

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 the aspects around bare electron proton capture. We then provide a numerical solution of the Fermi VA-Theory for 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 and the Compton wavelength of the electron. We also examine the implications for theoretical minimal power output for such a process.

PACS numbers: Valid PACS appear here

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I. BACKGROUND

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

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.)

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

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

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

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

When $Q < 1.02 MeV$, which is 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 β^+ (positron emission) to a lower 'magic number' of stable nuclei, and by β^- decay to achieve a higher

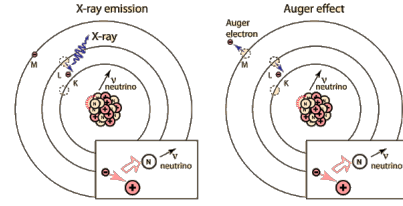


FIG. 1. orbital electron capture relaxation processes

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.

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

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

(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 Titanium¹. Since then, electron capture has been observed in about 150 radioactive isotopes.

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1. Effect of Chemical Environment of Electron Capture rate

The lightest element that E.C. has been observed in is ${}^7\text{Be}^2$. 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 $\tau_{EC} \sim 50 \text{ days}$.

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 pressure³⁻⁵. In particular, in 2004, Ohtsuki et. al. demonstrated a change of 0.83% by embedding Be in C-60 cages⁵.

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.

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) theory⁶⁻⁸. 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"⁹.

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

2. 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.

3. 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^+ .

4. Positron emission

In particular, 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.

5. Radiative Electron Capture

Also, in very rare cases, a gamma ray photon is emitted with the neutrino; this is called Radiative Electron Capture (REC)¹⁰⁻¹³. 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 neutrino¹⁴. It is traditionally been treated as a second order QED correction to the V-A theory¹². 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 details¹³.

C. Rate calculations

The electron capture rate can be computed using the Fermi VA-Theory^{7,8}. 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 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.

1. Bare proton-electron capture

We frequently write electron capture as if it were simply proton-electron capture

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

At zero energy, 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 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. 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 ${}^7\text{Be}$ in the Sun^{15,16}. 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).

3. Metallic Hydrides

It has been suggested that bare proton-electron capture could actually arise metallic hydrides, such as PdH and NiH, as a result of some exotic, here-to-fore unrecognized physical mechanism. Widom and Larsen, in particular, have proposed that the effective Q value for bare proton E.C. would be lowered because the surface electrons may undergo mass renormalization due surface plasmon radiation, leading to high order radiative corrections to the Weak interaction pair production process¹⁷. One may define an effective mass \tilde{m}_e using

$$\tilde{m}_e c^2 \cong -\overline{p^\mu p_\mu} = m_e c^2 + \left(\frac{e}{c}\right)^2 + \overline{A^\mu A_\mu}$$

where A^μ is the gauge potential for the fluctuating surface plasmon radiation, and assuming $\overline{p^\mu A_\mu} = 0$

They argue that such a renormalization may be possible because the neutron scattering experiments on PdH show a collective proton oscillation that would be resonate with electronic surface plasmons.

Outside of any new physics, is there any other plausible mechanism for E.C. in a metallic hydride? Any such process would be energetically bound by the uncertainty principle, meaning that the hydrogen atom would be under extreme confinement.

Curiously, neutron scattering experiments do show that in PdH, that the hydrogen atoms have a root-mean-square vibrational amplitude of $0.25A$ (at $T = 293K$), which is anomalously small¹⁸.

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.

A. 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^{7,8}, perhaps with some relativistic corrections to the electronic Hamiltonian¹⁹.

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 electron²⁰⁻²². 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 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 $L \geq \lambda_e$.

1. 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^{23,24}. And while this is usually taught as being simply particle-antiparticle creation,

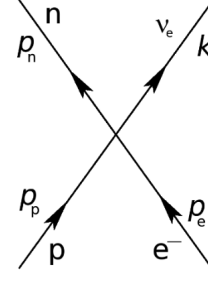


FIG. 2. EC particle production process

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 debate²⁵. Still, we will assume the traditional interpretation and that we can ignore the Klein paradox.

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

B. Theory

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 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.

C. 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 $|\Psi_{ep}(0)|^2$ 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 (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

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

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

2. Rate

This gives the (differential) rate as

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

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 ρ 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.

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

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_{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 Fock¹⁹. 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

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

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 (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]

D. Weak Interaction Hamiltonian and Matrix Elements

The Hamiltonian for the V-A theory for E.C. is^{7,8}

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

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 $\lambda = -\frac{G_A}{G_V}$, 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 $G_A = 1^{26}$.

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^{27} . 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 $(\dots \gamma^\mu \dots \gamma_u \dots)$ is the Einstein summation convention.

Writing the matrix elements in terms of the currents gives

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

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

[Express power in terms of real part of current]

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.

[how much more to describe here? Specify the 4-norm / gamma metric tensor convention?]

2. Sum over all 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.

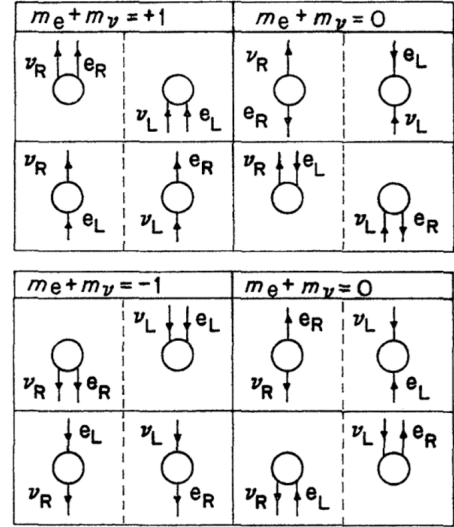


Fig. 1.1. The sixteen possible allowed transitions.

FIG. 3. Allowed spin transitions

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 V-A theory, as depicted in Figure⁷ (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 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.

E. 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.

1. Power Calculations

[Again, I have not worked this out in detail. In particular, we discuss the power above, so this is just for understanding the code, and I may leave this to the python notebook. It is necessary, however, to really grok all the pseudocode]]

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

F. 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 $L > 0.004\text{\AA}$, with a maximum of almost a factor of 3.

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Algorithm 1 Rate and Power Calculations

<pre> 1: for $\mathbf{p}_{ep} \in [\mathbf{p}_{max}, \mathbf{p}_{min}]$ do 2: $Tran(\mathbf{p}_{ep}) = 0$ 3: $Power_n(\mathbf{p}_{ep}) = 0$ 4: for $w_x, w_\phi \in \mathbb{Q}[1, 8]$ do 5: for $s_n, s_p, s_\nu, s_e \in [0, 1]$ do 6: for $s_x, s_y, s_z \in [-1, 1]$ do 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: for $u \in [1, 4]$ do 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: $Power_n(\mathbf{p}_{ep}) = Tran(\mathbf{p}_{ep}) * (2.2 + (E_n - M_n))$ </pre>	<pre> ▷ $\mathbf{p}_{ep} = \ \mathbf{p}_{ep}(L)\$ ▷ Transfer ▷ Neutron Power ▷ quadrature weights ▷ $s_{up}, s_{down} = 0, 1$ ▷ $\mathbf{p}_{ep} = \mathbf{p}_{ep}[s_x, s_y, s_z]$ ▷ 4 vectors \leftarrow rel. kinematics ▷ spinors by p, s-index ▷ 4-vector indices ▷ Hadronic current ▷ Leptonic current ▷ Current Amplitude ▷ Matrix Element Factor ▷ Integrated Rate ▷ Neutron Power estimate </pre>
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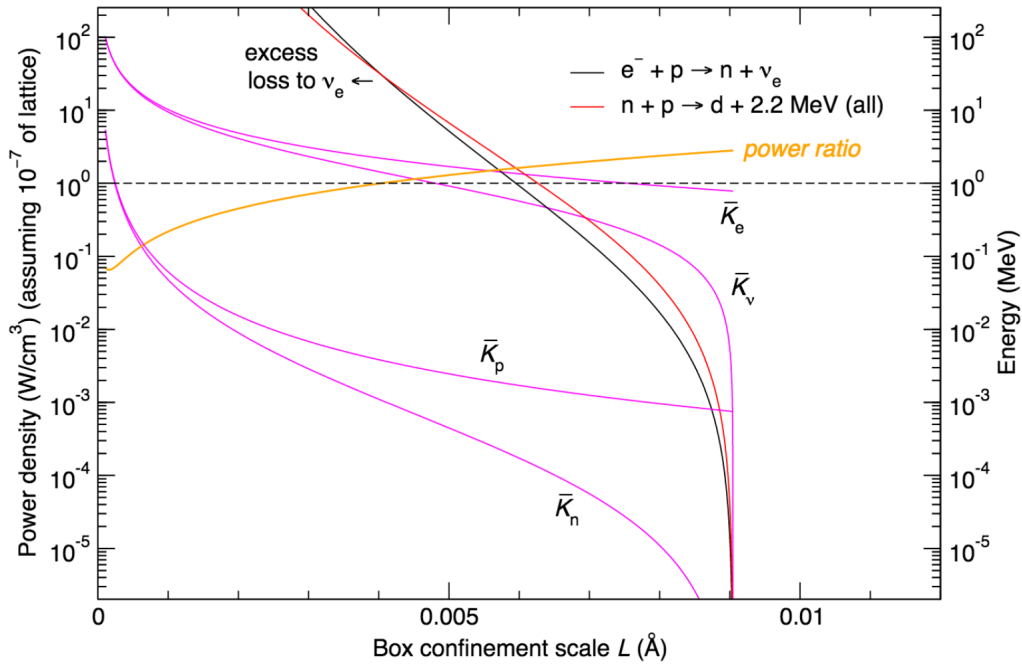


FIG. 4. Kinetic Energy and Power as a function of Box Length

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