EVALUATION OF THE ANOMALOUS X-RAY ENERGY IN VIP EXPERIMENT

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Abstract

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 $K_{\alpha}$ ($K_{\beta}$) 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 $\beta^2$ 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:

$$
\sigma_c = \frac{4\pi^2\alpha}{\hbar} E_{if} \left| \langle \Psi_f | \mathbf{\hat{r}} | \Psi_i \rangle \right|^2 \delta\left(\hbar \omega - E_{if}\right)
$$

(1)

where $\alpha$ 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 $\left| \langle \Psi_f \right| \text{ and } \left| \Psi_i \right\rangle$ 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 $\langle \Psi_f \rangle$ represents the final-decay state, which is always the $1s$ state, while $\left| \Psi_i \right\rangle$ can represent either a $2p$ state ($K_{\alpha}$ emission), a $3p$ state ($K_{\beta}$ 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 $\Delta E \approx 8000$ eV. Thus, such transitions occur in a time of the order of $\Delta t \approx \hbar/\Delta E \approx 10^{-19}$ 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 $K_{\alpha}$- and $K_{\beta}$-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 $K_{\alpha}$ -line. More difficult is the direct comparison between $K_{\alpha}$ -emission and K-edge transition, as this latter is a characteristic of the solid state. One might argue that $K_{\alpha}$ -emission should be
anyway favoured, because conduction electrons are at the Fermi energy, where the dipolar matrix element of Eq. (1) is strongly suppressed and a direct quadrupolar $3d$-$1s$ transition occurs, whose rate is usually negligible, compared to a $K_\alpha$-line. For this reason, even though in the following we consider all transitions as possible, we take the $K_\alpha$-emission as the most probable channel for the Pauli-violating-electron decay.

II. RESULTS.

A. $K_\alpha$-emission.

Referring to Fig. 1, we are interested in the energy difference $\Delta E = E_3 - E_4$. If we consider the usual $K_\alpha$ transition, which is given by $\Delta E' = E_2 - E_1 \cong 8042$ 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 $K_\alpha$-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:

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

(2)

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

(3)

Here $V_{nl}$ 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:

\[
\Delta E = \Delta E' - (V_{1s-1s} - V_{2p-2p}) \approx 7665 \text{ eV}
\]

(4)

where we used the values \( V_{1s-1s} \approx 483 \text{ eV} \) and \( V_{2p-2p} \approx 110 \text{ eV} \) 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. \( K_\beta \)-emission.

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

\[
\Delta E = \Delta E' - (V_{1s-1s} - V_{3p-3p}) \approx 8442 \text{ eV}
\]

(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 \( \text{Cu}^{1+} \) 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 $K_{\alpha}$-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 $\Delta E \equiv E_3 - E_4$, while the usual $K$-edge transition is given by $\Delta E' \equiv E_2 - E_1 \approx 8979$ eV. If we write, like before, $\Delta E \equiv E' - \bar{k}$, where the term $\bar{k}$ 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 $E_3$ in terms of $E_1$ and $E_4$ in terms of $E_2$ as follows:

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

(6)

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

(7)

Thus, with the same idea of the previous two subsections, we get:
\[ \Delta E = \Delta E' - (V_{1s-1s} - V_{1s-3d}) \approx 8534 \text{ eV} \]

(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 \(V_{1s-1s} \approx 483\) eV and \(V_{2p-2p} \approx 38\) 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 \(K_\alpha, K_\beta\) and K-edge,
are, respectively: $\Delta E_{K\alpha} = 7665$ eV; $\Delta E_{K\beta} = 8442$ eV; $\Delta E_{K\text{-edge}} = 8534$ 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 detriment of the precision.

In the next future we shall perform a more precise, \textit{ab-initio} evaluation of the x-ray energies by means of a Dirac-Fock numerical code\textsuperscript{(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 $K_{\alpha 1}$ and $K_{\alpha 2}$ ($E_{K\alpha 1} \cong 8048$ eV and $E_{K\alpha 2} \cong 8028$ eV), neglecting spin-orbit splitting, with the usual statistical weight 2:1=$K_{\alpha 1}:K_{\alpha 2}$.

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(3) R.D. Cowan, "The theory of atomic structure and spectra", pag. 165, University of California

(4) The adopted code is described in: J.V. Mallow, J.P. Desclaux, A.J. Freeman, Phys. Rev. A
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