§13. M1 Transition Energies and Probabilities between the Multiplets of the Ground State Ag-like Ions with Z = 47-92

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Background. The earlier systematic investigations on Ag-like ions were performed in the 1970-1980s. The energy level and electronic dipole (E1) transitions between $5s \to 5p$, $5p \to 5d$, $4f \to 5d$ and $4d \to 4f$ of most of the elements in $47 \le Z \le 67$ were determined. Recently, the investigation was extended to the higher Z elements because of the requirements on the atomic data relevant to the spectral analysis of fusion plasmas. The theoretical investigation on these ions can examine the relativistic effects, electron correlation effects and quantum electrodynamics (QED) effects as well as can check the feasibility and accuracy of modern atomic theory.

The ground state of Ag-like ion changes from $5s\,^2S$ to $4f\,^2F$ along with the increase of the atomic number. However, it is still in argument that when this change occurs. Due to the complexity of the $4f$ orbital and the electron correlation in many body system, the ground state for complex atoms is difficult to calculate. Meanwhile, the fine structure splitting between the ground state of highly charged ions can be observed directly by magnetic dipole (M1) transition with advanced electron beam ions trap facilities. The M1 transition can be used as a precise tool to diagnose the fusion plasma and a benchmark for the accuracy of atomic structure calculation.

Method of calculation. The present calculation has been performed in the framework of the MCDF method with implementation of the GRASP2K packages[1)]. To include the most important electron correlation effects, the multi-configuration expansion are constructed from single and double substitutions from $4d$ and $4f$ orbitals to an increasing active space of orbitals. The active space is labeled by the principal quantum number n, and the the active space n includes the atomic orbitals up to ns, np nd and (n-1)f. The active space sets were successively extended to $n = 7$. Only the new orbitals were optimized at each step.

Results and discussion. According to the present calculation, the ground state configuration of Ag-like ions with $47 \le Z \le 61$ are $5s\,^2S_{1/2}$. It moves to $4f\,^2F_{5/2}$ for $Z \ge 62$ (Sm XVI). The present result agrees well with experiments and other theories although another recent RMBPT calculation shows that $4f$ becomes lower at $Z = 61$(Pm XV).

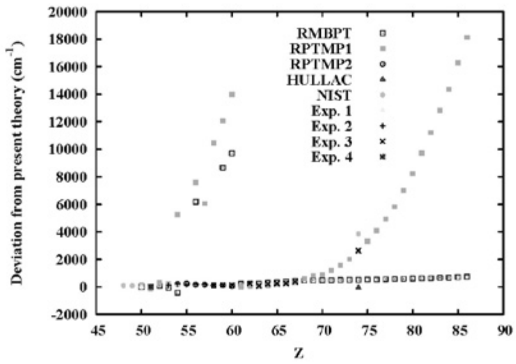

Fig. 1: Comparison of the fine structure splitting from various computations and experiments with the results of the present MCDF calculations. For the explanation of the labels in the figure, please see ref. 2.

The fine structure splitting of the ground configuration of Ag-like ions from various computations and experiments with the results of the present MCDF calculations are shown in fig. 1. The present calculation agrees with almost all of the experimental and the RMBPT theoretical results in high Z region. However, the RPTMP calculation obviously deviates from the present MCDF calculation and also from the RMBPT calculation in the high Z part. Because RPTMP is the theory using empirical model potentials, such deviations might be due to inappropriate choices of the experimental reference values. Another serious disagreement was found between the RMBPT and RPTMP calculation and present calculation for $52 \le Z \le 61$ ions, while in the same range another RPTMP calculation gives good agreement with present calculation.

The M1 transition energy and probability between $4d^{10}4f\ ^2F_{7/2,5/2}$ levels of Ag-like ions are given in fitting formula of $B = A(Z^*)^n$. For the transition energy, we have found that A = 0.01 cm^{-1}, $n = 4$, and $Z^* = Z - 32.78$. For the transition probability, we have found that $A = 1.88 \times 10^{-18} s^{-1}$, $n = 12.47$, and $Z^* = Z - 32.78$. As observed in other highly charged ions, the M1 transition probability increases rapidly with the increase of the transition energy and the nuclear charge number. These results may help to determine the lifetime of $4d^{10}4f\,^2F_{7/2}$ level of high Z Ag-like ions. However, it also indicates, for the lower Z Ag-like ions that the transition probability might be too small to be observed.

1) Jönsson P, He X, Fischer C F and Grant I, Comput. Phys. Commun., (2007) vol.177, pp.597.

2) Xiao-bin Ding et.al., J. Phys. B:At. Mol. Opt. Phys., (2012) vol 45, pp. 035003