Confinement Induced Electron Capture

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We describe a Gedankenexperiment in which a bare proton can capture an electron due solely to confinement. We first briefly review K orbital electron capture and related processes. We then describe the Fermi VA-Theory and how it can be applied to compute the cross section and rate for electron capture by a bare proton. We set the problem up as a (proton, electron) pair confined in classical box of size L, and compute the cross section using the full Weak Interaction Hamiltonian and relativisitic Kinematics. We provide numerical solutions for electron capture rate, and compare the power output relative to that of a neutron being captured in the port-reaction. We find that the capture is most likely for L=0.004-0.009 Angstroms, well beyond the radius of the proton and the Compton wavelength of the electron. We also examine the implications for theoretical minimal power output for such a process. Finally, we discuss some interesting applications and proposals for future work.

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I. BACKGROUND

As a student, we learn that the nucleus can not contain an electron; this is a simple application of the Heisenberg Uncertainty Principle[?] . If an electron were confined to volume of nuclear radius, it would have a (relativisitic) kinetic energy of order 10 MeV. But this is not observed experimentally. In Beta decay, a nucleus emits an electron with energy of order 1 MeV.

$$beta\ decay:\ n^0 \rightarrow p^+ +\ e^-\ +\ \bar{\nu_e}$$

We can describe beta decay using the Fermi VA theory for the Weak Interaction, which assumes a phenomenological contact force *with no range*.

A related Weak process is orbital electron capture, where a nucleus captures a bound, low lying electron, and emits a neutron and an electron anti-neutrino.

$$electron\ capture:\ p^+ +\ e^- \rightarrow\ n^0\ +\ \nu^e$$

Orbital electron capture is a fundamental nuclear process, on pair with the more familiar beta decay and positron production. It is, however, usually treated as an afterthought to beta decay, and there are no modern reviews of how to treat the the problem numerically. Indeed, the most complete reference dat back to the 1960s and 70s[1,2]. Still, electron capture displays its own unique, rich structure and subtlety. For example, the rate is effected chemical environment by nearly 1%. This is because the rate depends on the electronic density on the surface of the nucleus (i.e. $|\Psi_e(r \rightarrow 0)|^2$) since the interaction has no range.

But if we apply the Heisenberg Uncertainty Principle for electron capture, we would find the electron can still be captured even if it confined to a volume $100X$ the nuclear radius.

It can also emit Bremsstrahlung radiation. In fact, this is actually discussed in Jackson with a classical model[3]– although it is more properly treated using QED corrections to the Weak interaction[4]. In fact, technically, electron capture is a 2-body, relativistic bound state problem, although we model it by computing the non-relativistic atomic electronic wavefunctions of the parent and daughter nuclei, and then use them to evaluate the matrix elements of the Weak Interaction Hamiltonian using the Fermi-VA theory. And very rarely do we do a complete treatment of the Kinematics.

We are interested in the reviewing the basic electron capture process to understand how to apply the Fermi-VA theory to compute the cross section and capture rate as completely as possible. We will examine electron capture in its simplest form: a bare proton capturing an electron while confined in a classical box. We don't believe this has been discussed elsewhere and would serve as a great instructional example for students.

We begin by briefly reviewing both orbital electron capture and the Fermi VA Theory.

A. 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.

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

This may be called orbital electron capture, K-electron capture, or just electron capture (E.C.)

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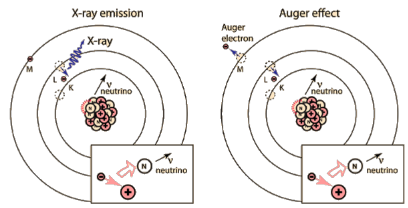

FIG. 1. orbital electron capture relaxation processes

Electron capture usually occurs in unstable radioisotopes which lack the nuclear binding energy Q to decay by the more familiar Beta decay processes (β^-, β^+). The typical Q energies necessary are

$$Q_{\beta+} \sim 2 - 4MeV$$

$$Q_{\beta-} \sim 0.5 - 2(MeV)$$

$$Q_{E.C.} \sim 0.2 - 2.0MeV$$

When $Q < 1.02MeV$, which is twice the rest mass of an electron $(2m_ec^2)$, a proton rich nucleus must decay by electron capture.

In particular, heavy elements may decay by E.C. and/or β^+ (positron emission) to a lower 'magic number' of stable nuclei, and by β^- decay to achieve a higher magic number. E.C. is favored for high Z nuclei, but because of the energetic constraint, very light elements, such as ^7Be, decay by primarily by E.C. Lacking any binding energy and/or internal nucleon structure, bare proton electron capture is not observed, and requires extreme, exotic conditions.

1. Experimental Evidence

We observe electron capture by observing the resulting transmuted nuclei and/or the radiative relaxation processes. The captured electron is bound to the atom, and it is usually a K-shell electron, but may be L or higher. The nucleus may then absorb some energy, becoming excited, and then undergo internal conversion. During this, another higher lying, bound atomic electron is absorbed, and either 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

$$^ZX_A + e^- \rightarrow \; ^{Z-1}X_A \; + \; h\nu_{X-ray}$$

(where Z is the total number of protons and neutrons, A the number protons, and $h\nu_{X-ray}$ 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 activated Titanium[5]. Since then, electron capture has been observed in about 150 radioactive isotopes.

2. Environment Effects on Electron Capture rates

The lightest element that E.C. has been observed in is ^7Be[6]. In fact, there is so little energy that the competing β^+ positron emission process (described below) is prohibited, leading to a fairly long E.C. half-life of $\tau_{EC} \sim 50\ days$.

Being so light, and having such a large rate, electron capture in ^7Be can be slightly modified by both changing the chemical environment and/or the external pressure[7–9]. In particular, in 2004, Ohtsuki et. al. demonstrated a change of 0.83% by embedding Be in C-60 cages[9].

How could such changes occur? The nuclear energy levels are in the keV to MeV region, and it is generally thought to be very difficult to impossible to effect. But the electron capture rate is proportional to electronic density at the surface of the nucleus–*the nuclear charge*. The electronic energy levels are in the eV range, so intense EM fields can alter the electronic structure and therefore slightly affect the E.C. rate.

3. Bare proton-electron capture

We frequently write electron capture as if it were simply proton-electron capture. But at zero energy, bare proton electron capture is not possible because it violates energy-momentum conservation. 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, and, presumably, in stellar environments.

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. Still, we have good reason to beleive it occurs.

4. Stellar Nucleosynthesis

Bare proton-electron capture is thought to occur in the early stages of the big bang and in stellar nucleosynthesis. It is thought to drive the formation of primordial elements, and to occur in the forming of neutron stars.

At very high temperatures, the proton electron collisions have sufficient energy to overcome the reaction barrier. For example, Bachall and coworkers have studied the electron capture rate in stellar media, and have computed the electron capture rate of ^7Be in the Sun[10,11]. And it is believed that ionized Hydrogen captures an electron during 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 $\rho \sim 10^2 - 10^3\ g\ cm^{-3}$ [?] As important, the reverse reaction is prohibited because, inside the dense neutron star, it is impossible to create a new electron; the Fermi sea is *full*.

So electron capture can occur by bare protons, but, presumably, only under extreme confinement (and with the reverse reaction is suppressed).

B. The Weak Interaction and V-A theory

Electron capture is mediated by the Weak interaction, described most concisely by the Fermi V-A (Vector Axial) theory[1,2,12]. The V-A theory is a simple phenomenological approach, readily amenable to numerical calculations. While It is now understood in terms of ElectroWeak Unification and can be derived from the Standard Model, the original paper by Fermi, for which he won the 1938 Nobel Prize in Physics, was initially rejected by *Nature* because "It contained speculations too remote from reality to be of interest to the reader"[13].

V-A theory is used to compute cross sections for scattering experiments and decay rates for electron capture for various atoms, even in different environments, chemical and otherwise. We can use machinery of the V-A theory to explore E.C. in a simple, idealized environment. To properly describe any reaction, however, we need to understand what reactions we can apply the theory to, and the other, potential competing reactions.

1. Electron Capture and other Weak processes

The Weak interaction describes several related processes within a single framework. *Neutron-rich* nuclei may become more stable as a result by undergoing one or more of the following:

- orbital electron capture $\quad p^+ + e^- \rightarrow n^0 + \nu_e$
- positon emission (β^+ decay) $\quad p^+ \rightarrow\ n^0 +\ e^+\ +\ \nu_e$
- β decay $\quad n^0 \rightarrow p^+ +\ e^-\ +\ \bar{\nu_e}$

There are also several related reactions, including

- reverse electron capture $\quad n^0 + \nu_e \rightarrow p^+ + e^-$
- free neutron decay $\quad n^0 \rightarrow p^+ + e^- + \bar{\nu_e}$
- inverse beta decay $\quad p^+ + \bar{\nu_e} \rightarrow n^0 + e^+$

Let us briefly review these.

2. Beta decay

Beta decay is the most familiar Weak process, and is discussed in great detail in a number articles and books. In contrast, electron capture, which is significantly more difficult to describe in detail, is a rare topic. Indeed, the most recent review is from 1976[1].

3. Positron emission

In any high energy relativisitic process, we have to worry about positron emission. We noted above, however, that in ^7Be, the competing positron decay reaction can not occur 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.

4. Neutron Decay

By detailed balance, reverse electron capture has the same rate as orbital electron capture–but is more favorable energetically. Indeed, inside the nucleus, the neutron is relatively stable. Free neutron decay has mean lifetime of $\tau = 881.5 \pm 1.5\ sec$, or about 15 minutes.

In contrast, orbital electron capture by a free proton is unspoken-of outside of a stellar environments. Even if the bare reaction could proceed, the reverse reaction would still dominate un less it is suppressed or is kinetically unfavorable.

5. Inverse Beta Decay

Electron capture is also sometimes called inverse β decay, but, here, we mean this to be the scattering of a proton and an electron anti-neutrino $\bar{\nu}_e$. It is characterized by emission of a positron e^+.

C. Higher order corrections

1. Orbital effects

Highly accurate E.C. calculations must treat the electronic structure of the initial and final electronic states. The capture rate is strongly affected by the overlap between the initial and final atomic states. But when Hydrogen is strongly confined, the atomic electron effectively detaches from the proton, and effectively behaves like a particle-in-a-box (depending on the shape of the box)[?] . So we do not need to consider atomic orbital effects here, and this greatly simplifies the analysis.

2. Radiative Electron Capture

The Weak interaction, as presented here, does not include higher order QED contributions. There are 2 dominant effects: positron emission and Internal Bremsstrahlung[4].

In particular, in very rare cases, a gamma ray photon is emitted with the neutrino; this is called Radiative Electron Capture (REC)[4,14–16]. This can be thought of as a kind of Internal Bremsstrahlung (or so-called *braking*) radiation, caused by the electron accelerating toward the nucleus during capture, taking energy away from outbound neutrino[3]. It is traditionally been treated as a second order QED correction to the V-A theory[4]. REC is 1000X less likely, but does occur. The resulting gamma rays are called soft because they do not exhibit sharp spectral lines. Recent, detailed rate calculations have elucidated the quantum mechanical details[16].

II. CONFINEMENT INDUCED ELECTRON CAPTURE

We pose the following Gedankenexperiment: Suppose we confine a bare proton (and an electron) in a particle-in-a-box of volume L^3. What box size L will 'induce' electron confinement ? Here, we examine what do detailed calculations look like that employ the full machinery of the Weak interaction, as an illustrative exercise.

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.

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 MeV of energy in the process. This post-process contributes to the power output, and prevents the reverse reaction. Realistically, we expect this to happen at the maximum box size, at the energy threshold, where the outbound neutron has very low momentum and therefore a very small mean free path.

Still, for illustrative purposes, we will compute the power output, assuming this post-reaction, at all box sizes.

2. Compton length

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

Most electron capture rate calculations use *ab initio* classical wavefunctions[1,2], perhaps with some relativisitic corrections to the electronic Hamiltonian[17].

We argue that 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[18–20]. The Compton wavelength sets the scale, accounting for both quantum mechanics and special relativity.

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

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

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

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

In any high energy, relativisitic system, positrons can be produced; here it is through β^+-decay. This generally occurs at or below the Compton length. We are seeking the maximum box size which can induce electron capture, and we assume that, at the max, positron emission will be very rare.

We also 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 $L \geq \lambda_e$.

3. Klein Paradox

Klein noted that a relativistic (Dirac) particle-in-a-box will *leak out* at box sizes near the Compton wavelength; this called the Klein paradox[21,22]. And while this is usually taught as being simply particle-antiparticle creation, it has been suggested that the Klein paradox it can occur even at larger boxes sizes, and it is a general phenomena of confined relativistic particles. And recent experiments on Graphene have reopened the debate[23]. Still, we will assume the traditional interpretation and that we can ignore the Klein paradox.

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

III. THEORY AND CALCULATIONS

The electron capture rate can be computed using the Fermi VA-Theory[1,2]. The most basic calculations require a only specifying the electronic wavefunctions(s), averaging over the possible electron-proton momenta, and numerically integrating over the outbound neutrino momentum. We describe this below.

The V-A theory is based on second order perturbation theory. It assumes an incoherent nuclear process, it is local, and that the interaction is phenomenological. It is treated as a simply a contact potential at the surface of

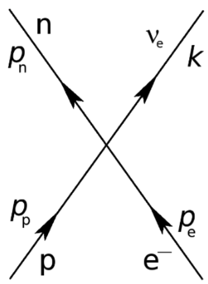

FIG. 2. EC particle production process

the nucleus. Here, this means we need to compute the nuclear charge–the electron density on the surface of the nucleus $\|\psi_e(R=0)\|$, which we obtain from a classical particle-in-the-box wavefunction (below).

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.

A. 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 2). It requires *at least* 0.511 MeV energy to overcome the reaction barrier, which, here, is *provided* by the box.

$$0.782MeV + p^+ + e^- \rightarrow n^0 + \nu_e$$

We want to compute the rate of E.C. and the (minimum) power generated, as a function of the box size (L), using the full Weak Interaction Hamiltonian. To do this, we need to express the rate in terms of the differential cross section, and in a form suitable for numerical calculations.

B. Transition Rates and Power Calculations

Orbital electron capture and other Beta-decay processes follow first order kinetics, so the capture rate is described by a single number. To calculate the rate, we require a full relativistic, quantum mechanical treatment because the capture process involves both creating particles and the kinetic energy spectrum is of order $m_e c^2$.

The capture rate Γ_{EC} is given by multiplying the cross section σ_{EC} by the incident velocity $\mathbf{v}_{ep}^{in}$ and electronic (box) density $\left|\Psi_{ep}(0)\right|^2$ of the (e^-, p^+) pair at the origin

$$\Gamma_{EC} = \left|\Psi_{ep}(0)\right|^2 \mathbf{v}_{ep}^{in} \sigma_{EC} \quad .$$

We will compute the electronic density classically, using box wavefunctions, and, for each box size, determine the incident velocity (really momentum). We then compute the cross section using full relativistic kinematics and Dirac spinors.

1. Cross Section

We write the differential cross section in the C.M. frame as

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

where $\mathcal{M}_{fi}$ is a matrix element of the weak interaction Hamiltonian, $\mathbf{k}$ represents the neutrino momentum components $(k^0, \mathbf{k}) = (E_\nu, \mathbf{k}) = p_\nu^4$, and we use natural units $(\hbar = 1, c = 1)$.

2. Rate

This gives the (differential) rate as

$$d\Gamma_{EC} = \left(\frac{1}{2\pi}\right)^2 \frac{\sum_{fi}\left|\mathcal{M}_{fi}\left[p_{ep}\rightarrow i\nabla\right)\right]\psi_{ep}(\mathbf{x})\big|_{\mathbf{x}=0}\Big|^2}{16E_pE_e\left|\mathbf{k}\cdot(E_n\mathbf{k} - k^0\mathbf{p}_n)\right|} k^3 d\Omega_k \tag{2}$$

where we explicitly specify the electronic wavefunction.

We represent the (e^-, p^+) pair using a 3D box wavefunction, and obtain the Energies and 3-momenta from the relativistic kinematics. We then average over all 8 permutations of the incident velocities (really momenta $\mathbf{p}_{ep}$) for the 3D box, and integrate over outbound neutrino solid angle $d\Omega_k$ using numerical quadrature. The final rate is computed as, for each box size, as a function the kinematics, using

$$\Gamma_{EC} = \frac{1}{8}\sum_{\mathbf{p}_{pe}} \int_{d\Omega_k} d\Gamma_{EC}$$

where $\left|\mathbf{p}_{ep}\right|$ is given by the box size (described below).

3. Power

We estimate the excess power generated by the confined electron capture, resulting if/when the outbound neutron reacts with the environment. The power $\mathcal{P}$ is

$$\mathcal{P} = \Gamma_{EC} * Q * \rho$$

where is the nuclear decay energy, or Q-value, and ρ is the density of confined elements. We choose the density to that of a typical material, of order Avogadro's number, $\mathrm{N_A} \sim 6.02 \times 10^{23}$.

We estimate the power for both the bare proton-electron capture

$$\mathcal{P}_{pe} = \Gamma_{EC} * [(\mathbf{E}_e - m_e) + (\mathbf{E}_p - M_p)] * \rho$$

and the subsequent neutron post-reaction

$$\mathcal{P}_n = \Gamma_{EC} * [2.2 + (\mathbf{E}_n - M_n)] * \rho$$

.

We also define an excess power as

$$\mathcal{P}_{XS} = \mathcal{P}_{pe} - \mathcal{P}_n$$

which we argue is a good measure of the potential reactive power output of the confined E.C. process. We are interested in box lengths where the excess power is significant enough to drive the reaction.

4. Particle-in-the-box Wavefunctions

While most electron capture calculations assume a specific, bound, atomic electronic wavefunction(s), we perform a much simpler calculation; we treat the electron-proton pair as classical particle-in-a-box, and analyze the problem just above the Compton scale using the low order VA theory.

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

.

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 proton wavefunction explicitly, and to treat the electron-proton coupling at the level of Hartree Fock[17]. This has proved useful, for example, 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

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

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

and we consider all 8 permutations for a given box size L:

$$\pm\mathbf{p}_{pe}(1), \pm\mathbf{p}_{pe}(1), \pm\mathbf{p}_{pe}(3)$$

5. Relativistic Kinematics and Energetics

For consistency with the particle production process, we treat all kinematics and energetics relativistically. Given energy-momentum conservation

$$E^2 = m^2 + \mathbf{p}^2$$

and the 3D particle-in-the-box energy ground state energy

$$E_{gs} = \frac{3\pi^2}{2mL^2} \quad ,$$

we use $E = \dfrac{\mathbf{p}^2}{2m}$ to write

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

and

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

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

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

which is approximately 781.6 KeV (or 783.1 KeV in the proton rest frame).

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 minimum momentum is

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

For the final state, the neutrino (ν) 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 (n) kinetic energy is

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

At this point, we can compute the relativistic energies for all particles, simply as a function of box length (L), for a confined (e^-, p^+) pair. Of interest is the shape of the curve, and when the excess power output becomes favorable. To compute the exact rate and estimate the power, we need to evaluate the matrix element(s) of the Weak Interaction Hamiltonian. While most practitioners simply estimate this, for our purpose, we can simply compute them exactly.

[maybe show the curve, and state the maximum box size. or wait until later ?]

[say something about estimating the size of the interaction here, which should be enough for a baseline calculation]

C. Weak Interaction Hamiltonian and Matrix Elements

The Hamiltonian for the V-A theory for E.C. is[1,2]

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

where J^μ and L_μ are (in modern parlance) the Hadron and Lepton currents, resp., and are given by

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

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

where u_n, u_p, u_e, u_ν are Dirac (free-particle) wavefunctions.

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 $G_V = 1.2767(16)$, and $G_A = 1$[24].

1. VA Matrix Elements

In our calculations, however, we use a slightly different, more modern convention for the matrix elements, multiplying through by G_V[25]. The matrix elements $\mathcal{M}_{fi}$ are then given by

$$\mathcal{M}_{fi} = \frac{G_F}{\sqrt{2}} \bar{u}(p_n, s_n)(G_V - G_A\gamma^5)\gamma^\mu u(p_p, s_p) \times \\ \bar{u}(p_\nu, s_\nu)\gamma_u (1 - \gamma^5) u(p_e, s_e) \quad (3)$$

where $u(p, s)$ are Dirac 4-spinors, with the convention

$$u(p, s=1) = \sqrt{E+m} \begin{bmatrix} 1 \\ 0 \\ \frac{p_3}{E+m} \\ \frac{p_1 + ip_2}{E+m} \end{bmatrix}$$

$$u(p, s=2) = \sqrt{E+m} \begin{bmatrix} 0 \\ 1 \\ \frac{p_1 - ip_2}{E+m} \\ \frac{p_3}{E+m} \end{bmatrix}$$

$$\langle \bar{u} | u \rangle = \bar{u}_0 u_0 - \bar{u}_1 u_1 - \bar{u}_2 u_2 - \bar{u}_3 u_3$$

and $\bar{u} = u^\dagger \gamma^0$. The γ are 4-component Gamma matrices, and $(\cdots \gamma^\mu \cdots \gamma_u \cdots)$ is the Einstein summation convention.

Writing the matrix elements in terms of the currents gives

$$\mathbf{J}_{had} = \bar{u}(p_n, s_n)(G_V - G_A\gamma^5)\gamma^\mu u(p_p, s_p)$$

$$\mathbf{L}_{lep} = \bar{u}(p_\nu, s_\nu)\gamma_u (1 - \gamma^5) u(p_e, s_e)$$

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.

2. Sum over spin combinations

Electron capture is similar to Beta decay in that there are allowed (Singlet-like) and disallowed (Triplet-like) transitions, as well as some very low order disallowed contributions. These are, of course, different from Beta decay since we need to consider the total angular momentum of the initial $(p^+ + e^-)$ and final $(n^0 + \bar{\nu_e})$ states.

By Singlet-like states, we effectively mean total spin 0, and by Triplet-like, we mean total spin -1 or 1. Since

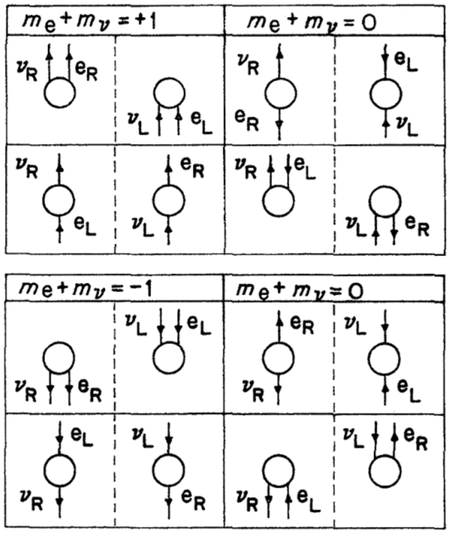

Fig. 1.1. The sixteen possible allowed transitions.

FIG. 3. Allowed spin transitions

we are using particle-in-the-box electronic wave functions, we do not consider orbital angular momentum, and therefore only have to consider if $s_p = s_e$ and $s_n = s_\nu$. Notice, however, we use the Dirac-spinor convention for $s = 1$ (*up*) and $s = 2$ (*down*), so total $s = 0$ corresponds to $(up, down)$ or $(down, up)$, etc.

We sum over the 16 allowed transitions in the V-A theory, as depicted in Figure? (taken from Beta Decay for Pedestrians; we need to replicate , but use p-e as the states, not e-k)

Similar to Beta, s, we have four spin dominate (*allowed*) spin combinations, consisting of Singlet-like (or Fermi-like) initial and final states, which is of order 50 (in natural units)

$$s_p \neq s_e; \quad s_n \neq s_\nu$$

$$\bar{u}(p_n, 1)u(p_p, 1)\ \bar{u}(p_\nu, 2)u(p_e, 2)$$

$$\bar{u}(p_n, 2)u(p_p, 2)\ \bar{u}(p_\nu, 1)u(p_e, 1)$$

,

$$\bar{u}(p_n, 2)u(p_p, 1)\ \bar{u}(p_\nu, 1)u(p_e, 2)$$

$$\bar{u}(p_n, 1)u(p_p, 2)\ \bar{u}(p_\nu, 2)u(p_e, 1)$$

.

There are two weaker (*dis-allowed*) combinations, similar to Gamow-Teller transitions, where are all spins are the same (Triplet-like states), and are of order 10^{-1} (that is, 10^{-3} smaller in magnitude)

$$s_n = s_p = s_\nu = s_e$$

$$\bar{u}(p_n, 1)u(p_p, 1)\ \bar{u}(p_\nu, 1)u(p_e, 1)$$

$$\bar{u}(p_n, 2)u(p_p, 2)\ \bar{u}(p_\nu, 2)u(p_e, 2)$$

.

There are four remaining, non-zero contributions, consisting of a single spin flip in the initial or final state, and is of order 10^{-3} in magnitude

$$s_p \neq s_e \ or \ s_n \neq s_\nu$$

$$\bar{u}(p_n, 1)u(p_p, 1)\ \bar{u}(p_\nu, 1)u(p_e, 2)$$

$$\bar{u}(p_n, 2)u(p_p, 2)\ \bar{u}(p_\nu, 2)u(p_e, 1)$$

.

$$\bar{u}(p_n, 2)u(p_p, 1)\ \bar{u}(p_\nu, 2)u(p_e, 2)$$

$$\bar{u}(p_n, 1)u(p_p, 2)\ \bar{u}(p_\nu, 1)u(p_e, 1)$$

The remaining (single and double flip) transitions have zero amplitude.

D. Numerical Calculations

The full calculations sums of over all 8 possible incident momenta permutations $(\pm\mathbf{p}_{ep}(1), \pm\mathbf{p}_{ep}(2), \pm\mathbf{p}_{ep}(3))$, and the 16 allowed spin transitions (see figure below). By conservation of momenta, we can eliminate the neutron and only need to average over the outbound neutrino momenta solid angle $(d\Omega_k)$; we do this using an 8-point gaussian quadrature.

Let us write the Real part of the current density as

$$C^2_{Re} = Re(\bar{C}^2_{amp} C^2_{amp})$$

where

$$C^2_{amp} = (\mathbf{J}_{had})^\mu (\mathbf{L}_{lep})_\mu = J^0_{had} L^0_{lep} - J^1_{had} C^1_{lep} - J^2_{had} L^2_{lep} - J^3_{had} L^3_{lep} \quad (4)$$

We can express the rate as

$$\Gamma_{EC} = C^2_{Re}(\mathcal{F})$$

Algorithm 1 Rate and Power Calculations

for $\mathsf{p}_{ep} \in [\mathsf{p}_{max}, \mathsf{p}_{min}]$ **do** ▷ $\mathsf{p}_{ep} = \|\mathbf{p}_{ep}(L)\|$
    $Tran(\mathsf{p}_{ep}) = 0$ ▷ Transfer
    $Power_n(\mathsf{p}_{ep}) = 0$ ▷ Neutron Power
    for $w_x, w_\phi \in \mathbb{Q}[1, 8]$ **do** ▷ quadrature weights
        for $s_n, s_p, s_\nu, s_e \in [0, 1]$ **do** ▷ $s_{up}, s_{down} = 0, 1$
            for $s_x, s_y, s_z \in [-1, 1]$ **do** ▷ $\mathbf{p}_{ep} = \mathsf{p}_{ep}[s_x, s_y, s_z]$
                $p_n, p_p, p_\nu, p_e, \leftarrow pekin(w_x, w_\phi, \mathbf{p}_{ep})$ ▷ 4 vectors ← rel. kinematics
                $\bar{u}(p_n, s_n), u(p_p, s_p), \bar{u}(p_\nu, s_\nu), u(p_e, s_e)$ ▷ spinors by p, s-index
                for $u \in [1, 4]$ **do** ▷ 4-vector indices
                    $\mathbf{J}_{had} = \bar{u}(p_n, s_n) \cdot (G_V - G_A\gamma^5) \cdot \gamma^\mu \cdot u(p_p, s_p)$ ▷ Hadronic current
                    $\mathbf{L}_{lep} = \bar{u}(p_\nu, s_\nu) \cdot \gamma_u \cdot (1 - \gamma^5) \cdot u(p_e, s_e)$ ▷ Leptonic current
                $\mathbb{C} = \langle \mathbf{L}^\dagger_{lep}, \mathbf{J}_{had} \rangle$ ▷ Current Amplitude
        $\mathcal{F}^2(\mathsf{p}_{ep}, p_p, p_e, p_n, p_\nu)$ ▷ Matrix Element Factor
        $Tran(\mathsf{p}_{ep}) += w_x w_\phi Re[\mathbb{C}^\dagger \mathbb{C}]\mathcal{F}^2$ ▷ Integrated Rate
    $Power_n(\mathsf{p}_{ep}) = Tran(\mathsf{p}_{ep}) * (2.2 + (E_n - M_n))$ ▷ Neutron Power estimate
¡

where

$$\mathcal{F} = r_c \left(\frac{p_{ep}}{2\pi}\right)^3 \left(\frac{G_F^2 (E_\nu^2 - m_\nu^2)^3}{512\pi^2 \; E_p E_e \hbar c \; \big| \; \mathbf{k}(E_n p_\nu - E_\nu p_n) \; \big|}\right) \tag{5}$$

We write power as

$$P1 = P_{pe} = C^2_{Re} \left[(\mathbf{E}_e - m_e) + (\mathbf{E}_p - M_p) \right] (\mathcal{F})$$

$$P2 = P_n = C^2_{Re} \left[2.2 + (\mathbf{E}_n - M_n) \right] (\mathcal{F})$$

and compute these as a function of the box size using the relativistic kinematic and Weak interaction matrix elements.

E. Results

Figure 4 presents the results of relativistic kinematics and excess power calculations, as a function of box length. For illustrative purposes, we include results box sizes even below the Compton length. The excess power ratio is positive for $L > 0.004\mathring{A}$, with a maximum of almost a factor of 3.

IV. DISCUSSION

A. Low energy electron-proton scattering resonances

We treat the electron-proton pair as if they are bound by the box potential; that is, we assume the box exists. We would like to observe a bound state directly, but describing bound states in relativistic field theory is a complex problem. Indeed, Steven Weinberg stated:

It must be said that the theory of relativistic effects and radiative corrections in bound states is not yet in satisfactory shape.

Ideally we would look for resonances, or quasi-bound states, in solutions of the Bethe Salpeter equation, or a related formulation of the relativistic two-body equations, for electron-proton scattering. This is significantly more complicated, requires some choice of approximation, and is prone to singularities that can lead to numerical instabilities. Still, there is some older work that suggests this may be successful.

In 1991, Spence and Vary claimed to have observed several (5) narrow, low energy, near threshold continuum resonances in numerical solutions of the Blankenbeckler-Sugar equation, a specific, relativistic (but not Gauge invariant) reduction of the two-body Bethe-Salpeter equation into a one-body equation. Their results suggested there could be short lived, quasi-bound electron-proton states up to 100 fm ($0.001\mathring{A}$) in extent. This is of order the box sizes we have investigated, and it would be very interesting to continue out study of confined electron capture using modern techniques.

B. Confinement-induced Nuclear Fusion in the Earth's Inner Core

We briefly mention a recent proposal for a confinement-induced nuclear reaction, namely, nuclear fusion at the Earth's core

The source of heat at the Earth's core remains controversial, although heat flow to the surfaces seemingly arises from both primordial and radiogenic sources. Moreover, signatures of antineutrinos have been detected emanating from the core. Recently (2016), Fukuhara proposed that the observed heat and geoneutrinos results from a three-body nuclear fusion of deuterons. They argue that the reaction occurs in D atoms confined in hexagonal FeDx crystals, at high pressure and temperature. Moreover, the D+D+D collision is modulated by a charge density wave instability which causes a breathing-mode-like displacement of the deuterons.

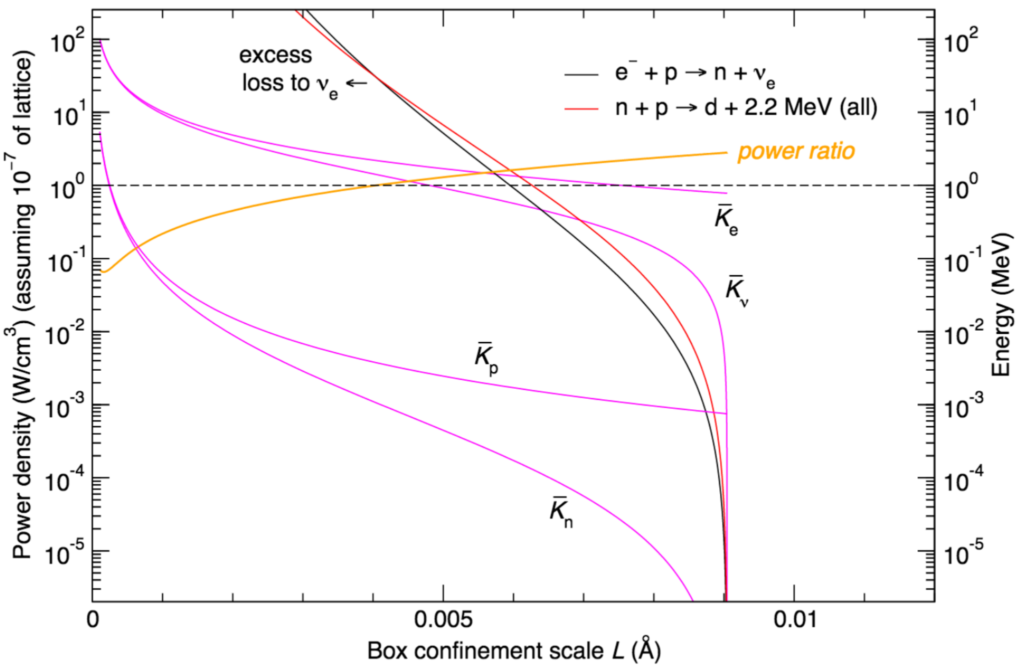

FIG. 4. Kinetic Energy and Power as a function of Box Length

It is noted that the confinement is estimated to be 37% of equilibrium lattice constant, of order a Bohr radius ($0.5\AA$). This is significantly larger than the L values here, although fusion requires a significantly smaller level of confinement than electron capture. And we do not consider temperature or pressure effects in our model, which Fukuhara estimates includes another 50% confinement in this model.

C.

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