

# Confinement Induced Electron Capture

C. Martin<sup>1, a)</sup> and R. Godes<sup>1, b)</sup>

*Authors' institution and/or address*

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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 relativistic 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 estimate the theoretical minimal power output for such a process, seeing that is feasible at large box lengths. Finally, we discuss proposals for future work and possible applications.

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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<sup>7</sup>. If an electron were confined to volume of nuclear radius, it would have a (relativistic) kinetic energy of order  $10\text{ MeV}$ . But this is not observed experimentally. In Beta decay, a nucleus emits an electron with energy of order  $1\text{ MeV}$ .

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

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.

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

Orbital electron capture is a fundamental nuclear process, on par 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 problem numerically. Indeed, the most complete reference date back to the 1960s and 70s<sup>1,2</sup>. 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 is 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<sup>3</sup>—although it is more properly treated using QED corrections to the Weak Interaction<sup>4</sup>. 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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<sup>a)</sup> Also at Physics Department, XYZ University.

<sup>b)</sup> Electronic mail: Second.Author@institution.edu.

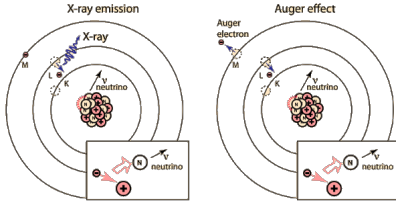


FIG. 1. orbital electron capture relaxation processes

Note that unlike Beta decay, which is a 1 body decay, and the emitted electron has a wide energy spectrum, E.C. is a 2 body reaction, and the emitted neutrino is mono-chromatic.

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

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

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

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

When  $Q < 1.02 \text{ MeV}$ , twice the rest mass of an electron ( $2m_e c^2$ ), a proton rich nucleus must decay by electron capture.

In particular, heavy elements may decay by E.C. and/or  $\beta^+$  (positron emission) to a lower 'magic number' of stable nuclei, and by  $\beta^-$  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  ${}^7\text{Be}$ , decay by primarily by E.C.

Note that lacking any binding energy and/or internal nucleon structure, bare proton electron capture is not readily observed, and requires extreme, exotic conditions such as strong confinement.

## 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, become excited, and then undergo internal conversion. During this, another higher lying, bound atomic electron is absorbed, and release an X-ray or Auger electron [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



(where  $Z$  is the total number of protons and neutrons,  $A$  the number protons, and  $h\nu_{X\text{-ray}}$  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<sup>5</sup>. 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  ${}^7\text{Be}$ <sup>6</sup>. In fact, there is so little energy that the competing  $\beta^+$  positron emission process (described below) is prohibited, leading to a fairly long E.C. half-life of  $\tau_{EC} \sim 50 \text{ days}$ .

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

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 Electron Proton Capture and Stellar Nucleosynthesis

At zero energy, bare proton electron capture is not possible because it violates energy-momentum conservation. Theoretically, a free proton can 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 such capture outside of an accelerator 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 believe it occurs, even if we don't understand the detailed mechanism.

Bare capture is thought to occur in the early stages of the big bang and in stellar nucleosynthesis. It drives the formation of primordial elements, and occur when neutron stars form. At very high temperatures, the proton electron collisions have sufficient energy to overcome the reaction barrier. For example, Bachall and coworkers have computed the electron capture rate of  ${}^7\text{Be}$  in the Sun<sup>10,11</sup>. 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 its temperature, these are also very dense systems, with  $\rho \sim 10^6 \text{ g cm}^{-3}$ . In contrast, the smallest star has density  $\rho \sim 10^2 - 10^3 \text{ g cm}^{-3}$  [?]. 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. We model this as a particle-in-a-box using the Femi VA theory.

## B. The Weak Interaction and Femi VA theory

Electron capture is mediated by the Weak Interaction, described most concisely by the Fermi VA (Vector Axial) theory<sup>1,2,12</sup>. The VA theory is a simple phenomenological approach, readily amenable to numerical calculations. 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*<sup>13</sup>.

VA 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 VA 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  $p^+ + e^- \rightarrow n^0 + \nu_e$
- positron emission ( $\beta^+$  decay)  $p^+ \rightarrow n^0 + e^+ + \nu_e$
- $\beta$  decay  $n^0 \rightarrow p^+ + e^- + \bar{\nu}_e$

There are also several related reactions, including

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

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 very rare topic. Indeed, the most recent review is from 1976<sup>1</sup>.

## 3. Positron emission

In any high energy relativistic process, we have to worry about positron emission. We noted above, however, that in  ${}^7\text{Be}$ , 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  $\tau = 881.5 \pm 1.5 \text{ sec}$ , 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 unless it is suppressed or is kinetically unfavorable.

## 5. Inverse Beta decay

Electron capture is also sometimes called inverse  $\beta$  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 rate calculations must treat the electronic structure of the initial and final electronic states, and it is strongly affected by their overlap. 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)<sup>?</sup>. 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<sup>4</sup>.

In particular, in very rare cases, a gamma ray photon is emitted with the neutrino; this is called Radiative Electron Capture (REC)<sup>4,14-16</sup>. 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 out-bound neutrino<sup>3</sup>. It is traditionally been treated as a second order QED correction to the VA theory<sup>4</sup>. 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<sup>16</sup>.

## 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.

Before we describe the theoretical approach, we address a few conceptual issues in setting up the problem.

### 1. Confined Atomic systems

Usually electron capture is described using the atomic orbitals of the parent and daughter nuclei<sup>1,2</sup>. This is very complicated and the basic physical insight can be lost in the details of various angular momentum selection rules and orbital overlap calculations. Moreover, when H atom is confined, the electron will detach from the proton and behave like a free particle in a box<sup>7</sup>.

### 2. Compton length

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

Most electron capture rate calculations use *ab initio* classical wavefunctions<sup>1,2</sup>, perhaps with some relativistic corrections to the electronic Hamiltonian<sup>17</sup>.

We argue that we can safely use a classical box as long as  $L_{min} \geq \frac{1}{2\pi}\lambda_e$ , where  $\lambda_e$  is Compton wavelength of an electron<sup>18-20</sup>. The Compton wavelength sets the scale, accounting for both quantum mechanics and special relativity.

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

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

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

$$L_{min} \sim 0.004 \text{ \AA}$$

In any high energy, relativistic system, positrons can be produced; here it is through  $\beta^+$ -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 ( $\sigma$ ) and rate ( $\Gamma$ ). 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<sup>21,22</sup>. 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 box sizes, and it is a general phenomena of confined relativistic particles. And recent experiments on Graphene have reopened the debate<sup>23</sup>. Still, we will assume the traditional interpretation and we will ignore the Klein paradox.

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

### 4. 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. 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.

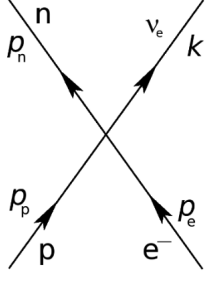


FIG. 2. EC particle production process

### III. THEORY AND CALCULATIONS

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

The VA 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 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.

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

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

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

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

##### 1. Cross Section

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

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

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

##### 2. Rate

This gives the (differential) rate as

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

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

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.

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

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  $\psi_{ep}^0$  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<sup>17</sup>. This has proved useful, for example, for describing isotope effects on electronic structure. It is may also be possible to eventually treat this problem using fully relativistic *ab initio* QFT methods, although this has only been applied to positronium so far<sup>?</sup>.

Here, we treat the confined electron, proton pair in the C.M. frame so that the 3-momentum of the electron and proton are related as

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

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

and we consider all 8 permutations for each 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

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

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

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

and

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

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

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

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 ( $\nu$ ) 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.

### C. Weak Interaction Hamiltonian and Matrix Elements

The Hamiltonian for the VA theory for E.C. is<sup>1,2</sup>

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

where  $J^\mu$  and  $L_\mu$  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  $u_n, u_p, u_e, u_\nu$  are Dirac (free-particle) wavefunctions.

$G_F$  is the Universal Fermi Weak Coupling Constant, and  $\lambda = -\frac{G_A}{G_V}$ , 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  $\gamma$  are 4-component Gamma matrices, and  $(\dots \gamma^\mu \dots \gamma_u \dots)$  is the Einstein summation convention.

Recall that the VA theory assumes that the electron-proton interaction is a contact potential, operating at the surface of the nucleus, and that the underlying quantum process is incoherent. We need simply compute the matrix elements in terms of the terms of the individual Hadronic and Leptonic currents

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

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

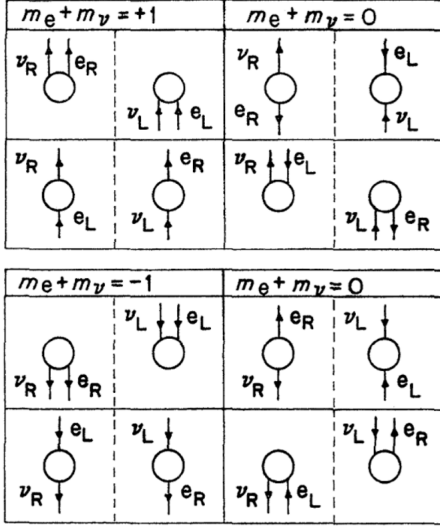


Fig. 1.1. The sixteen possible allowed transitions.

FIG. 3. Allowed spin transitions

## 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 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 VA theory, as depicted in Figure<sup>7</sup> (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 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 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

$$s_p \neq s_e \text{ or } s_n \neq s_\nu$$

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

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

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

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

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

## D. Numerical Calculations

We outline the calculations in pseudocode below.

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

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

where

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



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**Algorithm 1** Rate and Power Calculations
 

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1: <b>for</b> $\mathbf{p}_{ep} \in [\mathbf{p}_{max}, \mathbf{p}_{min}]$ <b>do</b> 2: $Tran(\mathbf{p}_{ep}) = 0$ 3: $Power_n(\mathbf{p}_{ep}) = 0$ 4: <b>for</b> $w_x, w_\phi \in \mathbb{Q}[1, 8]$ <b>do</b> 5: <b>for</b> $s_n, s_p, s_\nu, s_e \in [0, 1]$ <b>do</b> 6: <b>for</b> $s_x, s_y, s_z \in [-1, 1]$ <b>do</b> 7: $p_n, p_p, p_\nu, p_e \leftarrow pekin(w_x, w_\phi, \mathbf{p}_{ep})$ 8: $\bar{u}(p_n, s_n), u(p_p, s_p), \bar{u}(p_\nu, s_\nu), u(p_e, s_e)$ 9: <b>for</b> $u \in [1, 4]$ <b>do</b> 10: $\mathbf{J}_{had} = \bar{u}(p_n, s_n) \cdot (G_V - G_A \gamma^5) \cdot \gamma^\mu \cdot u(p_p, s_p)$ 11: $\mathbf{L}_{lep} = \bar{u}(p_\nu, s_\nu) \cdot \gamma_u \cdot (1 - \gamma^5) \cdot u(p_e, s_e)$ 12: $\mathbb{C} = \langle \mathbf{L}_{lep}^\dagger, \mathbf{J}_{had} \rangle$ 13: $\mathcal{F}^2(\mathbf{p}_{ep}, p_p, p_e, p_n, p_\nu)$ 14: $Tran(\mathbf{p}_{ep}) += w_x w_\phi Re[\mathbb{C}^\dagger \mathbb{C}] \mathcal{F}^2$ 15: $P_n(\mathbf{p}_{ep}) = Tran(\mathbf{p}_{ep}) * (2.2 + (E_n - M_n))$	$\triangleright \mathbf{p}_{ep} = \ \mathbf{p}_{ep}(L)\ $ $\triangleright$ Transfer $\triangleright$ Neutron Power $\triangleright$ quadrature weights $\triangleright s_{up}, s_{down} = 0, 1$ $\triangleright \mathbf{p}_{ep} = \mathbf{p}_{ep}[s_x, s_y, s_z]$ $\triangleright$ 4 vectors $\leftarrow$ rel. kinematics $\triangleright$ spinors by p, s-index $\triangleright$ 4-vector indices $\triangleright$ Hadronic current $\triangleright$ Leptonic current $\triangleright$ Current Amplitude $\triangleright$ Matrix Element Factor $\triangleright$ Integrated Rate $\triangleright$ Neutron Power estimate
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We express the rate as

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

in terms of an intermediate factor

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

We write the two power terms as

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

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

and compute these as a function of the box size using the relativistic kinematic and Weak Interaction matrix elements. We are interested in the estimated neutron output power ratio

$$power\ ratio : \frac{P_n}{P_{ep}}$$

as a function of box length  $L$ .

### 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 greater than unity for  $L > 0.004\text{\AA}$ , with a maximum of almost a factor of 3.

These simple calculations indicate that a confined electron capture reaction would be favorable as long as the produced neutrons react with environment at a high rate.

This is expected at the maximum box size, where the neutron has the smallest mean free path, although the reaction appears favorable for all box lengths larger than the Compton length,  $L > 0.004\text{\AA}$ .

### IV. DISCUSSION

We present calculations for a Gedankenexperiment describing confined orbital electron capture of a bare proton and an electron in a box

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

The intent is to model, conceptually, a confined proton, trapped in a field of free electrons, such that the kinetic energy of the proton is high enough to induce electron capture. We treat system as an electron-proton pair in a classical particle-in-the-box, and compute the capture rate using the Fermi VA theory. We use classical box wavefunctions to express the confinement, and compute relativistic proton momentum and kinetic energy resulting from the box. We then compute the rate by evaluating the Weak Interaction Hamiltonian matrix elements using the box wavefunction density at the origin, using a form of the cross section that takes into account the full relativistic Kinematics of the two-body  $e^- + p^+$  nuclear reaction. We compute the power generated by the E.C. process, as well as estimate the minimum excess neutron power, as a function of box size  $L$ . We find that the excess power ratio is greater than one for box sizes  $L > 0.004\text{\AA}$ , and increases rapidly as we approach the maximum box size  $L > 0.009\text{\AA}$ . We note we need a compression ratio of order 50X to induce capture.

While being pedagogic exercise, we would also like to discuss both directions for future work and a possible application.

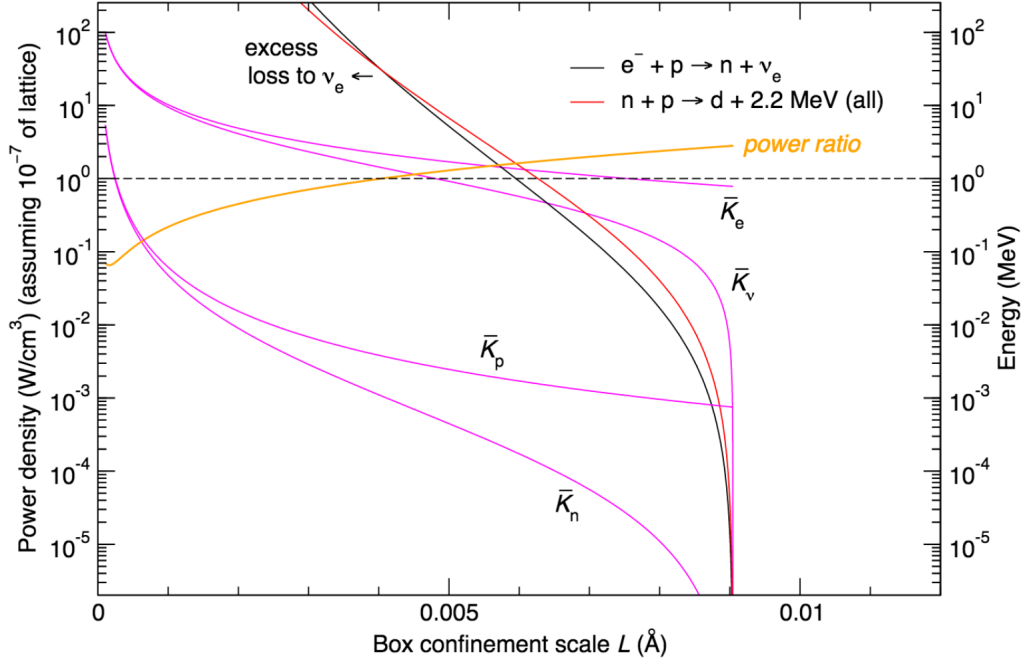


FIG. 4. Kinetic Energy and Power as a function of Box Length

#### 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 has stated<sup>?</sup>:

*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 Blankenbecker-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 (0.001Å) in extent. This is of order the box sizes we have investigated, and it would be very interesting to continue our study of confined electron capture using modern techniques.

The best, modern, relativistic *ab initio* techniques so far, also by Vary, have successfully treated positronium<sup>?</sup>,

and it would be interesting to try to extend such methods to electron-proton scattering. This is significantly more difficult since most *ab initio* many body methods can treat ground states, but to find quasi-bound states requires a powerful open shell method.

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

We briefly mention a recent proposal for another type of 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 result 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.

It is noted that the confinement is estimated to be 37% of equilibrium lattice constant, of order a Bohr radius (0.5Å). 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.

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