], 23.089[h]
$3d^2$	$^3F_3$	74.073	73.711	73.570	73.221	72.590[a], 72.456[b], 72.345[c], 72.264[d], 72.630[e], 72.009[f], 72.484[g], 72.499[h]
$3d^2$	$^3P_2$	84.234	83.872	83.742	83.393	82.882[a], 82.805[b], 82.772[c], 82.600[d], 82.822[e], 83.076[f], 82.784[g], 82.816[h]
$3d^2$	$^3P_1$	88.753	88.385	88.262	87.907	87.9[a], 87.613[b], 87.669[c], 87.460[d], 87.629[e], 88.160[f], 87.608[g], 87.625[h]
$3d^2$	$^1G_4$	89.260	88.883	88.716	88.351	86.4[a], 86.358[b], 86.429[c], 86.021[d], 86.385[e], 86.128[f], 86.306[g], 86.305[h]
$3d^2$	$^3F_4$	156.914	156.189	155.896	155.196	153.0[a], 153.158[b], 153.009[c], 152.704[d], 153.369[e], 152.591[f], 153.146[g], 153.191[h]
$3d^2$	$^1D_2$	164.347	163.617	163.356	162.651	161.1[a], 161.160[b], 161.006[c], 160.774[d], 161.214[e], 161.397[f], 161.115[g], 161.201[h]
$3d^2$	$^1S_0$	188.926	188.183	188.028	187.311	185.1[a], 185.139[b], 184.860[c], 184.927[d], 184.883[e], 186.772[f], 184.946[g], 185.196[h]
$3d4s$	$^3D_1$	2086.340	2085.242	2051.203	2050.737	–
$3d4s$	$^3D_2$	2087.497	2086.397	2052.365	2051.898	–
$3d4p$	$^3F_2$	2163.144	2162.820	2129.556	2128.736	–
$3d4s$	$^3D_3$	2164.797	2163.330	2131.640	2130.815	–
$3d4p$	$^3D_1$	2166.872	2165.404	2161.572	2161.255	–
$3d4s$	$^1D_2$	2166.876	2166.542	2165.269	2164.947	–
$3d4p$	$^1D_2$	2243.250	2242.557	2240.904	2240.231	–
$3d4p$	$^1F_3$	2244.332	2243.637	2242.368	2241.694	–
$3d4p$	$^3D_2$	2297.002	2295.625	2294.704	2293.334	–
$3d4p$	$^3P_1$	2300.618	2299.253	2298.163	2296.804	–
$3d4p$	$^3F_3$	2301.124	2299.755	2299.091	2297.731	–
$3d4p$	$^3P_0$	2302.788	2301.432	2300.422	2299.072	–
$3d4p$	$^3P_2$	2376.940	2375.203	2373.758	2372.041	–
$3d4p$	$^3F_4$	2377.144	2375.411	2374.466	2372.753	–
$3d4p$	$^3D_3$	2377.606	2375.860	2374.831	2373.108	–
$3d4p$	$^1P_1$	2383.961	2382.229	2381.117	2379.406	–
$3d4d$	$^3D_1$	2417.458	2415.892	2418.680	2417.102	–
$3d4d$	$^3G_3$	2417.596	2416.028	2418.819	2417.240	–
$3d4d$	$^3F_2$	2428.155	2426.624	2428.767	2427.228	–
$3d4d$	$^3P_0$	2439.719	2438.201	2440.107	2438.585	–
$3d4d$	$^1F_3$	2448.819	2447.151	2448.850	2447.187	–
$3d4d$	$^3D_2$	2451.272	2449.607	2451.313	2449.652	–
$3d4d$	$^3G_4$	2453.447	2451.781	2453.473	2451.812	–
$3d4d$	$^3S_1$	2454.980	2453.325	2454.984	2453.334	–
$3d4d$	$^3F_3$	2500.039	2498.126	2500.317	2498.408	–
$3d4d$	$^1D_2$	2503.595	2501.694	2503.777	2501.879	–
$3d4d$	$^1G_4$	2505.758	2503.856	2505.869	2503.970	–

[a]Ref. [22], [b]Ref. [14], [c]Ref. [6], [d]Ref. [5], [e,f]Ref. [8], [g]Ref. [10], [h]Ref. [9]

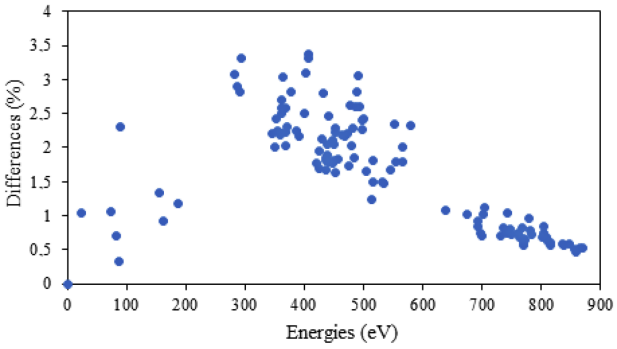

Fig. 1. Differences in percent between present AUTOSTRUCTURE results and MCDF [14].

TABLE II

Differences for energy levels of this work with [14] for W^{54+}

Levels		VV	VV+Breit +QED	CC	CC+Breit +QED
$3d^2$	$^3F_2$	0.000	0.000	0.000	0.000
$3d^2$	$^3P_0$	0.886	0.960	0.968	1.037
$3d^2$	$^3F_3$	2.231	1.732	1.537	1.055
$3d^2$	$^3P_2$	1.725	1.288	1.131	0.710
$3d^2$	$^3P_1$	1.301	0.881	0.740	0.335
$3d^2$	$^1G_4$	3.360	2.923	2.730	2.307
$3d^2$	$^3F_4$	2.452	1.979	1.787	1.330
$3d^2$	$^1D_2$	1.977	1.520	1.362	0.925
$3d^2$	$^1S_0$	2.045	1.644	1.560	1.173

4. Conclusion

A systematic study is carried out to investigate the effect of electron correlation, quantum electrodynamics, and the Breit relativistic contributions on the energy levels of Ca-like W. We show four different results for energies including different effects. When we compared our AUTOSTRUCTURE results with available theoretical and experimental data, a good agreement was observed. It is found that quantum electrodynamics, the Breit relativistic contributions, and configuration interaction effects play important roles on energy levels of highly ionized atoms. Hence, we hope that these present AUTOSTRUCTURE results will be useful for experimental researches in the future.

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