CONFINEMENT INDUCED ELECTRON CAPTURE

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1. Abstract

We describe a Gedandkenexperiment in which a bare proton can capture an electron due solely to confinement. We first briefly review the aspects around bare electron proton capture. We then provide a numerical solution of the Fermi VA-Theory for K-electron capture for an electron-proton pair confined in a classical box of size L. Interestingly, we find that the capture is most likely for L=0.004-0.009 Angstroms, well beyond the radius of the proton.

2. Background

We briefly review orbital electron capture and some considerations, like environmental effects on the rate, that motivate this study.

2.1. **Orbital Electron Capture.** In 1935, Yukawa proposed that a proton, bound in an atomic nucleus, could capture a low lying, bound atomic electron, transforming into a neutron, and releasing an electron neutrino [1,10]

$$p^{+} + \ e^{-} \rightarrow \ n^{0} \ + \ \bar{\nu}^{e}$$

K-electron capture usually occurs in unstable radioisotopes which lack the (nuclear binding) energy to decay by positron emission (standard Beta decay).

We can not observe electron capture directly, so we rely upon conservation of energy and momentum. We observe orbital electron capture by it's relaxation processes. It is usualy a K-shell electron, but maybe L or higher. The nucleus may absorb some energy, becoming excited. It then undergoes internal conversion. During this, a higher lying, bound atomic electron is aborbed, and an X-ray, or Auger electron released [see Figure 1].

Because electron capture occurs in (proton-rich) nuclei, and, subsequently, releases a X-Ray photon, the reaction is also sometimes written as

$$^{Z}X_{A} + \ e^{-} \rightarrow \ ^{Z+1}X_{A-1} \ + \ h\nu_{X-ray}$$

(where Z is the number of protons, A the number of neutons, and $h\nu$ is an X-ray photon)

Indeed, orbital electron capture is evidenced by high intensity x-rays and soft electrons. In 1938, Luis W. Alvarez observed the x-ray signature of orbital electron capture in ^{48}V (in activated Titanium). Since then, electron capture has been observed in about 150 radioactive isotopes.

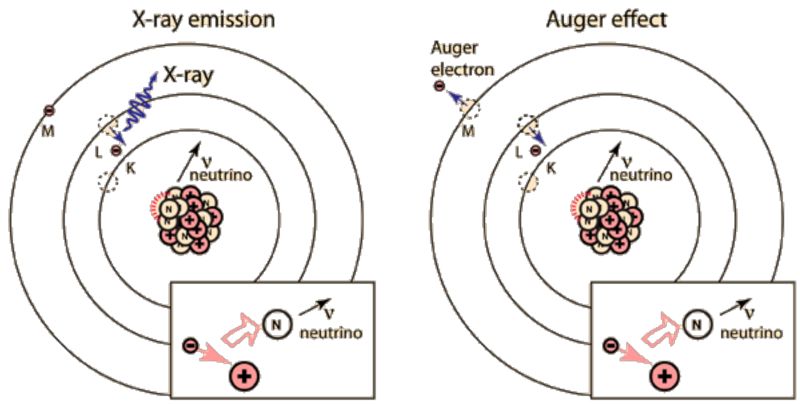

FIGURE 1. oribital electon capture relaxation processes

2.1.1. *Radiative Electron Capture.* In very rare cases, a gamma ray photon is emitted with the neutrino; this is called Radiative Electron Capture (REC) [10]. This can be thought of as a kind of Internal Bremsstrahlung radiation, caused by the electron accelerating toward the nucleus during capture. Recent, detailed rate calculatons have elucidated the details [11].

2.1.2. *Effect of Chemical Environment of Electron Capture rate.* The lightest element that K-electron capture has been observed in is ^{7}Be [3]. In fact, there is so little energy that the competing positron emission process is not possible (described below), and the half-life for electron capture is $\tau_{EC} \sim 50\, days$.

Being so light, and having such a large rate, electron capture in ^{7}Be can be slighlty modified by both changing the chemical environment and/or the external pressure [4-6]. In particular, in 2004, Ohtsuki et al demonstrated a change of 0.83How could such changes occur ?

The electronic energy levels are in the eV range, so intense EM fields can alter the electronic structure and therefore slighly affect the rate. In contrast, the nuclear energy levels are in the keV to MeV region, and it is generally thought to be very difficult to impossible to effect.

Of particular practical interest is using very large electric fields for accelerating Beta decay for disposing of nuclear waste [?].

Generally speaking, rates of nuclear processes can be enhanced by providing additional avenues for energy release, thereby increasing the entropy of the total reaction. For example, in bound state β^{-} decay, the rate of decay is greatly enhanced in heavy, bare ions. ^{187}Re decays with half life of $\tau_{\beta^-} \sim 42 \times 10^9$ years, but fully ionized $^{187}Re^{+}_{75}$ undergoes bound state β decay, with a half-life of only $\tau_{\beta^-} \sim$ 32.9 years. [7]

2.2. **The Weak Interaction and V-A theory.** Orbital electron capture is mediated by the Weak interaction. The simplest theory for the Weak Interaction is the Fermi V-A (Vector Axial) theory [8]. The V-A theory is a simple phenomenological approach, although it is now understood in terms of ElectroWeak Unification and can be derived from the Standard Model [9]. But we don't need all this machinary to do calculations.

One can use V-A theory to compute cross sections for scattering experiments and decay rates and electron capture for various atoms in chemical different environments. To properly desrcibe any reaction, however, we need to understand what reactions we can apply the theory to, and the other reactions that might also occur.

2.2.1. *Electron Capture and other (weak) processes.* The Weak interaction describes a variety of processes including:

- orbital (K) electron capture $p^+ + e^- \rightarrow n^0 + \nu_e$,
- positon emission, or β^+ decay $p^+ \rightarrow \ n^0 + \ e^+ \ + \ \nu_e$,
- the related (electron) β decay ; $n^0 \rightarrow p^+ + \ e^- \ + \ \bar{\nu_e}$

A neutron-rich nucleus may undergo electron capture, positron emission, and/or β decay, becoming more stable as a result.

2.2.2. *neutron decay.* Furthermore, there is the competing, reverse reaction, where a neutron interactions with a neutrino:

- reverse electon capture $n^0 + \nu_e \rightarrow p^+ + e^-$.

By detailed balance, it has the same rate as orbital electron capture by a free proton, but is more favorable energetically. This is similar to

- free neutron decay $n^0 \rightarrow p^+ + e^- + \bar{\nu_e}$,

Inside the nucleus, the neutron is stable. But, free neutron decay has mean lifetime of $\tau = 881.51.5$ *sec*, or about 15 minutes. This is the for nuclei with high atomic number, which usually have more neutrons than protons.

In contrast, orbital electron capture by a free proton is unheardof outside of a stellar environments, so in order for orbital capture to occur by a free proton, some external energy is necessary, and the free neutron decay must be suppressed or kinetically unfavorable. inverse beta decay

2.2.3. *inverse beta decay.* Note that K-electron capture is also sometimes called inverse β decay, but we this to be the scatterinf of a proton and an electron anti-neutrino

$$p^+ + \bar{\nu_e} \rightarrow n^0 + e^+ \quad ,$$

and is characterized by emission of a positron.

2.2.4. *positron emission.* In particular, any high energy relativisitc process, we have to worry about positron creation. We noted above, however, that in ^7Be, the competing positron decay reaction can not occue because there is not enough energy.

Generally, this occurs at length scales below the Compton length of the electron, which, is smaller than we will need to consider.

2.2.5. *internal Bremsstrahlung.* Electron capture and Beta decay events may also emit Bremsstrahlung (or so-called *braking*) radiation, in the form of soft gamma rays. this is 1000X less likely, but does occur. In electron capture, the electron emits this as it *accelerates* toward the nucleus, taking energy away from outbound neutrino. The resulting gamma rays are called soft because they do not exhibit sharp spectral lines.

2.2.6. *Rate calculations.* The rate of EC can be computed using the Fermi VA-Theory [8,10]. The most basic calculations require a only specifying the electronic wavefunctions(s), and integrating over the outbound neutrino momentum.

Note that the V-A theory assumes an incoherent nuclear process, it is local, and that the interaction is phenomonological. It is treated as a simply a contact potential at the surface of the nucleus. This means one only needs compute the nuclear charge–the electron density on the surface of the nucleus.

More complicated calculations are used for larger nuclei, second order processes, etc. They only require modifications to treat either atomic electronic structure of reactant and product atoms, and/or specific considerations for nuclear internal conversion and other second order processes.

2.3. **Bare proton-electron capture.** We frequently write K-electron capture as if it were simply proton-electron capture

$$p^+ + e^- \rightleftarrows n^0 + \nu_e \ \ .$$

Theoretically, a free proton can could capture an electron from the continuum, but the interaction energy must be above threshold for neutron production. This is a huge amount of energy, although this happens regularly in accelerators.

Observing proton electron capture outside of an accelerator, "on the desktop", so to speak, would be an incredibly hard experiment because both final particles are neutral, and the neutrino is extremely weakly interacting.

2.3.1. *Stellar Nucleosynthesis.* Bare proton-electron Capture is thought to occur in stars. It is thought to drive the formation of primordial elements, and to occur in the forming of neutron stars [?].

For example, Bachall and coworkers have studied the electron capture rate in stellar media, and have computed the rate of EC of 7Be in the Sun [13].

It is believed that a Hydrogen undergoes EC is the core collapse supernovae and in neutron stars [14]; in fact, it is thought to create stellar instability. While we usually characterize a star by it's temperature, these are also very dense systems, with $\rho \sim 10^6\ g\ cm^{-3}$. In contrast, the smallest star has density $\rho \sim 10^2 - 10^3\ g\ cm^{-3}$ [?]

The reverse reaction is also suppressed because, inside the neutron star, it is impossible to create a new electron; the Fermi sea is 'full'.

Generally speaking, at zero energy, proton EC is not possible because it violates energy-momentum conservation. At very high Temperatures, however, the proton electron collisions have sufficient energy to overcome the reaction barrier, and one needs a large supply of high energy electrons to suppress the reverse reaction).

So electron capture can occur by bare protons, but, presumably, only under extreme confinement.

3. Confinement Induced Electron Capture

We pose the following Gedankenexperiment:

Suppose we confine an electron and a bare proton as a particle-in-a-box of volume L^3. What box size L will 'induce' electron confinement ?

We write this as

$$E_{box} + p^{+} + e^{-} \rightarrow n^{0} + \nu_e$$

where E_{box} is the *confinement energy*, which is induced by the box constraints.

3.0.1. *neutron-post reaction.* To prevent the reverse reaction, we assume that the free neutron subsequently combines with another proton, and gives us 2.2 GeV of energy in the process. This post-process contributes to the power output

3.1. **a Classical box and the Compton length.**

The first obvious question is, should we use a classical or a relativisitic box?

Most electron capture rate calculations use classical wavefunctions [10, 12].

We can safely use a classical box as long as $L_{min} \geq \frac{1}{2\pi}\lambda_e$, where λ_e is Compton wavelength of an electron [16-19]. The Compton wavelength sets the scale, accounting for both quantum mechanics and special relativity. [15]

$$\lambda_e = \frac{h}{m_e c} = \frac{e^2}{m_e c^2}$$

$$\lambda_e \approx 2.426 \times 10^{-12}\ m$$

For an electron, the minimum L is on the order of 0.004 Angstrom

$$L_{min} \sim 0.004\ \mathring{A}$$

Furthermore, in any high energy, relativisitic system, one has to worry about positron production, here β^{+}-decay. This generally occurs below the Compton length. We are seeking the maximum box size which can induce EC, and we assume that, at the max, positron emission will be very rare.

Finally, we assume that the electron wavefunction does not change appreciably during the interaction, so that we may use a very simplified form for the cross section (σ) and rate (Γ). Again, this is reasonable for boxes $L \geq \lambda_e$.

So we use a classical box, with minimum size $L_{min} = 0.004\ \mathring{A}$; we compute the maximum size below.

3.2. **Theory.**

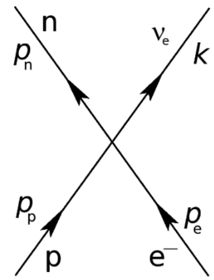

FIGURE 2. article production

3.2.1. *Particle production under the Weak interaction.* Electron capture is mediated by the Weak Interaction, through the particle production process, given by the 4-point Interaction (see Figure **??**)

$$p^+ + e^- \rightarrow\ n^0\ +\ \nu_e$$

which requires 0.511 MeV more energy–which is *provided* by the box. We do not consider the β^+-decay process here either.

3.2.2. *Hamiltonian.* The Hamiltonian for the V-A theory is [?]

$$\mathcal{H}(x) = -\frac{G_F}{\sqrt{2}}\left[J^\mu(x)L^+_\mu(x) + h.c.\right]$$

where J_μ and L_μ are the Hadron and Lepton currents, resp, and are given by

$$J_\mu = \bar{u}_n\gamma_\mu(1+\lambda\gamma_5)u_p$$

$$L_\mu = \bar{u}_\mu(1+\gamma_5)u_e$$

where u_n, u_p, u_e, u_ν are Dirac Spinors.

G_F is the Universal Fermi Weak Coupling Constant, and $\lambda = -\dfrac{G_A}{G_V}$, which is determined by experiment (and subject to minor changes). G_V is the Axial-Vector Weak Coupling Constant, and G_A is the vector weak coupling constant. The most recent value is $G_V =$ $?1.27590^{+0.00409}_{?0.00445}$, and $G_A = 1$ ”under the conserved vector current (CVC) hypothesis of the Standard Model” [22].

3.2.3. *Transition Rates and Power Calculations.* We want to compute the power generated by confined electron capture, as a funciton of the box size (L) We need the rate of electon capture, Γ_{EC}. And we need to assume the reverse reaciton is suppressed. The rate is given by Fermi's Golden Rule (discussed in the Appendix)

$$\Gamma_{EC} = \Gamma_{fi} = 2\pi|\mathcal{M}_{fi}|^2\rho(E_f)$$

where the matrix element $\mathcal{M}_{fi}$and the density of states $\rho(E_f)$ must be Lorentz Invariant (L.I.)

The matrix elements are

$$\mathcal{M}_{fi} = \langle \Psi_{final} | \mathcal{H} | \Psi_{final} \rangle$$

3.2.4. *VA Matrix Elements.* We use a slghtly different convention for the matrix elements, multiplying by G_V, giving

The matrix elements $\mathcal{M}_{fi}$ are

$$\mathcal{M}_{fi} = \frac{G_F}{\sqrt{2}} \bar{u}(p_n, s_n)(G_V - G_A \gamma^5)\gamma^\mu u(p_p, s_p) \times \bar{u}(k, s_k)\gamma_u (1 - \gamma^5) u(s_e, p_e)$$

We use Dirac 4-Spinors

$$\bar{u}(p_n, s_n), u(p_p, s_p), \bar{u}(k, s_k), u(s_e, p_e)$$

where

$$s_n, s_p, s_e, s_k$$

are 2-component spin vectors for the neutron, proton, electron, and electron neutrino, resp.

The Dirac spinors assume the standard energy normalization $\frac{1}{\sqrt{2E}}$.

The γ are 4-component Gamma matrices, and $(\cdots \gamma^\mu \cdots \gamma_u \cdots)$ is the Einstein summation convention.

3.2.5. *Cross Section.* The cross section for the process

$$E_{box} + p^+ + e^- \to n^0 + \nu_e$$

is given by

$$d\sigma_{ep} = \left(\frac{1}{2\pi}\right)^2 \frac{\sum_{fi} \left|\mathcal{M}_{fi}\right|^2}{16 \left|\mathbf{k} \cdot (E_n \mathbf{k} - k^0 \mathbf{p}_n)\right|} \frac{k^3 p_e d\Omega_k}{\left|\mathbf{p}_e \cdot (E_p \mathbf{p}_e - E_e \mathbf{p}_e)\right|}$$

Notice that when applying the VA theory this way, we assume that the electron-proton interaction is a contact potential, operating at the surface of the nucleus, and that the underlying quantum process is incoherent.

3.2.6. *Particle-in-the-box Wavefunctions.* We treat the electron, proton pair as classical particle-in-a-box.

$$\psi_{ep}(\mathbf{x}) = \left(\frac{2}{L}\right)^{\frac{3}{2}} cos\left(\frac{\pi x}{L}\right) cos\left(\frac{\pi y}{L}\right) cos\left(\frac{\pi z}{L}\right)$$

expressions for momentum

Because the VA theory assumes an incoherent process, the electron, proton wavefunction is usually factored as an electron wavefunction, with a point-particle in the center

$$\psi_{ep}(\mathbf{x}) = \psi_p(0)\psi_e(\mathbf{x})$$

We only consider the ground state ψ^0_{ep} wavefunction.

We note, in *ab initio* electronic structure calculations, it is now generally possible to treat the Hydrogen prton wavefunction explicitly, and to treat the electron-proton coupling at the level of Hartree Fock (i.e. variational mean field) [12] This has proved useful for describing isotope effects on electronic structure

Here, we treat the confined electron, proton pair in the c.m. frame so that the 3-momentum of the electron and proton related

$$\mathbf{p}_e = \mathbf{p}_{pe}$$

$$\mathbf{p}_p = -\mathbf{p}_{pe}$$

3.2.7. *comment on our approach.* We note that Blatt and Weisskopf [20] describe the fermi VA theory in the non-relativisitic limit. Here, they use classical plane wave solutions ($e^{i\mathbf{px}}$), with just box normalization ($\frac{1}{L^3}$). In contrast, we use the full classical particle-in-the-box wavefunctions, and analyze the problem just above the Compton scale using the low order VA theory.

3.2.8. *Relativistic Kinematics and Energetics.* For consistency with the particle production process,

$$p + e \rightarrow n + \nu_e$$

we treat all kinematics and energetics relativisitcally, such that the 4-vectors satisify

$$\overrightarrow{P}_n + \overrightarrow{P}_e = \overrightarrow{P}_n + \overrightarrow{P}_{\nu_e}$$

$$E^2 = M^2 + p^2$$

This gives

$$E_e^2 = m_e^2 + 3\left(\frac{\pi}{L}\right)^2$$

$$E_p^2 = M_p^2 + 3\left(\frac{\pi}{L}\right)^2$$

The threshold Kinetic energy in the center of momentum (c.m.) frame is given as

$$EKe_{min}: \quad K_e = E_e - m_e = \frac{(M_n - m_e + m_\nu)^2 - M_p^2}{2(M_n + m_\nu)}$$

Giving the minimum momentum as

$$pmin: \quad \mathbf{p}_{min} = \sqrt{(K_e + m_e)^2 - m_e^2}$$

Of course, the proton rest frame is approximately the electron rest frame, but it should be mentioned that the in the electron rest frame, the threshold kinetic energy is 2000X greater. Therefore, it is assumed that the energy transfer to induce electron capture is in the c.m. frame of the (e,p) pair.

The total energy in the c.m. frame is

$$E_{tot} = E_n - E_e$$

For the final state, the neutrino kinetic energy is

$$K_\nu = k^0 - m_\nu = \frac{(E_p + E_e - m_\nu)^2 - M_n^2}{2(E_p + E_e)}$$

and the neutron kinetic energy is

$$K_n = E_n - M_n = \frac{(E_p + E_e - M_n)^2 - m_\nu^2}{2(E_p + E_e)}$$