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Evaluation of the anomalous x-ray energy in VIP experiment.

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In this communication we analyze three possible decay channels of an eventual Pauli-principle-violating electron in a copper wire. The electron can reach the lowest $1s$ state either through a direct transition from Cu conduction band (K edge), or by a $2p$ ($3p$) capture, with a subsequent K_α (K_β) emission. The energy of the produced x-ray depends on the path followed by the electron.

Here we calculate the three different energy values and try to give a plausible estimate for the relative transition rates.

I. INTRODUCTION.

In our model we suppose that the non-paulian electron capture in Cu atoms occurs as an usual $1s$ decay. However, it is suppressed by the β^2 factor measuring the probability of Pauli-forbidden events, and shifted in energy towards the analogous decay of Ni atoms, due to the shielding of the extra $1s$ electron. Such a decay is in general a radiative process, whose cross-section can be expressed by the matrix element for matter-radiation interaction. In the dipole approximation we have:

$$\sigma_c = \frac{4\pi^2\alpha}{\hbar} E_{if} |\langle \Psi_f | \hat{\epsilon} \cdot \vec{r} | \Psi_i \rangle|^2 \delta(\hbar\omega - E_{if}) \tag{1}$$

where α is the fine structure constant, $E_{if} > 0$ is the energy difference between the two levels, and $\hbar\omega$ is the photon energy. The energy conservation is expressed through the delta-function, and $\langle \Psi_f |$ and $|\Psi_i\rangle$ are the final and initial states, respectively. Quadrupole and higher order radial matrix elements are suppressed, in the x-ray region, by a factor 100 and more and are henceforth neglected. In our model $\langle \Psi_f |$ represents the final-decay state, which is always the $1s$ state, while $|\Psi_i\rangle$ can represent either a $2p$ state (K_α emission), a $3p$

state (K_β emission), or, finally, the Bloch state of the conduction electron, in which case the decay originates directly at K-edge.

Here we try to evaluate the x-ray energy in all three cases. We suppose that the orbitals have no time to relax during the transition process (the so-called "sudden approximation"), which is justified, as the energy differences involved in all transitions is around $\Delta E \simeq 8000$ eV. Thus, such transitions occur in a time of the order of $\Delta t \simeq \hbar/\Delta E \simeq 10^{-19}$ s, while the typical electron dynamics involves a much bigger time-scale, of the order 10^{-15} s.

For what transition rates are concerned, a direct calculation is not possible, in the absence of any detailed information about the anomalous-electron wave-function. However, a rough estimate can be obtained for K_α- and K_β-emissions in the "normal" electron decay to a $1s$ hole in copper atoms. In this situation the transition rates are usually a factor 10 in favour of the K_α-line. More difficult is the direct comparison between K_α-emission and K-edge transition, as this latter is a characteristic of the solid state. One might argue that K_α-emission should be anyway favoured, because conduction electrons are at the Fermi energy, where the dipolar matrix element of Eq. (1) is strongly suprressed and a direct quadrupolar $3d$-$1s$ transition occurs, whose rate is usually negligeable, compared to a K_α-line. For this reason, even though in the following we consider all transitions as possible, we take the K_α-emission as the most probable channel for the Pauli-violating-electron decay.

II. RESULTS.

A. K_α-emission.

Referring to Fig. 1, we are interested in the energy difference $\Delta E \equiv E_3 - E_4$. If we consider the usual K_α transition, which is given by $\Delta E' \equiv E_2 - E_1 \simeq 8042$ eV,[1] we can write $\Delta E = \Delta E' - k$, where the term k takes into account of the extra correlations. Such a term is necessarily positive because we expect a correction towards Ni K_α-line, due to the extra electron shielding of the nucleus potential. In order to evaluate k we express E_3 in terms of E_1 and E_4 in terms of E_2 as follows:

$$E_3 = E_1 + V_{1s-Z} + V_{2p-Z} + V_{1s-e^-} + V_{2p-e^-} + V_{1s-1s} + V_{2p-2p} + 3V_{1s-2p} \tag{2}$$

$$E_4 = E_2 + V_{1s-Z} + V_{2p-Z} + V_{1s-e^-} + V_{2p-e^-} + 2V_{1s-1s} + 3V_{1s-2p} \tag{3}$$

Here $V_{nl-n'l'}$ represent the Coulomb interaction between two electrons in the shells nl and $n'l'$, respectively, while V_{nl-Z} takes into account of the Coulomb attraction with the Z protons of Cu nucleus and V_{nl-e^-} counts the interactions with all electrons other than $1s$ and $2p$, as represented in red in Fig. 1. Notice that the two expressions (2) and (3) are not strictly correct, because orbitals are not frozen, and even neglecting the extra $1s$ and $2p$ electrons, the remaining electrons in the configuration E_3 are not exactly comparable to those of configuration E_1, because of the relaxation due to the extra shielding (and similarly for E_4 and E_2). However, as E_4 and E_3 are subtracted, and as both terms are characterized by this extra shielding, we can suppose that the neglected relaxation effects, being of the same order of magnitude, cancel out, so that what is left is the correct x-ray energy. Thus, we get:

$$\Delta E = \Delta E' - (V_{1s-1s} - V_{2p-2p}) \simeq 7665\ eV \tag{4}$$

where we used the values $V_{1s-1s} \simeq 483$ eV and $V_{2p-2p} \simeq 110$ eV for the direct Coulomb integrals. These latters, in their Slater F^{2n} form, are taken from the "Atomic Structure Calculations" of Ref. [2]. The connection between F^{2n} and $V_{nl-n'l'}$ can be found, e.g., in Ref. [3], and reads: $V_{1s-1s} = F^0$ and $V_{2p-2p} = F^0 - \frac{2}{25}F^2$.

B. K_β-emission.

We can follow exactly the same path as in the previous subsection, with the only difference that the "normal" energy for K_β emission is $E_{K_\beta} \simeq 8905$ eV, and that instead of V_{2p-2p}, one has to use $V_{3p-3p} \simeq 20$ eV. Thus in this case the corrected energy is:

$$\Delta E = \Delta E' - (V_{1s-1s} - V_{3p-3p}) \simeq 8442\ eV \tag{5}$$

C. K-edge decay.

Referring to Fig. 2, we can perform the same calculation as before, with the warning that now we are dealing with Cu atoms, instead of Cu^{1+} ions, when comparing with the "normal" case. Due to this and to the fact that the decaying electron comes from an outer valence shell and not from a core one, we expect a better result within our scheme of frozen orbitals.

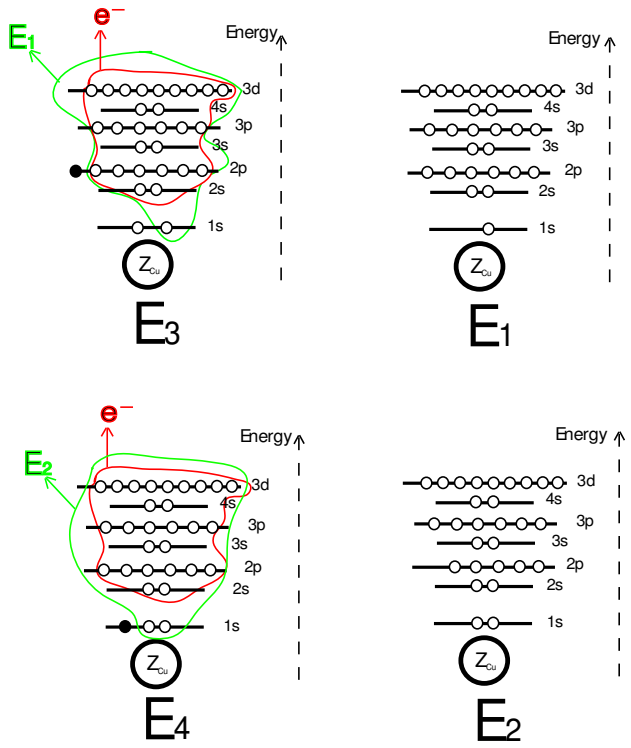

FIG. 1: Energy levels for K_α-emission. The ensemble of "spectator" electrons $(2s^2), (2p^5), (3s^2), (3p^6), (3d^{10}), (4s^1)$ are called e^-. The subset of E_4 and E_3 corresponding, respectively, to E_2 and E_1 is also indicated.

Again, we are interested in the energy difference $\Delta\tilde{E} \equiv \tilde{E}_3 - \tilde{E}_4$, while the usual K-edge transition is given by $\Delta\tilde{E}' \equiv \tilde{E}_2 - \tilde{E}_1 \simeq 8979$ eV. If we write, like before, $\Delta\tilde{E} = \Delta\tilde{E}' - \tilde{k}$, where the term $\tilde{k}$ takes into account of the extra correlations, and suppose again that the state of all electrons labelled by e^- (in red in Fig. 2) is not much affected by the presence of an extra $1s$ electron, we can express $\tilde{E}_3$ in terms of $\tilde{E}_1$ and $\tilde{E}_4$ in terms of $\tilde{E}_2$ as follows:

$$\tilde{E}_3 = \tilde{E}_1 + V_{1s-Z} + V_{1s-e^-} + V_{1s-1s} + V_{1s-3d} \tag{6}$$

$$\tilde{E}_4 = \tilde{E}_2 + V_{1s-Z} + V_{1s-e^-} + 2V_{1s-1s} \tag{7}$$

Thus, with the same idea of the previous two subsections, we get:

$$\Delta E = \Delta E' - (V_{1s-1s} - V_{1s-3d}) \simeq 8534\ eV \tag{8}$$

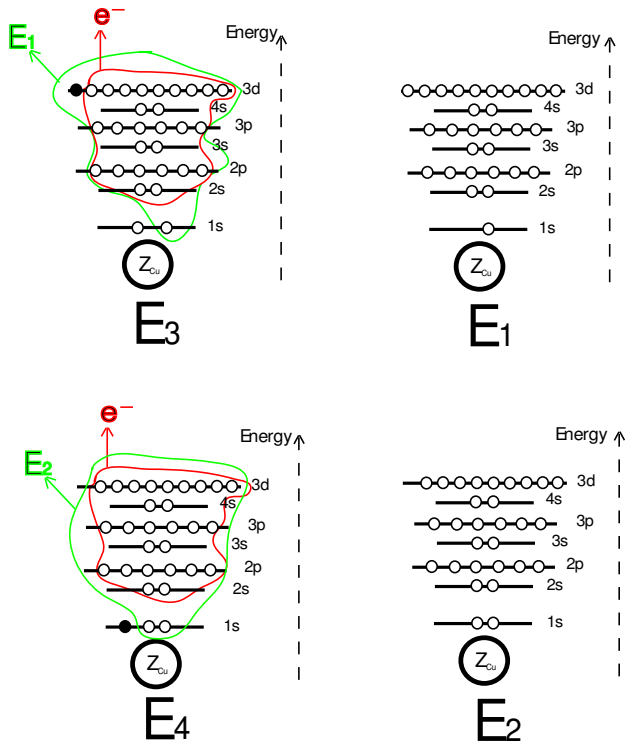

FIG. 2: Energy levels for K-edge transition. The ensemble of "spectator" electrons $(2s^2), (2p^6), (3s^2), (3p^6), (4s^2), (3d^{10}), (4s^2)$ are called e^-. The subset of E_4 and E_3 corresponding, respectively, to E_2 and E_1 is also indicated.

Again, we used the values $V_{1s-1s} \simeq 483$ eV and $V_{2p-2p} \simeq 38$ eV for the direct Coulomb integrals, as taken from Ref. [2]. The connection with F^{2n} in the case of V_{1s-3d} is taken from Ref. [3], without exchange term, as appropriate for a Pauli-principle-violating electron: $V_{1s-3d} = F^0$.

III. CONCLUSIONS.

In this Note we have calculated the energy of an emitted "Pauli-principle-violating" x-ray in the three more plausible decay channels. Our results, for the anomalous K_α, K_β and K-edge, are, respectively: $\Delta E_{K_\alpha} = 7665$ eV; $\Delta E_{K_\beta} = 8442$ eV; $\Delta E_{K-edge} = 8534$ eV. The approximations introduced here do not allow to get an uncertainty less than some tens of eV, and for this reason this calculation should be considered just as a first step. However, we believe that the importance of the present approach lies in its handiness, that allows a simple comprehension of the related physical ideas, even though to the detritement of the precision.

In the next future we shall perform a more precise, *ab-initio* evaluation of the x-ray energies by means of a Dirac-Fock numerical code[4], which should improve the uncertainty of a factor of about ten (from several tens of eV to several eV).

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[1] Here we just performed a weighted average of the two values for K_{α_1} and K_{α_2} ($E_{K_{\alpha_1}} \simeq 8048$ eV and $E_{K_{\alpha_2}} \simeq 8028$ eV), neglecting spin-orbit splitting, with the usual statistical weight 2:1=K_{α_1}:K_{α_2}.

[2] Joseph B. Mann, Los Alamos Scientific Laboratory report LA-3690, UC-34 Physics, TID 4500 "Hartree-Fock energy results for the elements Hydrogen to Lawrencium"

[3] R.D. Cowan, "The theory of atomic structure and spectra", pag. 165, University of California Press, 1981

[4] The adopted code is described in: J.V. Mallow, J.P. Desclaux, A.J. Freeman, Phys. Rev. A **17**, 1804 (1978)