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Calculation of relativistic corrections within the Hartree-Fock-Slater model

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Abstract

The aim of the project was to extend the XATOM toolkit by adding the relativistic correction. XATOM can calculate of cross section of photoionization, decay rates: fluorescence rates and Auger rates, elastic x-ray scattering form factor for all atomic species and all possible electronic configurations. All basic components have already been developed and the working non-relativistic Hartree-Fock-Slater code is available. However the relativistic effects have not been taken into account for atomic energy level calculations. I extended XATOM to include the relativistic effects via the first-order perturbation correction.

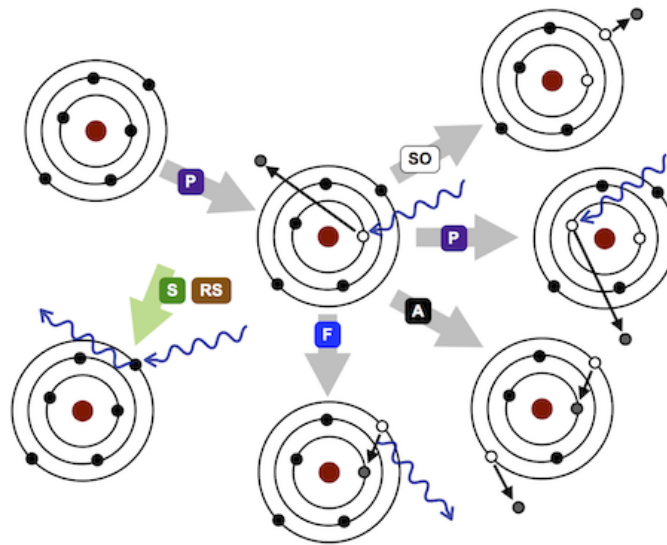
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Introduction

Future progress in the synchrotron radiation studies is connected with the progress in development of fourth generation synchrotron radiation sources which are related to the progress of Self-Amplified Spontaneous Emission Free-Electron Lasers (SASE FELs). The X-ray free electron laser (XFEL) produces X-ray radiation during a single pass of electron beam through a long undulator. XFEL offers many possibilities that have not been conceivable with conventional light sources. Because of their very high fluence within very short pulse duration, materials interacting with XFEL undergo significant radiation damage with ejection of electrons and possibly become highly ionized. A lot of different atomic processes can occur as the result of interaction of electromagnetic radiation generated by this laser with the matter (Picture 1). For instance, the most probable process in the range of VUV and soft X-ray is the photoionization process creates a core-level state, followed by another photoionization or relaxation process. In the process of relaxation from the excited state to the ground state the fluorescence and the Auger decay can be observed.

It is necessary to have a good theoretical base which can completely describe all these processes in order to understanding detailed ionization and relaxation dynamics in atoms during XFEL pulses. The XATOM toolkit was developed to treat detailed ionization, relaxation, and scattering dynamics for atoms during FEL pulses. It was employed a consistent theoretical framework based on non-relativistic quantum electrodynamics and perturbation theory, within the Hartree-Fock-Slater model. This program is useful because we can apply it for all possible n -hole and $+n$ charge electronic configurations of any elements. XATOM is used for calculating the following values: the photoionization cross sections, Auger decay rates, fluorescence rates, elastic x-ray scattering form factor and their dispersion correction. The ionization and relaxation dynamics are described by rate equations.



Picture 1. Diagrams of x-ray–atom interaction - **P**: photoionization, **A**: Auger (Coster-Kronig) decay, **F**: fluorescence, **SO**: shake-off, **S**: elastic x-ray scattering, **RS**: resonant elastic x-ray scattering. This figure is taken from [1].

The speed of the majority of the electrons in the atom is slow as compared to the speed of light. The velocity of electrons in the helium atom equals 0.02 speed of light. However the velocity of electrons, in the inner shells of heavy atoms increases significantly and equals a few tenths of the speed of light. Under these conditions, changing of mass is visible and must be taken into account. There are three important relativistic effects: the relativistic mass-velocity correction, the spin-orbit interaction correction, and the relativistic s-shift (Darwin term).

In the experiments of the multiphoton multiple ionization of xenon atoms, using SPring-8 Angstrom Compact free electron LAser (SACLA), experimental and theoretical charge states distributions of Xe were compared [2]. There is the discrepancy between experimental and theoretical data, which were obtained using XATOM with applying the Monte Carlo procedure, in this experiment and in other investigation on ionization dynamics of Xe atoms induced by XFEL pulses [3]. The discrepancy can be assigned to the non-relativistic treatment in the current theoretical model. Without including fine-structure splittings, some of possible transitions in Xe atom are energetically impossible and these transitions are completely missing in the HFS method [2], [3], [4]. Hence, it is necessary to include relativistic corrections into this calculation.

My main goal during my work is the calculation of the relativistic corrections of the atomic energy levels by the first order perturbation method. My studies throughout the programme can be separated into two parts. The first part is to investigate the main relativistic atomic effects and understand the way of solving equations with these additional terms within the framework of the first order perturbation theory. The second part of my work is to work with a program code. I analyze all necessary components of the XATOM code, and modify the program code by including the parts which describes the relativistic effects.

Non - relativistic Hartree-Fock-Slater method

For the pure hydrogen-like systems, it is possible to solve the Schrödinger equation analytically. More general many-electron systems cannot be treated with such precision. A majority of the elements in the periodic table are many-electron systems where the motion of every electron is coupled to the motion of all the other electrons as well as to the nucleus. To study such systems we have to rely on some approximation method. One widely used approximation method is the Hartree-Fock method. It is based on the natural approximation that every electron moves in the potential created by the nucleus plus the average potential of all the other electrons. This assumption leads to the independent-particle model, which essentially reduces the many-electron problem to the problem of solving a number of coupled single-electron equations.

The other major approximation is the replacement of the Hartree-Fock exchange potential terms with a simple exchange potential. The Hartree-Fock-Slater model employs a local density approximation to the exact exchange interaction, with the Latter tail correction.

Schrödinger equation with the non-relativistic Hamiltonian operator:

$$H_0\psi(r) = \left[-\frac{1}{2}\nabla^2 + v(r) \right] \psi(r) = E\psi(r) \quad (1)$$

Where $v(r)$ - the potential, which is defined like:
$$v(r) = \begin{cases} -\frac{Z}{r} + \int \frac{\rho(r')}{|r-r'|} d^3r' - \frac{3}{2} \left[\frac{3}{\pi} \rho(r) \right]^{1/3} \\ -\frac{Z - N_e + 1}{r} \text{ for } r > r_c \end{cases}$$

The potential can be separated into three parts: $-\frac{Z}{r}$ - coulomb interaction the electrons with

the nucleus, $\int \frac{\rho(r')}{|r-r'|} d^3r'$ - coulomb interaction defined by all the electrons, $-\frac{3}{2} \left[\frac{3}{\pi} \rho(r) \right]^{1/3}$ -

the Slater exchange potential, where Z - the atomic number, $\rho(r)$ - the electrons density

$$\rho(r) = \sum_{i=1}^{N_e} |\psi_i(r)|^2, \quad N_e - \text{the number of electrons, } \psi(r) - \text{wave function of electron, } E -$$

eigenvalue of Hamiltonian. For the case of $r > r_c$, we apply the Latter tail correction.

Theory of relativistic effects

For a hydrogenic atom, the structure of energy levels only depends on the principal quantum number n . However, for heavy atoms it is necessary to take into account relativistic and spin effects, which break the degeneracy of the energy levels and split the spectral lines. The scale of the fine structure splitting relative to the structure splitting is on the order of $(Z\alpha)^2$, where Z is the atomic number and α is the fine-structure constant, a dimensionless number equal to approximately $\alpha = 1/137.037$.

The Hamiltonian, including the relativistic corrections, can be separated into three corrective terms: the kinetic energy term, the spin-orbit term, and the Darwinian term [5]. The radial Pauli wave equation:

$$[H_0(r) + H_m(r) + H_d(r) + H_{so}(r)]R(r) = E R(r) \quad (2)$$

where $R(r)$ - radial wave function.

Here $H_0(r)$ is the non-relativistic Hamiltonian operator:

$$H_0(r) = -\left(\frac{1}{r^2}\right) \left(\frac{d}{dr} \right) \left(r^2 \frac{d}{dr} \right) + v(r) + \frac{l(l+1)}{r^2} \quad (3)$$

Where l - orbital quantum number, $v(r)$ is defined like (2).

The relativistic variation of the mass with velocity is accounted for by the term $H_m(r)$, which is most conveniently written form:

$$H_m(r) = -\left(\frac{\alpha^2}{4}\right)[E^0 - v(r)]^2 \quad (4)$$

where E^0 - zero order (the non-relativistic) energy eigenvalue. The relativistic mass-velocity correction is negative for all orbitals. This term is related to considering special relativity equation.

The relativistic Darwin correction produced by the operator $H_d(r)$:

$$H_d(r) = -\left(\frac{\alpha^2}{4}\right)\left(\frac{dv(r)}{dr}\right)\left(\frac{d}{dr}\right) \quad (5)$$

The Darwin term changes the effective potential at the nucleus. It can be interpreted as a smearing out of the electrostatic interaction between the electron and nucleus due to rapid quantum oscillations, of the electron. In the special case of a coulomb potential, the Darwin correction is positive for all orbitals with $l = 0$ and zero for all orbitals with $l \neq 0$. However, in my case, the potential is not the pure Coulomb potential and the Darwin correction is not zero for all orbitals with $l \neq 0$.

The spin-orbital energy is given by the term $H_{so}(r)$:

$$H_{so}(r) = -\left(\frac{\alpha^2}{4}\right)\left(\frac{1}{r}\right)\left(\frac{dv(r)}{dr}\right)\left[\begin{matrix} -l \\ l+1 \end{matrix}\right] \quad (6)$$

The upper quantity $[-l]$ refers to $j = l + 1/2$, and the lower quantity $[l+1]$ to $j = l - 1/2$ where $l \neq 0$. In the case of $l = 0$, spin-orbital correction equals zero. The spin-orbit interaction causes shifts in an electron's atomic energy levels due to electromagnetic interaction between the electron's spin and the magnetic field generated by the electron's orbit around the nucleus.

The zero-order non-relativistic wave equation has been solved for all orbitals (n,l):

$$H_0(r)R_{nl}^0(r) = E_{nl}^0 R_{nl}^0(r) \quad (7)$$

We solved our radial Pauli wave equation within the framework of the first-order perturbation theory, where α^2 plays role of the perturbation parameter. The energy, correct to order α^2 , is given by:

$$E_{nl}^1 = E_{nl}^0 + \int_0^\infty dr r^2 R_{nl}^0(r) [H_m(r) + H_d(r) + H_{so}(r)] R_{nl}^0(r) \quad (8)$$

where E_{nl}^0 - zero order (the non-relativistic) energy eigenvalue.

The notation for the energy corrections for each of these terms are following:

$$E_m = -\left(\frac{\alpha^2}{4}\right) \int_0^\infty dr r^2 [R_{nl}^0(r)]^2 [E^0 - v(r)]^2 = -\left(\frac{\alpha^2}{4}\right) \int_0^\infty dr [\chi(r)]^2 [E^0 - v(r)]^2 \quad (9)$$

$$\begin{aligned} E_d &= -\left(\frac{\alpha^2}{4}\right) \int_0^\infty dr r^2 [R_{nl}^0(r)] \left(\frac{dv(r)}{dr}\right) \left(\frac{dR_{nl}^0(r)}{dr}\right) = \\ &= -\left(\frac{\alpha^2}{4}\right) \int_0^\infty dr \chi(r) \left(\frac{dv(r)}{dr}\right) \left(\frac{d\chi(r)}{dr} - \frac{\chi(r)}{r}\right) \end{aligned} \quad (10)$$

$$E_{so} = \left(\frac{\alpha^2}{4}\right) \int_0^\infty dr r^2 [R_{nl}^0(r)]^2 \left(\frac{1}{r}\right) \left(\frac{dv(r)}{dr}\right) = \left(\frac{\alpha^2}{4}\right) \int_0^\infty dr [\chi(r)]^2 \left(\frac{1}{r}\right) \left(\frac{dv(r)}{dr}\right) \quad (11)$$

where E_m - the energy correction connected with the relativistic variation of mass with velocity, E_d - the energy correction connected with Darwin term, E_{so} - the energy correction connected with spin-orbital interaction, $\chi(r) = r \cdot R_{nl}^0(r)$ is the normalized non-relativistic self-consistent Hartree-Fock-Slater radial function corresponding to E_{nl}^0 .

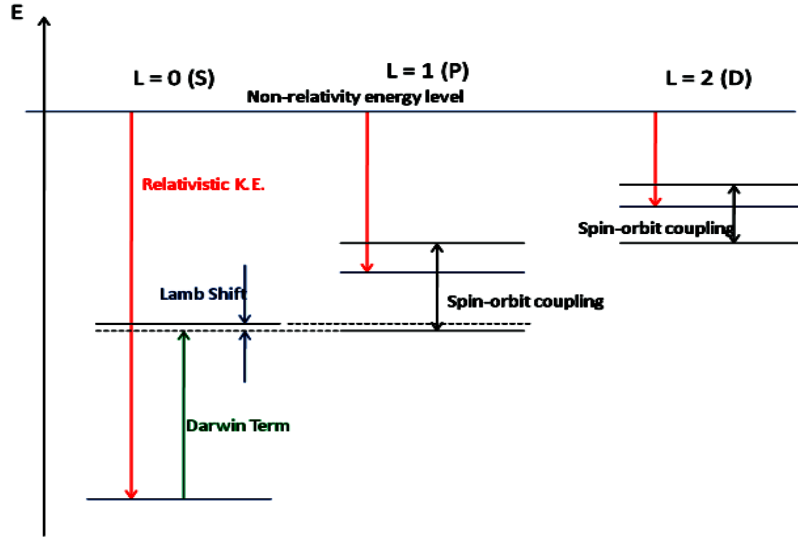
The total effect, obtained by summing the three components up, is given by the following expression:

$$\text{In case of } l = 0: \quad E(j) = E_0 + E_m + E_d$$

$$\text{In case of } l \neq 0: \quad E(j = l - 1/2) = E_0 + E_m + E_d + (-l - 1)E_{so}$$

$$E(j = l + 1/2) = E_0 + E_m + E_d + (l)E_{so}$$

The energy shifts are showed in *Picture 2*.



Picture 2. Energy levels of the fine structure with including Darwin, Kinetic and Spin-orbital correction. This figure is taken from [6].

XATOM program and GPS method

The XATOM program has wide application [7], and it provides good results for different atomic processes can occur as the result of interaction of electromagnetic radiation with the matter. The Herman-Skillman code is one of the simplest Self-Consistent Field computational codes for determining one-electron wave functions and the associated potential for any free atom or ion. Both of these programs were obtained within the same framework of first-order perturbation theory but with different numerical techniques.

There is one important numerical difference between XATOM and the Herman-Skillman code. XATOM uses non-uniform radial grids for bound states and uniform radial grids for continuum states instead of other kind of non-uniform grids with for both states in the Herman-Skillman code. The difference between these grids is different method of distribution of points. The main advantage of XATOM's non-uniform grid it is easy to increase the density of points near the origin; it is useful for heavy elements, the radial functions of electrons of these elements are very close to the origin and therefore it requires denser grid near this area.

For the solving a second-order differential equation, for instance, radial Schrodinger equation, it is applied a special technique - generalized pseudospectral method (GPS) is employed in the program XATOM [8]. The central part of the pseudospectral method is to approximate the exact function $f(x)$ defined on the interval $[-1, 1]$ by N th-order polynomial $f_N(x)$:

$$f''(x) + v(x)f(x) = \lambda f(x) \quad \text{or} \quad \hat{H}(r)\psi(r) = E\psi(r), \quad \psi(0) = \psi(\infty) = 0$$

$$f(x) \cong f_N(x) = \sum_{j=0}^N f(x_j) g_j(x) \quad (12)$$

Where λ - eigenvalue, $g_j(x)$ - are the cardinal functions defined by:

$$g_j(x) = -\frac{1}{N(N+1)P_N(x_j)} \cdot \frac{(1-x^2) \cdot P'_N(x)}{x-x_j} \quad (13)$$

where N – quantity of grid points, $P_N(x)$ - Legendre polynomials.

$$f(x_j) = P_N(x_j) A_j \quad (14)$$

for the frequently used Dirichlet boundary conditions,

$$A_0 = A_N = 0 \quad (15)$$

For atomic calculations involving the Coulomb potential, one typical problem with the grid methods is the Coulomb singularity at $r=0$ and the long-range nature of the interaction. First map the semi-infinite domain $r \in [r_{\min}, r_{\max}]$ is transformed into the finite domain $x \in [-1, 1]$ using the mapping transformation:

$$r = r(x) = L \frac{1+x}{1-x+\alpha} \quad (16)$$

where L – is a mapping parameter, $\alpha = \frac{2L}{(r_{\max} - r_{\min})}$.

The Darwin correction (5) and spin-orbital correction (6) include the first derivative of potential and the first derivative of radial wave function. In order to calculate this term we need to know the pseudospectral approximation for the first derivative of the wave function. It can be expressed through the coefficients A :

$$\left. \frac{d\psi(r)}{dr} \right|_{r(x_{j'})} = P_N(x_j) [r'(x_{j'})]^{-1/2} \sum_{j=0}^N D_{jj'}^{(1)} A_j \quad (17)$$

$$j' = 0, \dots, N$$

With the matrix $D_{jj'}^{(1)}$ represented by

$$D_{jj'}^{(1)} = [r'(x_{j'})]^{-1/2} d_{jj'}^{(1)} [r'(x_j)]^{-1/2} \quad (18)$$

where $d_{jj'}^{(1)}$ is the first derivative of the cardinal function (13) with respect to x :

$$\begin{aligned}
d_{j'j}^{(1)} &= \frac{1}{x_{j'} - x_j} (j' \neq j) & d_{00}^{(1)} &= -\frac{N(N+1)}{4} \\
d_{jj}^{(1)} &= 0 (j \neq 0, j \neq N) & d_{NN}^{(1)} &= \frac{N(N+1)}{4}
\end{aligned} \tag{19}$$

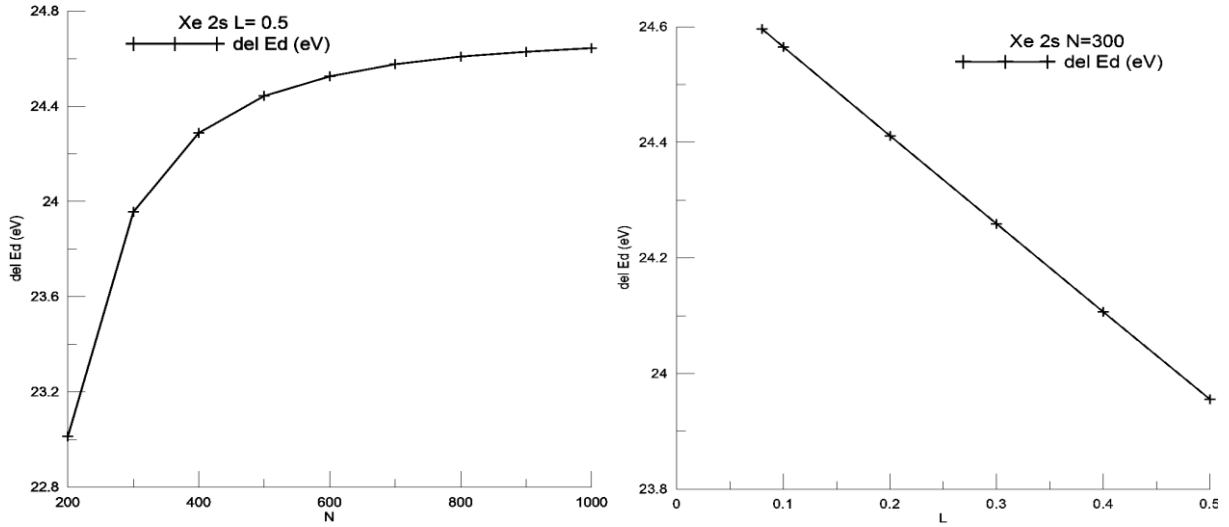
Results and discussion

I have modified the XATOM code with adding the extra module and obtained results of the calculations relativistic corrections. For reference, *Table 1* contains results for orbital energies of Fe and Xe without relativistic corrections.

1s	-7017.95	1s	-33121.49
2s	-829.40	2s	-5061.86
2p	-722.30	2p	-4776.21
3s	-98.95	3s	-1046.92
3p	-66.59	3p	-923.99
4s	-7.43	4s	-193.02
3d	-13.14	3d	-693.31
		4p	-148.65
		5s	-21.80
		4d	-71.56
		5p	-11.41

Table 1. Orbital energies for Fe (left) and Xe (right) without relativistic corrections. (all of these energy levels are presented in eV)

The relativistic corrections can be presented separately - three corrective terms: the kinetic energy term, the spin-orbit term, and the Darwinian term. *Table 2* contains results of the calculations of all of these terms and the comparison between data from the Herman-Skillman book [5] and findings for Fe and Xe. Even for very light elements near $Z = 10$ the relativistic effects make a contribution to the energy levels. The relativistic effects grow with increasing Z and become significant for all the shells in the atom, especially for the inner shells. I compared the results were obtained by the Herman-Skillman code and by the XATOM program in order to check my results, as both of these results were obtained within the framework of first order perturbation theory. For the kinetic energy term and the spin-orbit term the discrepancies between the two data are insignificant. If we consider the Darwinian term, the value of electrons energy levels in the inner shells from these different sources are different. For instance, difference between $E_d - E_d$ (book) = 24.625 eV for 2s shell of Xe. This difference varies depending on the parameters L – mapping parameter (15) and N - number of grid points. I tried the different variations of these parameters; dependence of the difference between $E_d - E_d$ (book) = ΔE_d and the parameter L and N is shown on the *Picture 3*.



Picture 3. Dependence of the difference between $E_d - E_d(\text{book})$ and the parameter L and N . ($E_d - E_d(\text{book}) = \text{delEd}$ is presented in eV).

The difference between the two values does not converge to zero. The value of $E_d - E_d(\text{book})$ grows with increasing of number of grid points N and decreasing of parameter L . The Darwin term includes the first derivative of potential. The shape of potential is the following:

$$\begin{cases} v(r) \rightarrow -\frac{1}{r} & r \rightarrow \infty \\ v(r) \rightarrow -\frac{Z}{r} & r \rightarrow 0 \end{cases} \quad (20)$$

The first derivative matrix in XATOM program is defined in the pseudospectral approximation (17). But we cannot use this matrix for calculating of the first derivative of potential because boundary conditions (15) for the function of potential are not satisfied. One of the probable way to solve this issue is to explicitly include end points with matrix $d_{jj}^{(1)}$ (19) or to find the derivative in the usual way, for example, the finite-difference method with grids equally-spaced.

Fe (Z=26)							
	E_m	E_m(book)	E_m - E_m(book)		E_d	E_d(book)	E_d - E_d(book)
1s	398.762	398.762	0	1s	-319.4454	-297.81345	-21.632
2s	46.556	46.556	0	2s	-29.4004	-29.4140	0.0136
2p	6.965	6.952	0.013	2p	0.19047	0.19047	0
3s	7.078	7.077	0.001	3s	-4.2747	-3.9931	-0.2816
3p	1.113	1.113	0	3p	0.0231285	0.0231285	0
4s	0.468	0.468	0	4s	-0.280263	-0.280263	0
3d	0.139	0.139	0	3d	0.0068025	0.0068025	0
	Eso	Eso(book)	Eso - Eso(book)				
1s	0	0	0				
2s	0	0	0				
2p	-4.231155	-4.231155	0				
3s	0	0	0				
3p	-0.529235	-0.5292345	0				
4s	0	0	0				
3d	-0.035373	-0.035373	0				
Xe (Z=54)							
	E_m	E_m(book)	E_m - E_m(book)		E_d	E_d(book)	E_d - E_d(book)
1s	7547.918	7548.1901	-0.2721	1s	-6041.8445	-6048.3749	6.5304
2s	1023.6402	1023.6538	-0.013605	2s	-638.6187	-613.99365	-24.625
2p	168.77003	168.77003	0	2p	2.462505	2.462505	0
3s	216.33991	216.33447	0.005442	3s	-127.7319	-127.90469	0.172784
3p	42.965951	42.961869	0.004082	3p	0.4693725	0.4693725	0
4s	48.274622	48.267819	0.006802	4s	-28.046708	-26.956947	-1.08976
3d	11.245893	11.244533	0.00136	3d	0.2897865	0.2897865	0
4p	9.341193	9.3398325	0.00136	4p	0.092514	0.092514	0
5s	7.1793585	7.1575905	0.021768	5s	-4.1536065	-4.1318385	-0.02177
4d	2.184963	2.1836025	0.00136	4d	0.043536	0.043536	0
5p	1.0516665	1.0516665	0	5p	0.010884	0.010884	0
	Eso	Eso(book)	Eso - Eso(book)				
1s	0	0	0				
2s	0	0	0				
2p	-99.62942	-99.629415	0				
3s	0	0	0				
3p	-18.95313	-18.954486	0.0013605				
4s	0	0	0				
3d	-2.701953	-2.701953	0				
4p	-3.832529	-3.8325285	0				
5s	0	0	0				
4d	-0.428421	-0.4282854	-0.000136				
5p	-0.424612	-0.42434	-0.000272				

Table 2. Table with data from two different sources: results were obtained by XATOM and results were obtained the Herman-Skillman code and difference between these results (all of these energy levels are presented in eV). These results were obtained for the following parameters of the grid: N=600, L=0.15

	<i>Enl (relativistic case)</i>	<i>HFS</i>	<i>RHFS</i>	<i>RHF</i>	<i>Experim ental*</i>	<i>k(%)</i>	<i>k1(%)</i>
1s	-34627.5635	-34,620	-34,555	-34,754	-34,561	0.022	0.19
2s	-5446.8815	-5578	-5417	-5509	-5453	2.351	0.11
2p1/2	-5166.5946	-5166	-5104	-5161	-5107	0.011	1.167
2p3/2	-4847.7064	-4848	-4774	-4835	-4787	0.006	1.268
3s	-1135.528	-1135.3	-1122.2	-1170	-1148.7	0.02	1.147
3p1/2	-1005.25	-1005.3	-989.7	-1025	-1002.1	0.0049	0.314
3p3/2	-948.3950	-948.4	-926.5	-961	-940.6	0.0005	0.828
4s	-213.2479	-214.3	-208.5	-229	-213.2	0.4909	0.022
3d3/2	-712.882	-712.9	-690.9	-708	-689	0.0025	3.466
3d5/2	-699.3704	-699.4	-677.4	-695	676.4	0.004	3.395
4p1/2	-165.797	-165.7	-160.8	-176	-	0.054	-
4p3/2	-154.2072	-154.2	-148.0	-163	-145.5	0	5.984
5s	-24.8257	-24.8	-23.7	-27.5	-23.3	0	6.548
4d3/2	-75.0315	-75.0	-69.9	-73.8	-69.5	0	7.958
4d5/2	-72.8928	-72.9	-67.7	-71.7	-67.5	0	7.989
5p1/2	-13.2942	-13.3	-12.4	-13.4	-13.4	0	0.789
5p3/2	-12.0214	-12	-11.0	-12	-12.1	0	0.649

*Table 3. Orbital energies of Xe for two cases: without relativistic corrections and taking into account the relativistic effects and data for level of energy for Xe from relativistic HFS calculation. The last column and penultimate column are $k = (HFS - Enl (relativistic case) * 100) / HFS$ and $k1 = (Experimental - Enl (relativistic case) * 100) / Experimental$ respectively in percent (all of these energy levels are presented in eV). *K. Siegbahn et al., ESCA Applied to Free Molecules, North Holland Publishing Co., Amsterdam (1969)*

In the Hartree-Fock-Slater (HFS) case and in my code the relativistic effect is added as a perturbation. It is interesting to compare eigenvalues obtained from other methods and with experimental binding energies of Xe. In the *Table 3* three different relativistic Self-Consistent-Field (SCF) solutions and experimental binding energies are presented [9]. My results from the XATOM are in the first column, results from Herman-Skillman book (Hartree-Fock-Slater method + relativistic correction) are in the second column; the relativistic Hartree-Fock-Slater (RHFS) solution which includes the relativistic effect in a self-consistent method but uses an approximate form for the exchange integral - results from applying Dirac-Fock-Slater method are presented in the third column; the relativistic Hartree-Fock (RHF) solution in which

exchange is properly calculated is based on the most sophisticated theory – results from Dirac-Fock method are presented in the fifth column. It can be seen that there is a difference between experimental data and calculated data. The last column and penultimate column are $k = (HFS - Enl \text{ (relativistic case)} * 100) / HFS$ and $k1 = (Experimental - Enl \text{ (relativistic case)} * 100) / Experimental$ respectively in percent. These columns are presented the difference between obtained results and HFS calculation – Hermann-Skillman, obtained results and experiment respectively. Hence, it is necessary to take into consideration other effects. To obtain substantial improvement for the outer shells, correlation effects need to be evaluated, and for the inner shells radioactive corrections must be calculated.

Conclusions

The primary purpose of this project was to make a modification of XATOM program, which would be used to calculate of the relativistic corrections by the first order perturbation method. The program written during this project has been tested in various setups and conditions; and the energy orbital levels of various atoms were obtained with relativistic corrections. The results were compared with the experimental data and with data obtained by other theoretical methods.

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