

A Straightforward Method of Calculating Finely the Soft X-Ray Spectra of Hydrogenlike Highly Ionized-States^{*}

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Abstract: A new method of calculating finely the soft X-ray spectra of hydrogenlike highly ionized-states is presented. It is based on the relation of the ionicity and the ionization energies of hydrogenlike atoms and the new model of potential function of hydrogenlike atoms. The relativistic revision and the spin-orbit coupling of excitation energy levels are taken into account. The calculated results are in good agreement with the experiments.

Key words: hydrogenlike ions, spectra of soft X-ray, effect of ionicity, relativistic effect

In the middle of 1970s, Chapline et al.^[1] predicted that the M → L shell transitions of highly ionized hydrogenlike atoms with medium atomic number were the most hopeful for the X-ray lasers. Recently, with the application of the accelerators, the experimental technology and the measure methods of the spectra of highly ionized heavy elements are developed^[2]. The studies of the X-ray laser, plasma physics and astrophysics are excited greatly^[3].

Because the probability of an electron near the nuclear is larger in the hydrogenlike atom, the relativistic effect, finite-nuclear-size effect, quantum-electrodynamics (QED) effect, and some unknown interactions are stronger. For example, the contribution of the non-Coulomb interaction to the ground state energy level is 309.9 eV for a hydrogenlike krypton ion^[4]. Therefore, the exact calculation of spectra is very difficult. What's more, it is not easy to identify the spectra due to the mixing of different ions or ion states. When the Hartree-Fock method is used, not only the process of calculation is complex, but also the results of calculation are limited. So it is necessary to find a straightforward and effective method to calculate the wavelength of the spectral lines.

The relation between the ionicity and the ionization energies of the hydrogenlike atoms has been studied and the new potential function model of hydrogenlike atoms has been set up^[4,5]. The ionicity included the relativistic effect, finite-nuclear-size, and QED effects of ground states of the ions. The calculated results of ionization energies for the hydrogenlike ions by the method are 0.01% less than that of the experiments and Hartree-Fock method. In

Ref. [6], the spin-orbit coupling was taken into account. But the change of the relativistic effect with the quantum number n and l was neglected.

In this paper, the relativistic effect varies with the quantum number n and l is considered, and the spin-orbit coupling of the electron is taken into account at the same time. The maximum relative error between the calculated and the experimental values reduces from 0.17% to 0.086% for the hydrogenlike sodium, magnesium^[6], and aluminium atoms. The method is satisfactory for calculating the soft X-ray spectra of other hydrogenlike atoms.

1 Theory

In the center force field, the Dirac equation of single electron in the nonrelativistic approximation is^[7]

$$[\hat{H}_0 + \hat{H}_s + \hat{H}_m + \hat{H}_d]\Psi = E\Psi \quad (1)$$

where

$$\hat{H}_0 = -\frac{\hbar^2}{2\mu}\nabla^2 + u(r) \quad (2)$$

is the Hamiltonian in nonrelativistic Schrodinger equation.

$$\hat{H}_s = \frac{1}{2\mu^2 c^2} \frac{1}{r} \frac{du(r)}{dr} \hat{L} \cdot \hat{S} \quad (3)$$

is the spin-orbit interaction.

$$\hat{H}_m = -\frac{\hat{P}^4}{8\mu^3 c^2} \quad (4)$$

and

$$\hat{H}_d = \frac{\hbar^2 e}{8c^2 \mu^2} \nabla^2 + u(r) \quad (5)$$

are the relativistic revision and Darwin term, respectively.

In the new potential function model of

hydrogenlike atoms, the form of the potential function is

$$u(r) = -\frac{\sqrt{Z^2 + f(\Delta Z)}}{4\pi\epsilon_0 r}e^2 \quad (6)$$

where Z is the atomic number; ΔZ is the ionicity; and $f(\Delta Z)$ is the function as ionicity. It is given by

$$\begin{aligned} f(\Delta Z) = & 1.40472 \times 10^{-5} \Delta Z^4 \\ & + 1.53677 \times 10^{-5} \Delta Z^3 \\ & + 8.49377 \times 10^{-4} \Delta Z^2 \\ & + 4.98974 \times 10^{-4} \Delta Z \end{aligned} \quad (7)$$

The function comes from fit to the experimental values of ionization energies of hydrogenlike ions, it includes the relativistic effect, finite-nuclear-size and QED effects of ground state of the ion.

Substituting Eqs. (6) and (7) into the Schrodinger equation corresponding to Eq. (2), the nonrelativistic energy levels of hydrogenlike ions are obtained as follows:

$$E_n = -\frac{Rhc[Z^2 + f(\Delta Z)]}{n^2} \quad (8)$$

where R, h, c are the Rydberg constant, Planck constant and the velocity of light in vacuum, respectively. The corresponding wave function is

$$\Psi = R_{nl}(r) Y_l^m(\theta, \varphi) \quad (9)$$

in which the angular function is

$$Y_l^m(\theta, \varphi) = A e^{\pm im\varphi}(\theta, \varphi) \Theta_{lm}(\theta) \quad (10)$$

where l, m are the angular and magnetic quantum numbers, respectively; $\Theta_{lm}(\theta)$ is the associated Legendre polynomials; A is the normalized constant. The radial function is

$$\begin{aligned} R_{nl} = & N_{nl} \exp\left(-\frac{\sqrt{Z^2 + f(\Delta Z)}r}{na_1}\right) \left(\frac{2\sqrt{Z^2 + f(\Delta Z)}r}{na_1}\right)^l \\ & \times L_{n-1}^{2l+1}\left(\frac{2\sqrt{Z^2 + f(\Delta Z)}r}{na_1}\right) \end{aligned} \quad (11)$$

where $L_{n-1}^{2l+1}\left(2\sqrt{Z^2 + f(\Delta Z)}r/na_1\right)$ is the Leguerre polynomials, $a_1 = \hbar/\mu e^2$ is the first Bohr's radius;

$$N_{nl} = -\left\{\left[\frac{2\sqrt{Z^2 + f(\Delta Z)}}{na_1}\right]^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}\right\}^{\frac{1}{2}} \quad (12)$$

Solving the Schrodinger equation corresponding to Eqs. (3) – (5) in the coupling picture $|nlsjm\rangle$, the energy of spin-orbit interaction is obtained as follows:

$$\begin{aligned} \Delta E_{ls} = & \frac{Rhc\alpha^2[Z^2 + f(\Delta Z)]^2}{n^3 l(l+1/2)(l+1)} \\ & \times \frac{j(j+1) - l(l+1) - s(s+1)}{2} \end{aligned} \quad (13)$$

where α is the fine-structure constant; j the total

angular quantum number; and s the spin angular quantum number.

The relativistic revision is

$$\begin{aligned} \Delta E_m = & -\frac{Rhc\alpha^2[Z^2 + f(\Delta Z)]^2}{n^3} \\ & \times \left(\frac{1}{l+1/2} - \frac{3}{4n}\right) \end{aligned} \quad (14)$$

and Darwin term (only adaptable to s state) is

$$\Delta E_d = Rhc\alpha^2[Z^2 + f(\Delta Z)]^2/n^3 \quad (15)$$

The sum of the relativistic revision and Darwin term for the $1s$ state of hydrogenlike atoms is

$$\begin{aligned} \Delta E_{ls} = & \Delta E_{m1s} + \Delta E_{d1s} \\ = & -Rhc\alpha^2[Z^2 + f(\Delta Z)]^2/4 \end{aligned} \quad (16)$$

It is evident that ΔE_{ls} has been included the ground energy level revised by the ionicity. Because ΔE_m varies with the quantum number n and l , and ΔE_d with n , Eq. (8) is adapt to the $1s$ state only. When we calculate the fine-structure energy levels of excited states, ΔE_{ls} should be subtracted from Eq. (8) and Eqs. (13) – (15) should be added to Eq. (8). Therefore, the formula of the energy levels of excited states is

$$\begin{aligned} E_{nlj} = & -\frac{Rhc[Z^2 + f(\Delta Z)] + Rhc[Z^2 + f(\Delta Z)]^2\alpha^2/4}{n^2} \\ & -\frac{Rhc\alpha^2[Z^2 + f(\Delta Z)]^2}{n^3} \left(\frac{1}{j+1/2} - \frac{3}{4n}\right) \end{aligned} \quad (17)$$

where $n > 1$; $j = l + 1/2$ or $j = l - 1/2$.

The energy level of ground state of hydrogenlike atoms is

$$E_{1s} = -Rhc[Z^2 + f(\Delta Z)] \quad (18)$$

The transition wavelength satisfying the selection rule of electrical dipole transition can be expressed as

$$\lambda = \frac{hc}{E_{nlj} - E_{n'l'j'}} = \frac{1.2397852 \times 10^3}{E_{nlj} - E_{n'l'j'}} \quad (19)$$

where $n > n'$; E_{nlj} is the energy of initial state, and $E_{n'l'j'}$ is that of final state, they are expressed in eV.

2 Calculated Results

According to Eqs. (17) – (19), we re-calculated the soft X-ray spectra of hydrogenlike sodium, magnesium, and aluminium atoms, and the soft X-ray spectra of hydrogenlike phosphorus, sulphur atoms are calculated too. The calculated results, the results of Ref. [6], and the experimental results are shown in Tab.1, respectively.

Tab. 1 A part of the soft X-ray spectra of hydrogenlike atoms

Ion symbol	nL, j		$n'L', j$		$\lambda/\text{nm}^{①}$	$\lambda/\text{nm}^{②}$	$\lambda/\text{nm}^{③}$
Na ⁺¹⁰	2P	1/2	1S	1/2	1.002?83	1.003?05	1.002?6 ^[8]
	2P	3/2	1S	1/2	1.002?29	1.002?51	1.002?6 ^[8]
	3P	1/2	1S	1/2	0.846?02	0.846?10	0.846?1 ^[8]
	3P	3/2	1S	1/2	0.845?91	0.845?98	0.846?1 ^[8]
	3D	3/2	2P	1/2	5.405?95	5.404?99	
	3D	5/2	2P	3/2	5.420?12	5.419?16	
Mg ⁺¹¹	2P	1/2	1S	1/2	0.842?43	0.842?65	0.842?53 ^[8]
	2P	3/2	1S	1/2	0.841?89	0.842?11	0.841?94 ^[8]
	3P	1/2	1S	1/2	0.710?69	0.710?76	0.710?62 ^[8]
	4P	3/2	1S	1/2	0.710?57	0.710?65	0.710?62 ^[8]
	4P	1/2	1S	1/2	0.673?82	0.673?86	0.673?60 ^[8]
	4P	3/2	1S	1/2	0.673?78	0.673?82	0.673?60 ^[8]
	5P	1/2	1S	1/2	0.658?03	0.658?06	0.657?60 ^[8]
	5P	3/2	1S	1/2	0.658?00	0.658?04	0.657?60 ^[8]
	6P	1/2	1S	1/2	0.649?76	0.649?78	0.650?30 ^[8]
	6P	3/2	1S	1/2	0.649?74	0.649?77	0.650?30 ^[8]
	4P	3/2	2S	1/2	3.365?54	3.368?82	3.367?80 ^[9]
	4P	1/2	2S	1/2	3.366?62	3.369?90	
	4D	5/2	2P	3/2	3.373?81	3.371?91	3.373?60 ^[9]
	4D	3/2	2P	3/2	3.374?18	3.372?27	
	4D	3/2	2P	1/2	3.365?54	3.363?65	
	3P	3/2	2S	1/2	4.539?81	4.546?84	4.539?2 ^[9]
	3P	1/2	2S	1/2	4.544?46	4.551?50	
	3D	5/2	2P	3/2	4.553?98	4.553?02	4.553?0 ^[9]
Al ⁺¹²	4F	5/2	3D	3/2	13.006?0	12.989?32	13.006?1 ^[9]
	4F	7/2	3D	5/2	13.016?1	12.999?33	13.014?1 ^[9]
	2P	3/2	1S	1/2	0.717?06	0.717?29	0.717?03 ^[8]
	2P	1/2	1S	1/2	0.717?60	0.717?83	0.717?59 ^[8]
	3P	3/2	1S	1/2	0.605?25	0.605?33	0.605?24 ^[8]
	3P	1/2	1S	1/2	0.605?36	0.605?44	0.605?24 ^[8]
	4P	3/2	1S	1/2	0.573?91	0.573?96	0.573?87 ^[8]
	4P	1/2	1S	1/2	0.573?96	0.574?00	0.573?87 ^[8]
	5P	3/2	1S	1/2	0.560?48	0.560?51	0.560?35 ^[8]
	5P	1/2	1S	1/2	0.560?50	0.560?54	0.560?35 ^[8]
	6P	3/2	1S	1/2	0.553?45	0.553?47	0.553?37 ^[8]
	6P	1/2	1S	1/2	0.553?46	0.553?48	0.553?37 ^[8]
	7P	3/2	1S	1/2	0.549?29	0.549?31	0.549?10 ^[8]
	7P	1/2	1S	1/2	0.549?30	0.549?32	0.549?10 ^[8]
P ⁺¹⁴	8P	3/2	1S	1/2	0.546?626	0.546?64	0.546?30 ^[8]
	8P	1/2	1S	1/2	0.546?631	0.546?65	0.546?30 ^[8]
	2P	3/2	1S	1/2	0.538?11		0.538?02 ^[8]
	2P	1/2	1S	1/2	0.538?65		0.538?59 ^[8]
S ⁺¹⁵	3P	3/2	1S	1/2	0.454?26		
	3P	1/2	1S	1/2	0.454?37		
	2P	3/2	1S	1/2	0.472?71		0.472?74 ^[8]
	2P	1/2	1S	1/2	0.473?25		0.473?34 ^[8]
	3P	3/2	1S	1/2	0.399?07		
	3P	1/2	1S	1/2	0.399?19		
	5G	9/2	4F	7/2	15.819?0		15.821?7 ^[10]
	4F	5/2	3D	3/2	7.310?1		7.309?1 ^[10]
	4D	3/2	3P	1/2	7.277?5		7.213?1 ^[10]

① Calculated results in the paper; ② The results of Ref. [6]; ③ Experimental results.

3 Conclusion and discussion

It is seen from Tab.1 that the influence of relativistic effect on the finely structure of excitation energy levels is larger. It makes the maximum relative error between the calculated and the experimental values reduces from 0.17% to 0.086% in Ref.[6] for the hydrogenlike sodium, magnesium, and aluminium atoms. For the hydrogenlike phosphorus, sulphur atoms, the relative error of most spectral lines is less than 0.019%, and that of only a spectral line ($S^{+15}, 4d^2 D_{3/2} \rightarrow 3P^2 P_{1/2}$) is 0.89%. In consideration of the limitation of the resolving power of the device in Ref.[10], we think the reason for the large relative error of the spectrum can come from the experiment. It can be proved in need of other experiments.

Because the relativistic, finite-nuclear-size and QED effects of ground state of ions have been included in the function as ionicity, and the change of relativistic effect of excited states with the quantum number is taken into account, the complex calculation process is simplified. The straightforward and effective method is afforded for the experimenters. They can know quickly their measured spectra and assess on the experimental error.

The revision of the finite-nuclear-size and QED effects of excited states will be studied in future.

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类氢高离化态软 X 射线谱精细计算的简捷方法

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摘 要 利用高离化态类氢离子电离能与电离度的关系及类氢离子的新势函数模型, 对离子激发能级进行了相对论效应修正并计及了电子自旋轨道耦合的影响. 给出了计算高离化态类氢离子软 X 射线谱的简捷方法, 计算结果与实验值吻合较好.

关键词 类氢离子, 软 X 射线谱, 电高度效应, 相对论效应

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