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EVALUATION OF THE ANOMALOUS X-RAY ENERGY IN VIP EXPERIMENT: SOME VALUES FROM DIRAC-FOCK METHOD

S. Di Matteo[1], L. Sperandio[2]

[1] *Groupe thèorie, Dèpartement Matèriaux et Nanosciences, Institut de Physique de Rennes UMR UR1-CNRS 6251, Universitè de Rennes 1, F-35042 Rennes Cedex, France*

[2] *IstitutoNazionale di Fisica Nucleare - Laboratori Nazionali di Frascati, P.O.Box 13, 00044 Frascati (RM), Italy*

Abstract

The goal of the VIP experiment was to improve the limit on the Pauli Exclusion Principle through the search of "anomalous" X-ray in copper atoms, produced by "fresh" electrons (introduced through electrical current that crosses our sample and thus "new" respect to the existing ones in the copper, that had already all the time to perform the allowed and "prohibited" transitions) which have the probability to do the Pauli-forbidden transition [1] [2]. Here we calculated the energy shift of the anomalous X-ray for three possible decay channels: direct transition to 1s (*K*-edge) and 2p (3p) capture with a subsequent K_α (K_β) emission [3].

Since we are considering a non-antisymmetrized electron then we can follow the case of a muonic atom. The reported values were obtained from Dirac-Fock calculations, as previously performed for a variety of muonic atoms by Mallow et al. [4]. Dirac-Fock approximation takes into account the relativistic corrections that are relevant for heavy ions, as we have considered our sample (Z_{Cu} = 29). Thanks to a numerical code it is possible to perform relativistic calculations for atoms, using the "multiconfiguration" approximation for the *N*-electron wave function. This scheme proceeds through the optimization of the parameters during a self-consistent process [5]. Muon and electron can be treated in analogous way through the self-consistent field theory, to obtain wave functions and energies. The most commonly used approximation to treat the Hamiltonian of an *N*-electron system is the so called "no pair" approximation that explicity excludes electron-positron pairs. The effects of the Breit operator, the Lamb shift and all sort of radiative corrections, as perturbations, are included.

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1. INTRODUCTION

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2. THEORETICAL METHOD

A lot of results from muonic atom experiments are explained, in first approximation, on the basis of two-body (muon and nucleus) "hydrogenic" models, with the muon so close to the nucleus that the effect of the atomic electrons could be ignored. Recent experiments show

that these models are not entirely satisfactory (for example the transition intensities are dependent on the atomic charge state).

We can follow the self-consistent Dirac-Fock method to determine the structure of muonic atoms with all the electrodynamic corrections to the electronic energy, used by Desclaux. Then we can put a different mass for the exchange between muon and electron.

We consider the energy eigenvalue equation for a many-electron atom:

$$H_I \Psi = E \Psi$$

where, in the relativistic case, H_I is the usual approximate Breit-Dirac Hamiltonian:

$$H_I = \sum_{j=1}^{N} \left[\vec{\alpha} \cdot c \vec{p}_j + V_n(r_j) \right] + \sum_{i<j} \left(\frac{1}{r_{ij}} + H_B(i,j) \right).$$

(N is the number of electrons). The first summation includes kinetic energy, spin-orbit interaction and the electron-nucleus Coulomb interaction. The potential V_n takes into consideration a finite-nuclear-charge distribution and not a non-physical nuclear point-charge one. The $1/r_{ij}$ term is the electron-electron Coulomb repulsion and $H_B(i,j)$ is the Breit operator which take into account magnetic interaction and retardation. This last is used only at the first-order perturbation to correct the relativistic interaction between the electrons. Another correction, as a perturbation for heavy atoms, is the Lamb-shift. Some approximations are made: antisymmetrizzation of the total wave function, central-field, application of the variational principle.

Adding to the N-electron atom a negative muon in a bound state, we had to add to the atomic Hamiltonian those terms which corresponds to the muon's kinetic energy and its Coulomb interaction with the nucleus and the electrons:

$$H_\mu = H_1 + \vec{\alpha} \cdot c\vec{p}_\mu + \beta E_0(\mu) + V_n(r_\mu) + \sum_{k=1}^{N} \frac{1}{r_{\mu k}}.$$

Since muon and electron are distinct particle there is no muon-electron exchange interaction. So, it is possible treat these systems as ordinary atoms.

To solve these coupled integro-differential equations a numerical code was developed by Desclaux and collaborators [4] [5]. We shall use the same code to perform our calculations.

3. RESULTS AND DISCUSSION

In a previous report we have showed some values about the energy of an emitted "Pauli-principle-violating" X-ray in three more plausible decay channels. Our results, for the anomalous K_α, K_β and K-edge in copper, are, respectively: $\Delta E_{K\alpha} = 7665$ eV, $\Delta E_{K\beta} = 8442$ eV,

Transition	Initial energy	Final Energy	Transition energy	Radiative transition rate (s-1)	Multipole order
core:	(1s)2(2s)2(3s)2(2p*)2(3p*)2(2p)4(3p)4(3d*)4(3d)6				
2p1/2-1s1/2	-45799	-53528	7729	2.63E+14	E1
2p3/2-1s1/2	-45780	-53528	7748	2.56E+14	E1+M2
3p1/2-1s1/2	-44998	-53528	8530	2.78E+13	E1
3p3/2-1s1/2	-44996	-53528	8532	2.68E+13	E1+M2
2p1/2-2s1/2	-44998	-45934	936	1.64E+12	E1
2p3/2-2s1/2	-44996	-45934	938	1.49E+12	E1+M2

eV.
y P.

Tab. 1 – Transition with "Pauli-violating electron" in Cu.

The results obtained through the Dirac-Fock numerical code take into account all the possible corrections (Breit operator, Lamb shift, radiative corrections,…). These values are in good agreement with our results. From the Tab.1 we can see that the K_α emission's transition energy, $(\Delta E_{K\alpha})_{DF}$, is about 7742 eV, given by its statistical ratio (2:4), due to the spin ($2p_{1/2}$: $2p_{3/2}$). In an analogous way we determine $(\Delta E_{K\beta})_{DF} \approx 8531$ eV. Both $\Delta E_{K\alpha}$ and $\Delta E_{K\beta}$ differ from our values of some tens of eV , in particular:

$$\{[(\Delta E_{K\alpha})_{DF} - \Delta E_{K\alpha}\,] / (\Delta E_{K\alpha})_{DF}\} \approx 9.95 \cdot 10^{-3} \approx 1\ \%$$

$$\{[(\Delta E_{K\beta})_{DF} - \Delta E_{K\beta}\,] / (\Delta E_{K\beta})_{DF}\} \approx 0.010 \approx 1\%$$

Also, it is interesting to note the radiative transition-rate values, as an indication of the probability of the decay: K_α emission is more probably than K_β one (they differ of one

order of magnitude). This induce us to put our attention on K_α emission rather than K_β one. Instead for the *K*-edge transition it is more difficult to calculate the radiative transition-rate because it is not a purely atomic process, but a solid state one, thus implying that an electron from infinity falls to 1s orbital. This makes extremely difficult the estimation of its transitions rate with the code of Ref. [5].

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