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THEORETICAL CALCULATION OF THE RELATIVISTIC SUBCONFIGURATION-AVERAGED TRANSITION ENERGIES*

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A method for calculating the average energies of relativistic subconfigurations in highly ionized heavy atoms has been developed in the framework of the multiconfigurational Dirac–Fock theory. The method is then used to calculate the average transition energies of the spin-orbit-split 3d–4p transition of Co-like tungsten, the 3d–5f transition of Cu-like tantalum, and the 3d–5f transitions of Cu-like and Zn-like gold samples. The calculated results are in good agreement with those calculated with the relativistic parametric potential method and also with the experimental results.

Keywords: subconfiguration-averaged transition energy, highly ionized heavy atom, spin-orbit-split array

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I. INTRODUCTION

Spectroscopic data concerning highly ionized heavy atoms are of great interest for plasma diagnostic studies in fusion experiments, and works of identification and interpretation of the spectra emitted from highly ionized heavy atoms have undergone significant developments in recent years.[1−3] In comparison with the typical spectra consisting of isolated lines emitted from medium or low Z elements, the spectra emitted from high Z elements are often characterized by some quasi-continuum bands, and the number of single lines is very small. This is a general characteristic of such spectra where, due to the various broadening mechanisms and the finite resolution of the spectrometer, the experimental resolution is low. For this reason a model has been developed describing the unresolved transition array (UTA) as a whole, and analytical formulae calculating the first and second moments of the wavenumber distribution, i.e. the mean wavelengths and the spectral width of the UTAs between whole configurations are given.[4,5] But, in many cases of highly ionized heavy atoms, the spin-orbit splitting of one (or several) of the electrons may be the dominant feature of the configurational structure, so that the lines are grouped in nearly pure-jj, well-separated subarrays. In this case, although the formulae given in Ref.[1] are still valid, they are not suitable for identifying the spectra, since the appearance of one theoretical peak is quite different from that of the experimentally distinctly separated subarrays. For these cases, new formulae have been established, which give the first and second moments of each of the spin-orbit-split arrays (SOSAs).

For identifying the unresolved structures in experimental spectra, it is necessary to compute the mean positions—the average transition energies of relativistic subconfigurations (in pure jj coupling), which requires that relativistic calculations of atomic structures be performed. Now, two programs for relativistic calculations of atomic structures are often used: the relativistic parametric potential method[6] (also called the RELAC program) and the multiconfigurational Dirac–Fock (MCDF) package of Grant.[7]

In this paper, in contrast to those papers[8,9] which focused on computing the fine structures of atomic energy levels, we treat subconfigurations as effective energy levels and calculate the average transition energies of these subconfigurations. For this purpose, a method for calculating the average transition energies of subarrays based on the MCDF method is presented. Then, the average transition energies

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of the subarrays belonging to the 3d–4p transition of W^{47+}, the average transition energies of the subarrays belonging to the 3d–5f transitions of Ta^{44+}, and the average transition energies belonging to the 3d–5f transitions of Au^{50+} and Au^{49+} are calculated. In the calculation, both the Coulomb interactions and the magnetic interactions between pairs of electrons are included. Finally, the calculated results are compared with those computed by the relativistic parametric potential method.

Ⅱ. CALCULATION METHOD

A. Average transition energy

According to the SOSA theory, the average transition energy of a subarray is defined as the first moment of the weighted wavenumber distribution, that is

$$\mu_1 = \sum_{a,b}[\langle b|H|b\rangle - \langle a|H|a\rangle]w_{ab} \Big/ \sum_{a,b} w_{ab}. \quad (1)$$

Here, H is the Hamiltonian of an atomic system, and w_{ab} is the weight of a transition and is defined as the Z part of its $E1$ strength. Generally speaking, the average transition energy of a subarray cannot be simply regarded as the energy spacing between the upper and lower subconfigurations. In fact, there is often a difference between them, and this is defined as

$$\delta E(Y \to X) = T_{\rm av}(Y \to X) - [E_{\rm av}(Y) - E_{\rm av}(X)], \quad (2)$$

where Y and X are, respectively, the upper and lower subconfigurations, $T_{\rm av}(Y \to X) \equiv \mu_1$, and $E_{\rm av}$ is the average energy of the subconfiguration.

Now, assuming pure jj coupling in both configurations, the configurations will be split into subconfigurations. Generally, there are two types of subarrays. These are:

(i) $(nl_j)^N n'l'_{j'}$–$(nl_j)^N n''l''_{j''}$. Here, (n,l,j) denotes a spin-orbit-split electronic orbit, and N denotes the number of electrons in the orbit. In this case, δE defined in Eq.(1) is zero; and

(ii)$(nl_j)^{N+1}$–$(nl_j)^N n'l'_{j'}$. Here, $(nl_j)^{N+1}$ usually denotes the ground configuration of a highly ionized heavy atom. In this case, δE is not zero, and it has an analytical expression given in Ref.[1].

B. Average energy of a relativistic subconfiguration

As given by Grant in Ref.[10], the total energy for the average of a configuration can be written in the form

$$E_{\rm av} = E^0 + E^{\rm C} + E^{\rm M} + E^{\rm R}, \quad (3)$$

where

$$E^0 = \sum_a q_a I(a) \quad (4)$$

is the single particle contribution;

$$\begin{aligned} E^{\rm C} = & \sum_a \Bigg\{ \frac{1}{2} q_a (q_a - 1) F^0_{\rm C}(a,a) \\ & - \frac{1}{2} q_a \left(\frac{q_a - 1}{[j_a] - 1} \right) \sum_{v>0} [j_a] \frac{1}{2} \Gamma_{j_a v j_a} F^v_{\rm C}(a,a) \Bigg\} \\ & + \frac{1}{2} \sum_{\substack{a,b \\ a \neq b}} q_a q_b \Bigg\{ F^0_{\rm C}(a,b) - \sum_v \frac{1}{2} \Gamma_{j_a v j_b} G^v_{\rm C}(a,b) \Bigg\} \end{aligned} \quad (5)$$

is the contribution of the Coulomb repulsion of a pair of electrons;

$$\begin{aligned} E^{\rm M} = & - \sum_a \frac{1}{2} q_a \left(\frac{q_a - 1}{[j_a] - 1} \right) \sum_{v \rm odd} \frac{1}{2} [j_a] \Gamma^{\rm M}_{j_a v j_a} F^v_{\rm M}(a,a) \\ & - \frac{1}{2} \sum_{\substack{a,b \\ a \neq b}} q_a q_b \sum_{v,\gamma} \frac{1}{2} \Gamma^{ab}_{j_a v j_b}(\gamma) G^{v\gamma}_{\rm M}(a,b) \end{aligned} \quad (6)$$

is the magnetic term of a pair of electrons. $E^{\rm R}$ denotes the retardation term which has a similar form to the magnetic term $E^{\rm M}$, only with the Γ coefficients replaced by their Λ coefficient equivalents.

With the coefficients given in Ref.[10], from Eqs.(3)–(6), the average energy of a given relativistic subconfiguration, and therefore the average transition energies between two subconfigurations, can be computed.

Ⅲ. RESULTS AND DISCUSSION

With the relativistic integrals calculated using the MCDF model in the averaged level (AL) scheme,[11] the average transition energies ($T_{\rm av}$) of the subarrays belonging to Co-like $3d^9$–$3d^8 4p$ transitions of tungsten are computed. The results are given in Table 1. Here, we notice that the correction terms δE given in the fifth column are not zero, and the nonrelativistic Slater integrals used are obtained from the relativistic integrals by employing the method proposed by Bauche *et al.*[12] In the third and the fourth column of this table the energy spacings between the upper and lower subconfigurations are given, with those in the fourth column including the magnetic interaction. Presented in the sixth column are the subconfiguration-averaged transition energies computed in this work. In the remaining columns are

the corresponding quantities computed with the relativistic parametric potential method. We find clearly from this table that the present calculations are in excellent agreement with those calculated by Bauche *et al.*[1] with the RELAC program. We have also calculated the $T_{\rm av}$ of some subarrays of the Cu-like 3d–5f transition of tantalum. The results are given in Table 2. Good agreement is found between the two methods once again. Here, the $3d_{5/2}$–$5f_{5/2}$ transition is not presented because it is often too weak to be identified in experimental spectra. The subconfiguration-averaged transition energies of the Cu-like and Zn-like 3d–5f transitions of gold are also calculated. In the calculation, a $4l(l \leq 3)$ spectator electron is considered for subconfigurations of Cu-like ions and two $4l(l \leq 3)$ spectator electrons are considered for those of Zn-like ions. The calculated results are given in Table 3. In this table, the mean wavenumbers of the experimentally observable peaks[13] are given. According to the SOSA model, an experimental peak is in fact the superposition of a series of homogeneous transition subarrays. In both Tables 2 and 3 the correction terms δE are neglected because in the two cases they are all zero.

Table 1. $T_{\rm av}$ of the Co-like 3d–4p transition of tungsten.

Subarrays		The present work				RELAC†		
Lower-subconf.(X)	Upper-subconf.(Y)	$E_{\rm av}(Y)-E_{\rm av}(X)$ /cm^{-1}	$E_{\rm av}(Y)-E_{\rm av}(X)^*$ /cm^{-1}	δE /cm^{-1}	$T_{\rm av}$ /cm^{-1}	$E_{\rm av}(Y)-E_{\rm av}(X)$ /cm^{-1}	δE /cm^{-1}	$T_{\rm av}$ /cm^{-1}
$3d^3_{3/2}3d^6_{5/2}$	$3d^2_{3/2}3d^6_{5/2}4p_{1/2}$	14343527	14349302	11013	14360315	14342800	11324	14354124
	$3d^2_{3/2}3d^6_{5/2}4p_{3/2}$	15203052	15239657	–4701	15234956	15193562	–4684	15188878
	$3d^3_{3/2}3d^5_{5/2}4p_{3/2}$	14662289	14672095	10117	14682212	14661202	11192	14672394
$3d^4_{3/2}3d^5_{5/2}$	$3d^3_{3/2}3d^5_{5/2}4p_{1/2}$	14342420	14321620	16519	14338139	14337452	16986	14354438
	$3d^3_{3/2}3d^5_{5/2}4p_{3/2}$	15210539	15220246	–7051	15213195	15196566	–7026	15189540
	$3d^4_{3/2}3d^4_{5/2}4p_{3/2}$	14648929	14656953	8094	14665047	14647942	8954	14656896

∗ denotes the results including the magnetic interaction between pairs of electrons.

† denotes the results calculated by Bauche *et al.*[1] with the RELAC program.

Table 2. $T_{\rm av}$ of the Cu-like 3d–5f transition of tantalum.

	$3d_{3/2}$–$5f_{5/2}$			$3d_{5/2}$–$5f_{7/2}$		
Spectators	The present work		RELAC†	The present work		RELAC†
	$T_{\rm av}$/cm^{-1}	$T^*_{\rm av}$/cm^{-1}	$T_{\rm av}$/cm^{-1}	$T_{\rm av}$/cm^{-1}	$T^*_{\rm av}$/cm^{-1}	$T_{\rm av}$/cm^{-1}
$4s_{1/2}$	22039057.0	22069684.5	22065314.0	21551377.7	21581681.5	21612276.0
$4p_{1/2}$	22035828.9	22066468.1	22060446.0	21543889.5	21574153.4	21602938.0
$4p_{3/2}$	22048937.9	22079560.3	22075054.0	21563139.3	21593767.8	21621622.0
$4d_{3/2}$	22041891.7	22072796.9	22065314.0	21541502.9	21572241.8	21598272.0
$4d_{5/2}$	22033331.8	22063997.4	22060446.0	21554407.7	21585344.5	21612276.0
$4f_{5/2}$	22021560.9	22052182.5	22050718.0	21519906.3	21550770.1	21579630.0
$4f_{7/2}$	22009682.3	22040287.3	22040996.0	21531206.1	21562374.9	21593608.0

∗ denotes the results including the magnetic interaction between pairs of electrons.

† denotes the results calculated by Audebert *et al.*[2] with the RELAC program.

IV. CONCLUSION

The calculation of the relativistic average energy of a jj-coupling subconfiguration is a very important step in the analysis of the quasi-continuum spectra of highly ionized heavy atoms. In the past the work has usually been done with the relativistic parametric potential method. The present computation shows that by employing the MCDF package, we can also obtain results with considerable precision. Therefore, the

Table 3. T_{av} of the Cu-like and Zn-like 3d–5f transition of gold.

	$3d_{3/2}$–$5f_{5/2}$			$3d_{5/2}$–$5f_{7/2}$		
Spectators	The present work		Experimental results†	The present work		Experimental results†
Cu-like	T_{av}/cm^{-1}	T_{av}^{*}/cm^{-1}	T_{av}/cm^{-1}	T_{av}/cm^{-1}	T_{av}^{*}/cm^{-1}	T_{av}/cm^{-1}
$4s_{1/2}$	27543897.8	27585244.2		26832860.2	26873071.6	
$4p_{1/2}$	27538747.4	27580105.1		26822982.9	26863149.8	
$4p_{3/2}$	27557193.5	27598539.5		26848136.4	26888809.9	
$4d_{3/2}$	27546777.5	27588498.5	27570995.3	26821597.3	26862453.8	26888948.6
$4d_{5/2}$	27538272.1	27579675.8		26837002.1	26878093.8	
$4f_{5/2}$	27522638.8	27563990.6		26795108.0	26836105.7	
$4f_{7/2}$	27509568.6	27550885.5		26809156.3	26850611.4	
Zn-like						
$4s4p_{1/2}$	27261296.2	27302719.3		26547105.4	26588348.6	
$4s4p_{3/2}$	27279444.0	27320855.5		26572013.6	26613584.4	
$4p_{1/2}^{2}$	27256546.9	27297992.1		26537703.5	26577922.8	
$4p_{1/2}4p_{3/2}$	27274997.9	27316416.3		26562812.4	26604329.0	
$4p_{3/2}^{2}$	27293531.9	27334929.5		26587964.2	26629091.6	
$4s4d_{3/2}$	27210081.6	27311882.7		26546540.1	26587979.5	
$4s4d_{5/2}$	27261105.9	27302576.8		26561159.1	26602958.5	
$4p_{1/2}4d_{3/2}$	27264453.5	27306260.9		26536123.3	26577505.8	
$4p_{1/2}4d_{5/2}$	27256509.4	27297994.6		26551873.1	26593618.8	
$4p_{3/2}4d_{3/2}$	27283683.2	27325470.9		26562149.6	26605563.1	
$4p_{3/2}4d5/3$	27274552.9	27316015.2		26576790.7	26620622.8	
$4d_{3/2}^{2}$	27273337.5	27315563.4		26535848.0	26576708.6	
$4d_{3/2}4d_{5/2}$	27265541.9	27307391.1	27270248.2	26551713.6	26595351.1	26609898.9
$4d_{5/2}^{2}$	27251825.3	27299336.9		26567454.5	26611534.7	
$4s4f_{5/2}$	27242096.1	27283767.0		26517595.7	26559257.0	
$4s4f_{7/2}$	27232677.9	27274065.6		26532922.3	26575120.3	
$4p_{1/2}4f_{5/2}$	27237104.6	27279078.9		26508162.7	26549764.1	
$4p_{1/2}4f_{7/2}$	27227751.1	27269150.3		26523332.1	26565472.1	
$4p_{3/2}4f_{5/2}$	27260056.9	27301472.4		26536332.0	26579929.2	
$4p_{3/2}4f_{7/2}$	27247393.6	27288774.9		26550357.9	26594478.6	
$4d_{3/2}4f_{5/2}$	27249995.5	27291833.4		26510335.4	26553738.9	
$4d_{3/2}4f_{7/2}$	27237609.1	27279366.5		26524554.3	26568491.9	
$4d_{5/2}4f_{5/2}$	27241643.6	27283156.7		26525651.4	26569484.7	
$4d_{5/2}4f_{7/2}$	27229058.1	27270501.3		26539298.2	26583667.8	
$4f_{5/2}^{2}$	27225996.3	27267555.5		26484746.7	26525919.7	
$4f_{5/2}4f_{7/2}$	27213766.7	27255221.2		26498422.3	26542543.9	
$4f_{7/2}^{2}$	27202944.2	27244284.9		26513554.2	26555662.7	

$*$ denotes the results including the magnetic interaction between pairs of electrons.

† denotes the mean wavenumber of the experimentally observable peak.

approach offers an alternative method for calculating the subconfiguration-averaged quantities needed in the identification of the unresolved spectra emitted by highly ionized heavy atoms.

Here, we have not tried to make any further attempt to improve the accuracy of our results because we think it is good enough for use in spectroscopic analysis or for diagnostic purposes when the magnetic interaction between pairs of electrons is included. In comparison, we find that our calculations are in excel-

lent agreement with those computed with the RELAC program. Of course, if more precise results are needed, the retardation term and other higher correction term have to be included.

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