

Appendix A4

Derivation of the Proton-Proton Capture Cross-Section to Form a Hypothetical Diproton (Helium-2)

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1. Introduction

In Appendix A2 we have derived the neutron-proton capture cross-sections. Both the magnetic dipole and electric dipole contributions were found to be non-zero, though the magnetic dipole (spin) contribution is dominant in neutron-proton capture at non-relativistic energies. Since the neutron is neutral, there is no Coulomb barrier to interfere with neutron-proton capture. In Appendix A3 we have derived the cross section for proton capture by deuterons to form helium-3 (the second reaction in the stellar nucleosynthesis sequence). This differed from the neutron-proton capture calculations in two ways. Firstly, the magnetic dipole contribution is identically zero (in first order perturbation theory) because only one spin state is available, and hence the cross section is determined by the electric dipole contribution alone. Secondly, a Coulomb barrier is present, necessitating a numerical evaluation of the electric dipole matrix element. Both these differences cause the proton-deuteron capture cross section to be smaller than the neutron-proton capture cross section.

Unlike Appendices A2 and A3, here we shall consider a reaction which is not a possibility in this universe. We consider two protons reacting to form a diproton, i.e., helium-2 (He^2). A diproton does not exist as a bound state in this universe (as discussed in Chapter 9C of the "Cosmic Coincidences"). So we are implicitly considering a hypothetical universe with a slightly stronger nuclear force, sufficient to bind the diproton.

Like proton-deuteron capture, proton-proton capture also has no magnetic dipole (spin) contribution. This is again because only one spin state is available (alternatively, we have seen in Appendix A2 that the spin term is proportional to the difference of the magnetic dipole moments of the two interacting particles, which is clearly zero for identical particles). Also like proton-deuteron capture, proton-proton capture involves a Coulomb barrier. However, unlike proton-deuteron capture, proton-proton capture has no electric dipole contribution either. The reason is that we are dealing with identical fermions whose wavefunction must be antisymmetric under interchange. Thus, the possible two-proton states are 1S , 3P , 1D , etc. Unlike the neutron-proton or proton-deuteron systems, there is no possible matrix element of the form $\langle ^N S | eE_0 r \cos \theta | ^N P \rangle$, where 'N' represents the same initial and final spin state, and $\langle ^1 S | eE_0 r \cos \theta | ^3 P \rangle$ is identically zero because the different spin states are orthogonal, and the electric dipole interaction Hamiltonian does not change the spin. Thus, the lowest order contribution arises from the electric quadrupole matrix element $\langle ^1 S | eE_0 r^2 P_2(\cos \theta) | ^1 D \rangle$. Evaluation of this matrix element including the Coulomb barrier again requires numerical calculation, but an algebraic expression is also derived for the case of no Coulomb barrier to facilitate checking the numerical program.

Appendices A2 and A3 used a method in which the photodisintegration cross section was evaluated first, and the capture cross section derived from it via the reciprocity theorem. These Appendices suffered from a mysterious missing factor of $1/4$. In this Appendix we use a different method, calculating the capture cross section directly and based on the classical expressions for the radiant energy emitted by oscillating multipoles. The method is developed first for the neutron-proton case and shown to give the correct result (i.e. no spurious factor of $1/4$), thus giving confidence in the result for the proton-proton cross section which follows.

2. Classical Multipole Fields and Radiant Power

The following development is taken largely from Blatt & Weisskopf, "Theoretical Nuclear Physics", Chapter XII, Section 3. Consider the following classical (but complex) charge and current densities,

$$\rho(\vec{r}, t) = e^{-i\omega t} \rho(\vec{r}) + e^{i\omega t} \rho(\vec{r})^* ; \quad \vec{J}(\vec{r}, t) = e^{-i\omega t} \vec{J}(\vec{r}) + e^{i\omega t} \vec{J}(\vec{r})^* \quad (1)$$

Since we have given these source distributions a harmonic time dependence we expect radiation to be produced. The exact solution for the electric and magnetic field strengths are, where $k_\gamma = \omega/2$,

$$\vec{E} = \frac{i}{k_\gamma} a_E^{Lm} \nabla \times \vec{F} + a_M^{Lm} \vec{F}, \quad \vec{H} = a_E^{Lm} \vec{F} - \frac{i}{k_\gamma} a_M^{Lm} \nabla \times \vec{F} \quad (2)$$

$$\text{where, } \vec{F} = \tilde{u}_L(kr) \bar{X}_{Lm}(\theta, \phi) \text{ and } \bar{X}_{Lm}(\theta, \phi) = \hat{L} Y_{Lm}(\theta, \phi) / \sqrt{L(L+1)} \quad (3)$$

where Y_{Lm} are the spherical harmonics with conventional normalisation (see below) and \hat{L} is the angular momentum (vector) differential operator, and,

$$\tilde{u}_L(kr) \equiv e^{-i\sigma_L} [j_L(kr) + i n_L(kr)] \equiv e^{-i\sigma_L} h_L^{(1)}(kr) \quad (4)$$

where j, n are the spherical Bessel / Neumann functions, and h the Hankel function. To complete the solution (2, 3, 4) the field amplitudes are given by,

$$a_E^{Lm} = -\frac{4\pi}{(2L+1)!!} \left(\frac{L+1}{L}\right)^{1/2} k_\gamma^{L+2} Q_{Lm}; \quad a_M^{Lm} = \frac{4\pi}{(2L+1)!!} \left(\frac{L+1}{L}\right)^{1/2} k_\gamma^{L+2} M_{Lm} \quad (5)$$

where Q_{Lm} and M_{Lm} are the multipole moments of order L (e.g. for $L = 1$ they are the dipole moments, up to some constant factor, for $L = 2$ the quadrupole moments, etc.), and are given by,

$$Q_{Lm} = \int r^L Y_{Lm}^*(\theta, \phi) \rho(\vec{r}) dV, \quad M_{Lm} = -\int r^L Y_{Lm}^*(\theta, \phi) \frac{\nabla \cdot (\vec{r} \times \vec{J})}{c(L+1)} dV \quad (6)$$

[NB: In MKSA units we interpret the charge and current densities as including the factor of $1/\sqrt{4\pi\epsilon_0}$]. Since the asymptotic form of the \tilde{u}_L functions for large r is $\propto \sin(kr + \alpha)/kr$, for some phase angle ' α ', the electric and magnetic fields also

become of order $1/kr$. Hence the Poynting vector is of order $1/(kr)^2$ and thus integrates to give a constant energy flux out of any sufficiently large sphere, as expected for a radiation field. The power radiated per second into solid angle $d\Omega$ is, for each of the electric and magnetic multipoles respectively,

$$dP_E^{Lm} = \frac{c}{2\pi k_\gamma^2} Z_{Lm}(\theta, \phi) |a_E^{Lm}|^2 d\Omega, \quad dP_M^{Lm} = \frac{c}{2\pi k_\gamma^2} Z_{Lm}(\theta, \phi) |a_M^{Lm}|^2 d\Omega \quad (7)$$

where, $Z_{Lm}(\theta, \phi) = |\bar{X}_{Lm}(\theta, \phi)|^2$. Note that if the current flux density is due to the charge density moving at some position-dependent velocity (i.e. $\bar{J} = \rho\bar{u}$) then the magnetic multipole power is of order $(u/c)^2$ times smaller than the electric multipole energy, and hence negligible for non-relativistic energies.

With the aid of the result $\int Z_{Lm}(\theta, \phi) d\Omega = 1$ the total power from (7) is,

$$P_E^{Lm} = \frac{c}{2\pi k_\gamma^2} |a_E^{Lm}|^2, \quad P_M^{Lm} = \frac{c}{2\pi k_\gamma^2} |a_M^{Lm}|^2 \quad (8)$$

2.1 Dipole Case

The spherical harmonics are normalised so that,

$$Y_{Lm}(\theta, \phi) = \left(\frac{2L+1}{4\pi} \right)^{1/2} P_L(\cos\theta) \quad (9)$$

so, with $L = 1$ for an electric dipole, Equ.(5) gives the field amplitude to be,

$$a_E^{10} = -\sqrt{\frac{8\pi}{3}} k_\gamma^3 p \quad (10)$$

where the electric dipole is defined as usual by,

$$p = \int r \cos\theta \cdot \rho(\bar{r}) dV \quad (11)$$

[NB: $Q_{10} = \sqrt{3/4\pi} \cdot p$]. Hence, Equ.(8) gives the power radiated by an oscillating dipole to be,

$$P_E^{10} = \frac{4}{3} c k_\gamma^4 p^2 = \frac{4}{3} \cdot \frac{\omega^4}{c^3} p^2 \quad (12)$$

[in MKSA units, insert a factor of $4\pi\epsilon_0$ in the denominator]. If we now consider the case of a real charge distribution, ρ , then Equ.(1) shows that the power, (12), corresponds to a time dependent charge density given by,

$$\rho(\bar{r}, t) = 2\rho(\bar{r}) \cos \omega t \quad \text{for real } \rho \quad (13)$$

Thus, in this case, $\rho(r)$ is actually only *half* the peak charge density, and hence p given by (11) is only half the peak dipole moment. Calling the peak dipole moment $p_0 = 2p$ we have,

$$P_E^{10} = \frac{1}{3} \cdot \frac{\omega^4}{c^3} P_0^2 \quad (14)$$

in agreement with Duffin, Equ.(4.80), for the mean radiated power of a dipole.

2.2 Electric Quadrupole Case

Eqs.(5, 6, 9) give,

$$a_E^{20} = -\sqrt{\frac{2\pi}{15}} k_\gamma^4 p_q \quad (15)$$

where,

$$p_q = \int r^2 P_2(\cos\theta) \rho(\bar{r}) dV \quad (16)$$

and,

$$P_2(\cos\theta) = (3\cos^2\theta - 1)/2 \quad (17)$$

[NB: $Q_{20} = \sqrt{5/4\pi} p_q$]. Hence, from (8), the power radiated by our oscillating electric quadrupole is,

$$P_E^{20} = \frac{1}{15} c k_\gamma^6 p_q^2 = \frac{1}{15} \cdot \frac{\omega^6}{c^5} p_q^2 \quad (18)$$

However, we note that, for a real charge distribution, Equ.(13) again holds and the actual peak charge density is twice $\rho(r)$. Thus, in terms of the peak quadrupole moment, $p_{q0} = 2p_q$, we have,

$$P_E^{20} = \frac{1}{60} \cdot \frac{\omega^6}{c^5} P_{q0}^2 \quad (19)$$

3. The Capture Cross Section Formulae

3.1 Electric Dipole Case (e.g. n-p capture)

The transition from the classical expression for radiant power to a quantum mechanical cross section is made in two steps. The first is to convert the classical power to a number of photons per second, simply by dividing by the energy per photon, i.e. $\hbar\omega$, giving, from Equ.(12),

$$w_d = \frac{4}{3} \cdot \frac{\omega^3 p^2}{\hbar c^3} \quad (20)$$

where w_d is the probability of a photon being emitted per second per nucleon, i.e. the reaction rate per nucleon. The second step is to convert the classical expression (11) for the dipole moment into its quantum equivalent, i.e.,

$$p^{(qm)} = Ze \int r \cos \theta \Psi_f^* \Psi_i \cdot dV \quad (21)$$

where $\Psi_{i,f}$ are the initial and final wavefunctions of the nucleons and Z is the number of protons (i.e. the total charge). Note that we are only dealing with the 2-body problem here. More generally (21) would involve a sum over wavefunctions dependent upon $3(N-1)$ coordinates. The capture cross section is related to the reaction rate by,

$$w = v \sigma_{cap} \times \text{particle density} \quad (22)$$

where v is the relative velocity of collision of the two nucleons. If the particle density is one particle per volume V_{max} , then,

$$\sigma_{cap} = \frac{w}{v(1/V_{max})} = \frac{4}{3} \cdot \frac{V_{max} \omega^3 p^{(qm)2}}{v \hbar c^3} \quad (23)$$

in agreement with Blatt & Weisskopf Ch.XII, Equ.(4.4), noting that the latter assume $V_{max} = 1$.

Care must be exercised in using (23), however, due to the potential trap of introducing an error of a factor of 2 in the dipole moment (and hence a factor of 4 in the cross section). This is a consequence of Equ.(13), which derives from Equ.(1). When translating (11) into its quantum equivalent, Equ.(21), we have effectively assumed that the quantum states in question also consist, like (1), of two conjugate parts, i.e.,

$$\Psi_{i,f}(\vec{r}, t) = \Psi_{i,f}(\vec{r})e^{-i\omega t} + \Psi_{i,f}^*(\vec{r})e^{i\omega t} \quad (24)$$

i.e. a combination of particles and anti-particles in field-theory speak. The wavefunction is therefore twice the real part of one of these terms, like Equ.(13). If we used a time dependent wavefunction (LHS of 24) normalised to unity, it would follow that the time independent functions on the RHS would be normalised to $1/2$. Thus, the dipole moment from (21) is actually only half the size that would be derived on the basis of Schrodinger states normalised to unity. Equivalently, we can agree to evaluate (21) using Schrodinger states but replace (23) by the counterpart of (14), i.e.,

$$p_0^{(qm)} = Ze \int r \cos \theta \Psi_{f,Sch}^* \Psi_{i,Sch} \cdot dV \quad (25)$$

$$\text{(polarised)} \quad \sigma_{cap} = \frac{1}{3} \cdot \frac{V_{max} \omega^3 p_0^{(qm)2}}{v \hbar c^3} \quad (26)$$

where the subscript $_{Sch}$ refers to Schrodinger states normalised to unity in volume V_{max} . We expect this to resolve the factor of 4 problem from Appendix 2.

In writing (26) we have assumed that any n-p pair may combine. This is not true since the transition is from a free nucleon state 3P to the bound state 3S (deuteron). For two unpolarised nucleons, there are four equally likely spin states, one of which is the singlet state, plus three orientations of the triplet state. Only the triplet states can react

via the electric dipole interaction to form deuteron. Thus, on average, only $\frac{3}{4}$ of the nucleons can combine. Thus, for unpolarised nucleons the cross section is,

$$\text{(unpolarised)} \quad \sigma_{\text{cap}} = \frac{1}{4} \cdot \frac{V_{\text{max}} \omega^3 p_0^{(\text{qm})2}}{v \hbar c^3} \quad (27)$$

When evaluating the quantum dipole moment, (25), i.e. the matrix element, the bound state wavefunction will be independent of the normalisation volume but the initial free state wavefunction, since it has been chosen to normalise in volume V_{max} , will be proportional to $1/\sqrt{V_{\text{max}}}$. The normalisation volume thus cancels out from the cross section formula, (27), as it must.

A conundrum arises when the matrix element, (25), is evaluated using spherical wave states – as is natural. If a spherical wave is normalised to unity within the volume V_{max} , its wavefunction will be proportional to $k/\sqrt{r_{\text{max}}}$, where $V_{\text{max}} = (4\pi/3)r_{\text{max}}^3$. Using Equ.(27) would then result in a cross section proportional to $V_{\text{max}} / r_{\text{max}}$, and hence divergent as the normalisation volume is increased. The resolution of this paradox lies in noting that, whilst such a spherical wavefunction has an average particle density of $1/V_{\text{max}}$ (being normalised to unity in this volume), unlike the plane wave case the particle density is highly non-uniform. The decrease in the spherical wavefunction as $1/kr$ means that the particle density is much greater near the origin. Thus, it is simply not valid to evaluate the reaction rate from the cross section by multiplying by the average particle density. The reaction rate will be far bigger due to the concentration near the origin. Indeed, there is no direct means (as far as I can see) of deriving the cross section from the reaction rate for a spherical wave state, since the reaction rate derives from the cumulative effects of a spatially varying particle density. Instead, we merely translate the plane wave state formula. To do this we start by noting the algebraic identity,

$$\sqrt{V_{\text{max}}} \Psi_i(\mathbf{r} \rightarrow \infty) \rightarrow e^{i\mathbf{k}\cdot\mathbf{r}} = j_0(kr) + 3ij_1(kr)P_1(\cos\theta) - 5j_2(kr)P_2(\cos\theta) - 7ij_3(kr)P_3(\cos\theta) + \dots \quad (28)$$

Note that this implies that a single particle in a plane wave state can be regarded as the sum of an infinite number of different spherical wave particles, each contributing an infinitesimal amount. Consider firstly a spherical wave state normalised according to,

$$\tilde{\Psi}_{i,\text{Sch}}(\mathbf{r} \rightarrow \infty) \rightarrow j_1(kr)P_1(\cos\theta)/\sqrt{V_{\text{max}}} \quad (29)$$

noting that this is *not* normalised to unity in volume V_{max} . Define a matrix element using this free wavefunction,

$$\tilde{p}_0^{(\text{qm})} = Ze \int \mathbf{r} \cos\theta \cdot \Psi_{f,\text{Sch}}^* \tilde{\Psi}_{i,\text{Sch}} \cdot dV \quad (30)$$

Due to the orthogonality of the Legendre polynomials it is clear that the $L = 1$ term is the only one that survives in (25) in any case, and hence (28) gives,

$$p_0^{(\text{qm})} = 3i\tilde{p}_0^{(\text{qm})} \quad (31)$$

Thus, the use of a spherical free wave normalised according to (29) results in a cross section formula,

$$\text{(unpolarised)} \quad \sigma_{\text{cap}} = \frac{9}{4} \cdot \frac{V_{\text{max}} \omega^3 \tilde{p}_0^{(qm)2}}{v \hbar c^3} \quad (32)$$

Alternatively, using a spherical wave normalised to unity in volume V_{max} , i.e.,

$$\Psi_i^S = a j_1(kr) P_1(\cos \theta) \text{ gives } a^2 = \frac{3k^2}{2\pi r_{\text{max}}} \quad (33)$$

and defining a matrix element accordingly,

$$p_0^{(qm)S} = Ze \int r \cos \theta \cdot \Psi_{f,\text{Sch}}^* \Psi_i^S \cdot dV \quad (34)$$

it is clear that the matrix elements (30) and (34) differ only in the normalisation constants, i.e.,

$$p_0^{(qm)S} = a \sqrt{V_{\text{max}}} \tilde{p}_0^{(qm)} \quad (35)$$

Thus, substituting (35), with (33) for ‘a’, into (32) gives the cross section as,

$$\text{(unpolarised)} \quad \sigma_{\text{cap}} = \frac{9}{4} \cdot \frac{\omega^3 (p_0^{(qm)S})^2}{a^2 v \hbar c^3} = \frac{3\pi}{2} \cdot \frac{\omega^3 r_{\text{max}} (p_0^{(qm)S})^2}{v \hbar c^3 k^2} \quad (36)$$

where ω and k relate to the photon and the nucleons respectively. Thus, the photon energy is $E_\gamma = \hbar\omega$ and the sum of the initial kinetic energies of the two nucleons is E where $(\hbar k)^2 = 2M_R E \approx M_p E$, where M_R is the reduced mass (roughly half the mean of the neutron and proton masses).

The important feature of (36) is that the matrix element defined by (34) is proportional to $1/\sqrt{r_{\text{max}}}$, and hence the cross section from (36) is independent of the normalisation volume, as required. [NB: the free state wavefunction defined by (33) is proportional to $1/\sqrt{r_{\text{max}}}$, and the bound state is independent of the normalisation volume – providing it is sufficiently large].

Also note that the velocity ‘v’ appearing in (36), and indeed in (32), carries its meaning unchanged from its origin in the plane-wave formula (27), i.e., it is the relative velocity of approach of the two nucleons in an assumed plane wave state. Note that both the nucleons initially have momentum $\hbar k$, at least in the approximation that $M_n \approx M_p$. This can be seen by writing the total kinetic energy as,

$$\text{K.E.} = \frac{p_n^2}{2M_n} + \frac{p_n^2}{2M_n} \approx 2 \cdot \frac{(\hbar k)^2}{2M_p} \approx E \text{ as required.} \quad (37)$$

Thus, the relative velocity is,

$$v = |v_n| + |v_p| \approx 2 \cdot \frac{\hbar k}{M_p} \approx \frac{\hbar k}{M_R} \quad (38)$$

assuming collinear initial motion. Substituting into (36) gives,

$$\text{(unpolarised)} \quad \sigma_{\text{cap}} = \frac{3\pi}{2} \cdot r_{\text{max}} \left(p_0^{(\text{qm})S} \right)^2 \frac{M_R}{\hbar^2} \cdot \left(\frac{k_\gamma}{k} \right)^3 \quad (39)$$

We may now evaluate the electric dipole capture cross section for the n-p system by using the matrix element for spherical wave states normalised to unity in V_{max} already derived in Appendix 2, i.e.,

$$r_{\text{max}} \left(p_0^{(\text{qm})S} \right)^2 = e^2 \cdot \frac{16\beta k^4}{3(k^2 + \beta^2)^4} \quad (40)$$

(ignoring the correction term linear in the nuclear force range), where $(\hbar\beta)^2 = 2M_R B$ and B is the binding energy (of the deuteron in this case). Thus, substituting (4) into (39) we get the result for the n-p electric dipole capture cross section to be,

$$\sigma_{\text{cap}}^E = 4\pi\alpha(\hbar c)^2 \frac{\sqrt{BE}}{(M_p c^2)^2 (B + E)} \quad (41)$$

consistent with Evans, “Nuclear Physics”. [NB: Evans does not derive (41) explicitly but it can be deduced simply from his photodisintegration cross section].

3.2 The Electric Quadrupole Case (p-p capture)

The transition from the classical expression for the radiant power of an oscillating quadrupole to a quantum mechanical cross section is again made in two steps, following the development of the dipole case (Section 3.1). The first is to convert the classical power to a number of photons per second, simply by dividing by the energy per photon, i.e. $\hbar\omega$, giving, from Equ.(18),

$$w_q = \frac{\omega^5 p_q^2}{15\hbar c^5} \quad (42)$$

where w_q is the probability of a photon being emitted per second per nucleon, i.e. the reaction rate per nucleon. The second step is to convert the classical expression (16) for the quadrupole moment into its quantum equivalent, i.e.,

$$p_q^{(\text{qm})} = Ze \int r^2 P_2(\cos\theta) \cdot \Psi_f^* \Psi_i \cdot dV \quad (43)$$

where $\Psi_{i,f}$ are the initial and final wavefunctions of the nucleons and Z is the number of protons (i.e. the total charge), which is 2 in this case. Note that because we are now dealing with identical particles the range of the angular integration in (43) is over a solid angle of only 2π steradians, not 4π . [However, if the normalisation constant has been found by integrating over 4π then (43) should also be, since the factor of 2 error then cancels].

The capture cross section is related to the reaction rate by,

$$w = v\sigma_{\text{cap}} \times \text{particle density} \quad (44)$$

where v is the relative velocity of collision of the two nucleons. If the particle density is one particle per volume V_{max} , then,

$$\sigma_{\text{cap}} = \frac{w}{v(1/V_{\text{max}})} = \frac{V_{\text{max}} \omega^5 (\mathbf{p}_q^{(\text{qm})})^2}{15v\hbar c^5} \quad (45)$$

in agreement with Blatt & Weisskopf Ch.XII, Equ.(4.4), noting that the latter assume $V_{\text{max}} = 1$.

Care must be exercised in using (45) however, due to the potential trap of introducing an error of a factor of 2 in the dipole moment (and hence a factor of 4 in the cross section). This is a consequence of Equ.(13), which derives from Equ.(1). When translating (16) into its quantum equivalent, Equ.(43), we have effectively assumed that the quantum states in question also consist, like (1), of two conjugate parts, i.e.,

$$\Psi_{i,f}(\vec{r}, t) = \Psi_{i,f}(\vec{r})e^{-i\omega t} + \Psi_{i,f}^*(\vec{r})e^{i\omega t} \quad (46)$$

i.e. a combination of particles and anti-particles in field-theory speak. The wavefunction is therefore twice the real part of one of these terms, like Equ.(13). If we used a time dependent wavefunction (LHS of 46) normalised to unity, it would follow that the time independent functions on the RHS would be normalised to $1/2$. Thus, the quadrupole moment from (43) is actually only half the size that would be derived on the basis of Schrodinger states normalised to unity. Equivalently, we can agree to evaluate (43) using Schrodinger states but replace (45) by the counterpart of (19), i.e.,

$$p_{q,0}^{(\text{qm})} = Ze \int r^2 P_2(\cos\theta) \Psi_{f,\text{Sch}}^* \Psi_{i,\text{Sch}} dV \quad (47)$$

$$\text{(polarised)} \quad \sigma_{\text{cap}} = \frac{V_{\text{max}} \omega^5 (p_{q,0}^{(\text{qm})})^2}{60v\hbar c^5} \quad (48)$$

where the subscript Sch refers to Schrodinger states normalised to unity in volume V_{max} . In view of the success of this interpretation in resolving the factor of 4 problem from Appendix 2 as regards the n-p dipole cross sections we have some confidence that it is correct.

In writing (26) we have assumed that any n-p pair may combine. This is not true since the transition is from a free nucleon state 1D to the bound state 1S (the diproton). The spin states must be singlets due to the exclusion principle. For two unpolarised protons, there are four equally likely spin states, one of which is the singlet state, plus three orientations of the triplet state. The triplet states are possible only for certain spatial states. In particular, if a pair of widely spaced protons have aligned spins they will not approach close to each other in an even L state. Only the singlet state can react via the electric quadrupole interaction to form diproton. Thus, on average, only $1/4$ of the protons can combine. Thus, for unpolarised protons the cross section is,

$$\text{(unpolarised)} \quad \sigma_{\text{cap}} = \frac{V_{\text{max}} \omega^5 (\mathbf{p}_{q,0}^{(\text{qm})})^2}{240v\hbar c^5} \quad (49)$$

When evaluating the quantum dipole moment, (47), i.e. the matrix element, the bound state wavefunction will be independent of the normalisation volume but the initial free state wavefunction, since it has been chosen to normalise in volume V_{max} , will be proportional to $1/\sqrt{V_{\text{max}}}$. The normalisation volume thus cancels out from the cross section formula, (49), as it must.

The same conundrum arises when the matrix element, (49), is evaluated using spherical wave states as we encountered for the dipole case, Section 3.1. If a spherical wave is normalised to unity within the volume V_{max} , its wavefunction will be proportional to $k/\sqrt{r_{\text{max}}}$, where $V_{\text{max}} = (4\pi/3)r_{\text{max}}^3$. Using Equ.(49) would then result in a cross section proportional to $V_{\text{max}} / r_{\text{max}}$, and hence divergent as the normalisation volume is increased. The resolution of this paradox lies in noting that, whilst such a spherical wavefunction has an average particle density of $1/V_{\text{max}}$ (being normalised to unity in this volume), unlike the plane wave case the particle density is highly non-uniform. The decrease in the spherical wavefunction as $1/kr$ means that the particle density is much greater near the origin. Thus, it is simply not valid to evaluate the reaction rate from the cross section by multiplying by the average particle density. The reaction rate will be far bigger due to the concentration near the origin. Indeed, there is no direct means (as far as I can see) of deriving the cross section from the reaction rate for a spherical wave state, since the reaction rate derives from the cumulative effects of a spatially varying particle density. Instead, we merely translate the plane wave state formula. To do this we again start from the algebraic identity, (28)

$$\sqrt{V_{\text{max}}} \Psi_i(\mathbf{r} \rightarrow \infty) \rightarrow e^{i\mathbf{k}\cdot\mathbf{r}} = j_0(kr) + 3ij_1(kr)P_1(\cos\theta) - 5j_2(kr)P_2(\cos\theta) - 7ij_3(kr)P_3(\cos\theta) + \dots$$

Consider firstly a spherical wave state normalised according to,

$$\tilde{\Psi}_{i,\text{Sch}}(\mathbf{r} \rightarrow \infty) \rightarrow j_2(kr)P_2(\cos\theta) / \sqrt{V_{\text{max}}} \quad (50)$$

noting that this is *not* normalised to unity in volume V_{max} . Define a matrix element using this free wavefunction,

$$\tilde{p}_{q,0}^{(\text{qm})} = Ze \int r^2 P_2(\cos\theta) \cdot \Psi_{f,\text{Sch}} \cdot \tilde{\Psi}_{i,\text{Sch}}^* \cdot dV \quad (51)$$

Due to the orthogonality of the Legendre polynomials it is clear that the $L = 2$ term is the only one that survives in (47) in any case (noting that the final nucleon state is spherically symmetric), and hence (28) gives,

$$p_{q,0}^{(qm)} = -5\tilde{p}_{q,0}^{(qm)} \quad (52)$$

Thus, the use of a spherical free wave normalised according to (50) results in a cross section formula,

$$\text{(unpolarised)} \quad \sigma_{\text{cap}} = \frac{5}{48} \frac{V_{\text{max}} \omega^5 (\tilde{p}_{q,0}^{(qm)})^2}{v\hbar c^5} \quad (53)$$

Alternatively, using a spherical wave normalised to unity in volume V_{max} , i.e.,

$$\Psi_i^S = aj_2(kr)P_2(\cos\theta) \quad \text{gives } a^2 = \frac{5k^2}{2\pi r_{\text{max}}} \quad (54)$$

and defining a matrix element accordingly,

$$p_{q,0}^{(qm)S} = Ze \int r^2 P_2(\cos\theta) \cdot \Psi_{f,\text{Sch}}^* \Psi_i^S \cdot dV \quad (55)$$

it is clear that the matrix elements (51) and (55) differ only in the normalisation constants, i.e.,

$$p_{q,0}^{(qm)S} = a\sqrt{V_{\text{max}}} \tilde{p}_{q,0}^{(qm)} \quad (56)$$

Thus, substituting (56), with (55) for ‘a’, into (53) gives the cross section as,

$$\text{(unpolarised)} \quad \sigma_{\text{cap}} = \frac{5}{48} \frac{\omega^5 (p_{q,0}^{(qm)S})^2}{a^2 v\hbar c^5} = \frac{\pi}{24} \frac{\omega^5 r_{\text{max}} (p_{q,0}^{(qm)S})^2}{v\hbar c^5 k^2} \quad (57)$$

where ω and k relate to the photon and the nucleons respectively. Thus, the photon energy is $E_\gamma = \hbar\omega$ and the sum of the initial kinetic energies of the two protons is E where $(\hbar k)^2 = 2M_R E = M_p E$, where M_R is the reduced mass (exactly half the proton mass).

The important feature of (57) is that the matrix element defined by (55) is proportional to $1/\sqrt{r_{\text{max}}}$, and hence the cross section from (57) is independent of the normalisation volume, as required. [NB: the free state wavefunction defined by (54) is proportional to $1/\sqrt{r_{\text{max}}}$, and the bound state is independent of the normalisation volume – providing it is sufficiently large].

Also note that the velocity ‘v’ appearing in (36), and indeed in (32), carries its meaning unchanged from its origin in the plane-wave formula (27), i.e., it is the relative velocity of approach of the two protons in an assumed plane wave state. Note

that both the protons initially have momentum $\hbar k$. This can be seen by writing the total kinetic energy as,

$$\text{K.E.} = 2 \times \frac{p_p^2}{2M_p} \approx E \text{ as required.} \quad (58)$$

Thus, the relative velocity is,

$$v = 2|v_p| = 2 \cdot \frac{\hbar k}{M_p} = \frac{\hbar k}{M_R} \quad (59)$$

assuming collinear initial motion. Substituting into (57) gives,

$$\text{(unpolarised)} \quad \sigma_{\text{cap}} = \frac{\pi M_p \omega^5 r_{\text{max}} \left(p_{q,0}^{(qm)S} \right)^2}{48 \hbar^2 c^5 k^3} \quad (60)$$

To evaluate the electric quadrupole capture cross section for the p-p system we now need to calculate the matrix element for spherical wave states normalised to unity in V_{max} , i.e. Equ.(55).

4. Evaluation of Quadrupole Matrix Element Without Coulomb Potential

<<<Insert Derivation>>> *This was never typed up.* Result is...

$$r_{\text{max}} \left| \langle {}^1 S(\text{bound}) | r^2 P_2(\cos \theta) | D(\text{free}) \rangle \right|^2 = \frac{256}{5} \cdot \frac{\beta k^6}{(k^2 + \beta^2)^6} \quad (X1)$$

Substitution of (X1) into the cross section formula, (60), and noting that the quadrupole moment of Equ.(55) is Ze times the above matrix element, and further that $Z = 2$ in this case, we have,

$$\sigma_{\text{cap}}^E = \frac{64\pi\alpha}{15} \cdot \frac{M_p \omega^5 \beta k^3}{\hbar c^4 (\beta^2 + k^2)^6} = \frac{64\pi\alpha}{15} \cdot (\hbar c)^2 \cdot \frac{B^{1/2} E^{3/2}}{(M_p c^2)^3 (E + B)} \quad (X2)$$

5. Evaluation of Quadrupole Matrix Element With Coulomb Potential

In this Section we use numerical solutions of the Schrodinger equation to evaluate the matrix element $\left| \langle {}^1 S(\text{bound}) | r^2 P_2(\cos \theta) | D(\text{free}) \rangle \right|$ including the Coulomb potential.

The EXCEL based program used, NSW1d, is essentially the same as NSW1b used previously (Appendix 3) to calculate the matrix element for p-D capture, the difference being accommodation of the D-wave state. Before proceeding, we first discuss the nuclear potential to be used and carry out checks that the analytical result of Equ.(X2) is reproduced by NSW1d when the Coulomb potential is switched off.

5.1 The Nucleon-Nucleon Singlet Nuclear Potential

We shall again assume the nuclear force can be adequately represented by a square well potential. For the p-p system we are concerned with the spin singlet state, both for the bound diproton and the initial free state (1D), as discussed above. We shall take the best estimate of the singlet nuclear potential to be $V_0 = 16.1$ MeV with $a = 2.4$ fm. This is taken from Evans, who also gives an alternative: be $V_0 = 11.8$ MeV with $a = 2.8$ fm. Bound states for the dineutron or diproton do not exist with these potentials. The amount by which the potential must be increased to cause nn and pp to be stable are given below (derived using NSW1a),

a (fm)	Actual V_0	g/g_{actual}^*	Increased V_0^*	Just stable...
2.8	11.8	1.096	14.17	nn
2.4	16.1	1.088	19.06	nn
2.8	11.8	1.138	15.29	pp
2.4	16.1	1.128	20.49	pp

$$* V_0 = (g / g_{\text{actual}})^2 V_0 (\text{actual})$$

For the pp system, the Coulomb potential (\tilde{e}^2 / r) is applied only for $r > a$ (where $\tilde{e}^2 = e^2 / 4\pi\epsilon_0$ in MKSA units). The binding energies of the dineutron and diproton for a range of increasing nuclear force strengths are given below (again derived from NSW1a):-

For a = 2.4 fm, $V_0(\text{nom}) = 16.1$ MeV

g/g_{actual}^*	Increased V_0^*	B(nn), MeV	B(pp), MeV
1.15	21.292	0.3578	0.14368
1.2	23.184	0.81592	0.59178
1.25	25.156	1.43603	1.21207
1.3	27.209	2.21463	1.99683
1.4	31.556	4.2215	4.02317
1.5	36.225	6.79069	6.61384

A spot check was made using the analytic result for a 3D spherical 'square' well, for the nn system without Coulomb potential only, suggesting that NSW1a gives binding energies accurate to ~0.2%. The above results used a reduced mass of 469.46 MeV, and integration parameters within NSW1a of $r_0 = 0.001$, $\Delta r = 0.01$, $r_{\text{max}} = 30$.

We shall also wish to explore the sensitivity of our results to the assumed range, a , of the nuclear force. To this end we shall need a set of pairs of (a , V_0) values which all produce the same nn binding energy. In the case of a nuclear coupling constant increased by 30% (i.e. g/g_{actual}) we find, using the same integration parameters as above in NSW1a,

a (fm)	V₀ (MeV)	B(nn), MeV
2.4	27.209	2.21463
2.0	36.644	2.21469
1.5	59.806	2.21451
1.0	123.298	2.21456
0.5	451.3	2.21449
0.25	1728.826	2.21451

5.2 Checks on Program NSW1d

Checks were first carried out by evaluating the matrix element contributing to the np system electric dipole interaction, i.e. $\langle {}^3S | r \cos \theta | {}^3P \rangle$, confirming that the program had not been corrupted by the modifications. This check was repeated with a Coulomb potential switched on, again with results unchanged from NSW1b.

We now wish to check the incorporation of the D-wave state into NSW1d by comparing results against the analytic results, Equ.(X1) – noting that the latter applies only for no Coulomb potential and in the limit of zero range, $a \rightarrow 0$. The numerical program cannot be run at zero range ($a = 0$), and instead we have obtained results at a range of decreasing ‘a’ values. These ranges, and the corresponding potential well depths, V_0 , are given by the last table in Section 5.1. They relate to a strong nuclear coupling constant increased by 30%. Nucleon energies, E , of 0.1, 0.01 and 0.001 MeV were used in the checks. Results can be sensitive to a parameter R_{exp} used in NSW1d as the radius at which the numerical evaluation of the bound state wavefunction is replaced by the assumption of an exponential decay (with known decay constant β). Suitable values for R_{exp} are chosen simply by checking that the wavefunction looks smooth over the whole range of radii. This will introduce some error, but this appears to be small at the lower energies. Tabular results follow, obtained for a normalisation radius of $r_{\text{max}} = 57.32 \text{ fm}$ and $g/g_{\text{actual}} = 1.3$:-

a (fm)	R_{exp} (fm)	$\langle {}^1S r^2 P_2(\cos \theta) {}^1D \rangle$ no Coulomb potential		
		E = 0.1 MeV	E = 0.01 MeV	E = 0.001 MeV
2.4	13	0.4818	0.01711	5.47×10^{-4}
2.0	13	0.4782	0.01422	4.55×10^{-4}
1.5	9	0.3940	0.01337	4.28×10^{-4}
1.0	9	0.3827	0.01258	4.02×10^{-4}
0.5	4.5	0.3393	0.01185	3.79×10^{-4}
0.25	2.25	0.3263	0.01151	3.68×10^{-4}
0 (Equ.X1)	-	0.3106	0.01106	3.54×10^{-4}

Thus, the numerical results from program NSW1d do extrapolate nicely to the analytical results from Equ.(X1) as ‘a’ reduces to zero, thus effectively checking both the program and the analytical expression. In particular, note that the matrix element without Coulomb interaction reduces to zero at low energies proportional to $E^{3/2}$.

5.3 Numerical Results for $\langle {}^1S | r^2 P_2(\cos \theta) | {}^1D \rangle$ With Coulomb Potential

Results have been obtained for the best estimate range, $a = 2.4 \text{ fm}$, and for three illustrative nuclear force strengths, namely increases in g of 20%, 30% and 40%.

These correspond to pp binding energies, B, of 0.59178, 1.99683 and 4.02317 MeV respectively. The results were derived using a reduced mass of 469.136 MeV, and integration parameters of $r_0 = 0.001$, $\Delta r = 0.01$, $r_{\max} = 30$, and a normalisation radius of $r_{\max} = 57.32$ fm.

E (MeV)	$\langle {}^1 S r^2 P_2(\cos \theta) D \rangle$ with Coulomb potential		
	$g/g_{\text{actual}} = 1.2$	$g/g_{\text{actual}} = 1.3$	$g/g_{\text{actual}} = 1.4$
0.0005	4.64E-8	2.92E-9	4.33E-10
0.001	5.96E-6	3.75E-7	5.58E-8
0.002	2.11E-4	1.33E-5	1.98E-6
0.005	6.556E-3	4.15E-4	6.18E-5
0.01	0.04792	3.053E-3	4.56E-4
0.02	0.2542	0.01642	0.002471
0.05	1.5601	0.1050	0.01612
0.075	3.1197	0.2173	0.03394
0.1	4.9360	0.3560	0.05655
0.25	16.349	1.4641	0.2561
0.5	26.119	3.4007	0.6892
1	23.561	5.9544	1.5400
2	16.814	7.3175	2.6523
5	6.770	5.1790	3.1920
10	2.520	2.6843	2.403

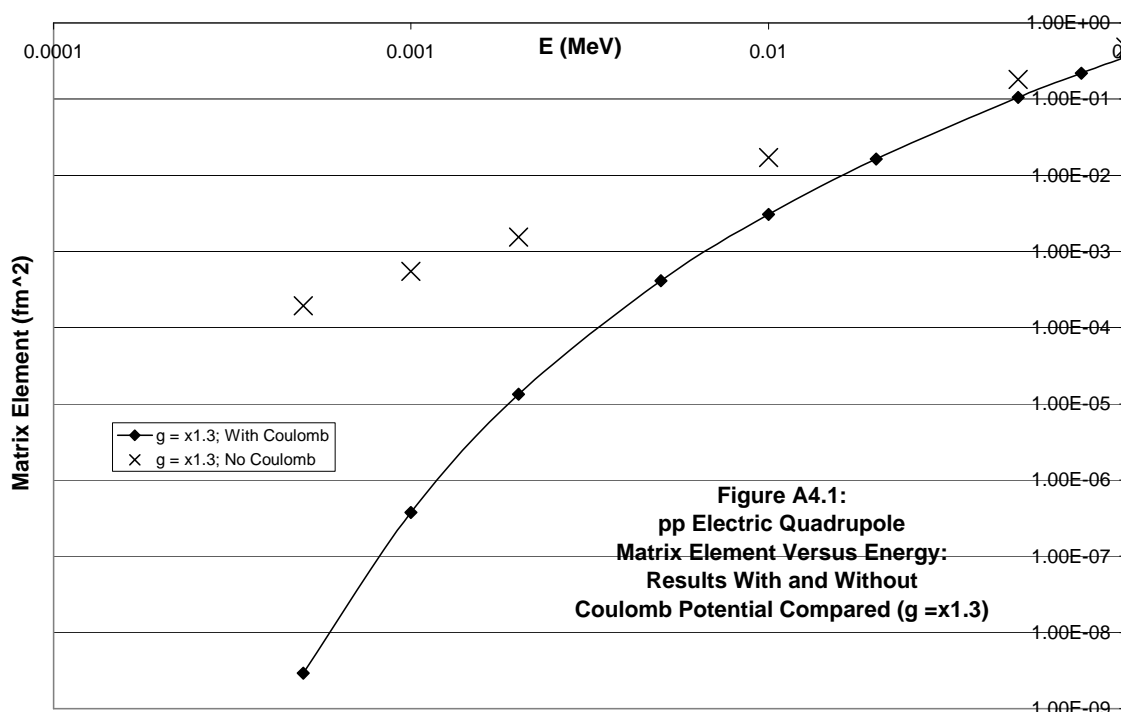


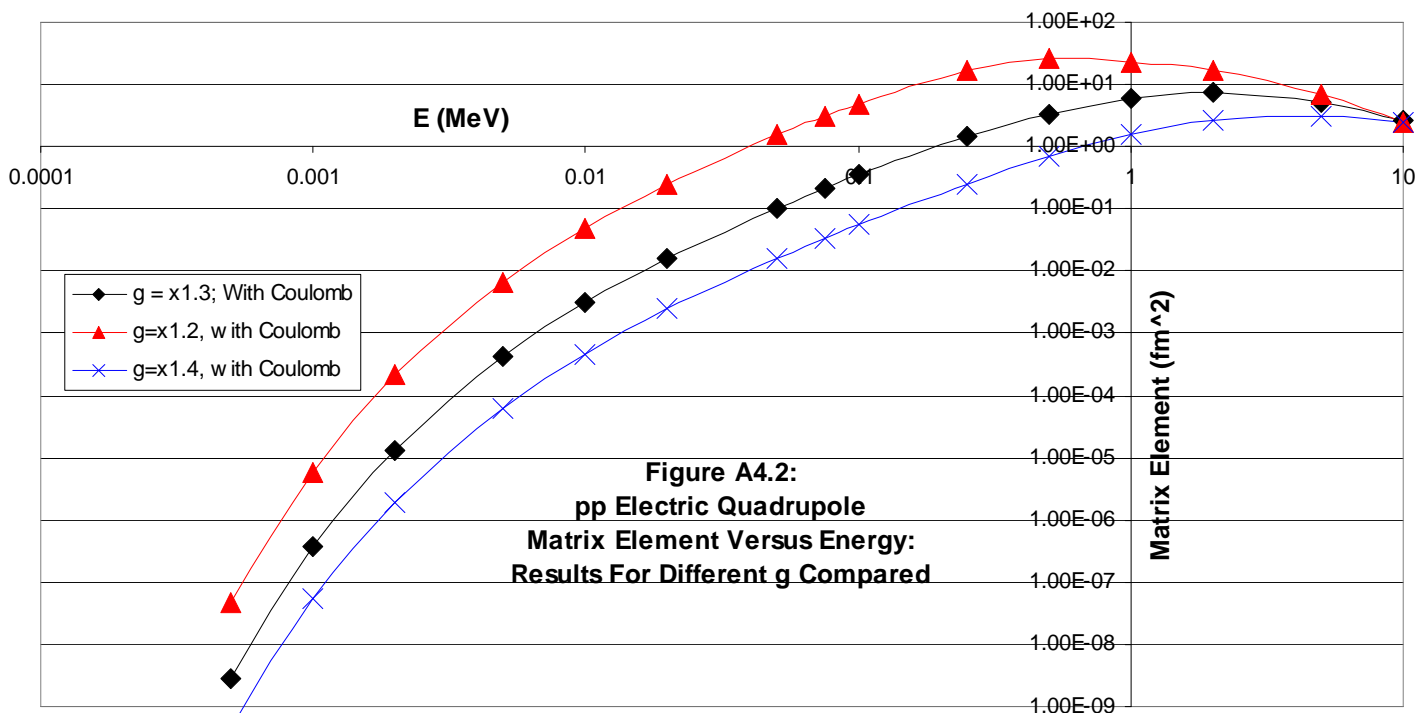
Figure A4.1 compares the low energy behaviour of the matrix element with and without the Coulomb potential. Without the Coulomb potential we have already seen that the quadrupole matrix element reduces as $E^{3/2}$. [NB: Recall from Appendices 2

and 3 that the corresponding low energy behaviour for the S-S (magnetic dipole) matrix element is $\propto E^{1/2}$, whereas the S-P electric dipole matrix element is $\propto E$. Including the Coulomb barrier causes the actual pp quadrupole matrix element to reduce towards zero much faster, namely exponentially proportional to $e^{-b/\sqrt{E}}$, where, from Appendix 3, we expect $b = \pi\alpha\sqrt{M_p}/2 = 0.351 \text{ MeV}$. The last two data points in the above graph give $b = 0.371$ (the second and third from last points giving $b = 0.385$), in reasonable agreement with expectation. Thus, the matrix element rapidly falls away to virtually zero below about 1keV, which corresponds roughly with the temperature at the centre of typical solar mass stars.

The analytic result for the matrix element without the Coulomb potential, Equ.(X1), implies that the matrix element reaches a maximum when $E = B$. This appears to hold also for the matrix element including the Coulomb interaction, as born out by the tabulated results above. Moreover, the magnitude of the matrix element at its

maximum (without the Coulomb potential) is $M.E. = \sqrt{\frac{4}{5\beta^5 r_{\max}}}$, and this expression

is in good order of magnitude agreement with the greatest values in the above Table (i.e. 24.1, 5.3 and 2.2 for the three g values).



6. Evaluation of the pp Capture Cross Section

We may write the cross section for unpolarised pp capture in a number of different but equivalent ways. Following (60) we have,

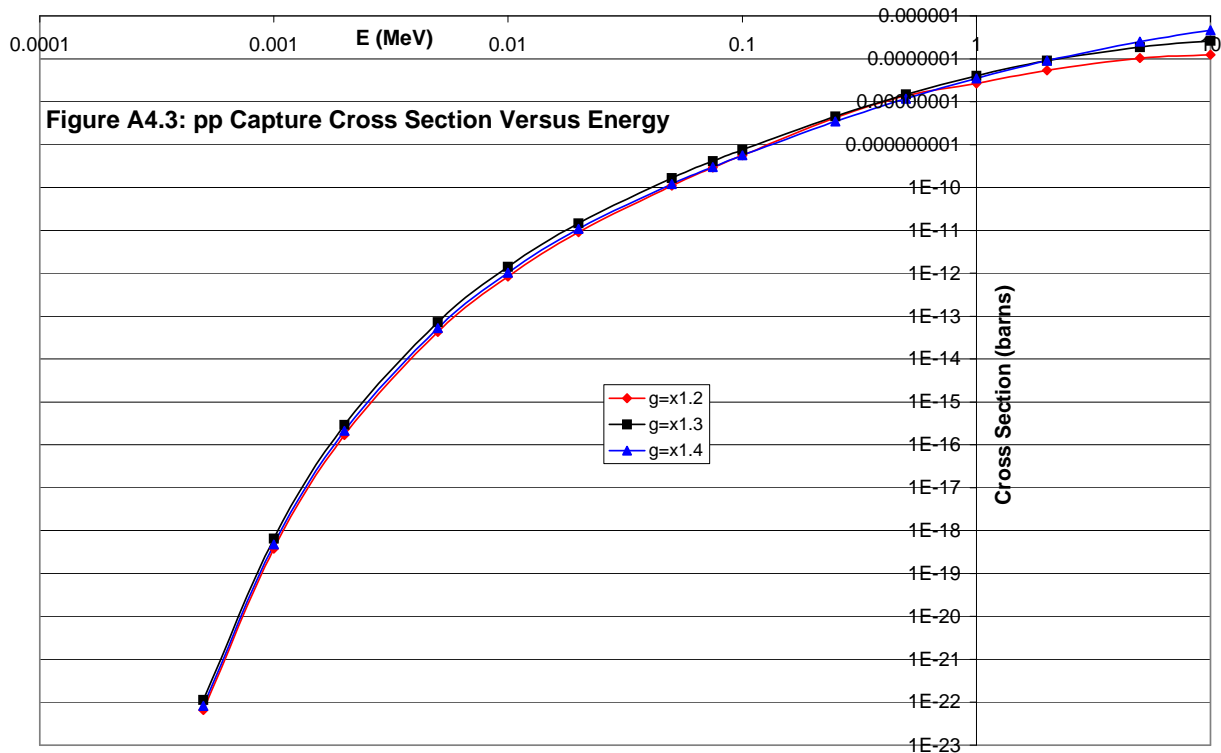
$$\begin{aligned}\sigma_{\text{cap}} &= \frac{\pi}{48} \cdot \frac{M_p \omega^5 r_{\text{max}} \left(p_{q,0}^{(\text{qm})S} \right)^2}{\hbar^2 c^5 k^3} = \frac{\pi \alpha}{6} \cdot \frac{\omega^5 r_{\text{max}} (\text{M.E.})^2}{vc^4 k^2} = \frac{\pi \alpha}{12} \cdot \frac{M_p \omega^5 r_{\text{max}} (\text{M.E.})^2}{\hbar c^4 k^3} \\ &= \frac{\pi \alpha}{12} \cdot \frac{(E+B)^5 r_{\text{max}} (\text{M.E.})^2}{(\hbar c)^3 (M_p c^2)^{1/2} E^{3/2}}\end{aligned}\quad (\text{X3})$$

where,

$$\text{M.E.} = \int r^2 P_2(\cos \theta) \cdot \Psi_{f,\text{Sch}} [{}^1S] \cdot \Psi_i^S [{}^1D] \cdot dV \quad \text{and} \quad p_{q,0}^{(\text{qm})S} = Ze(\text{M.E.}) \quad (\text{X4})$$

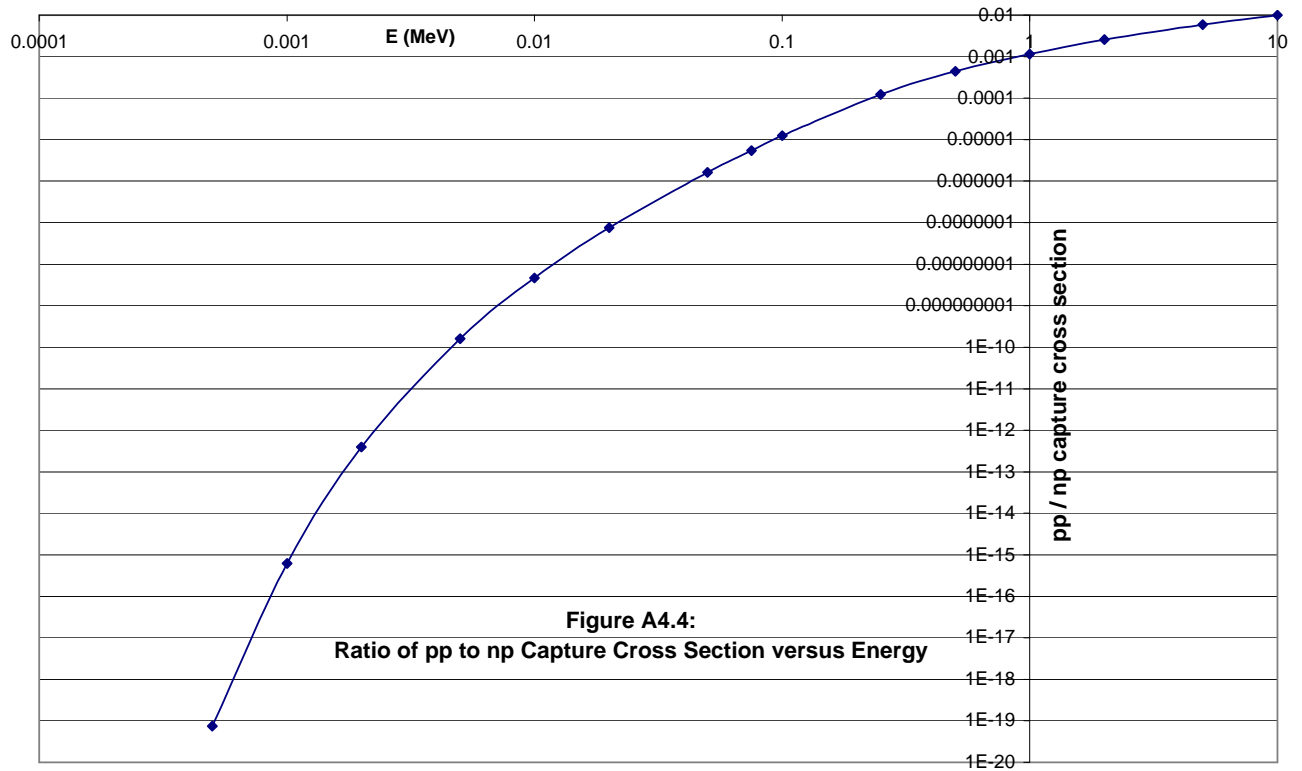
and $Z = 2$ for the pp system, and B is the binding energy of the diproton. In deriving the last form of (X3) we have used the approximation that the photon carries away all the excess energy (i.e. the kinetic energy of the diproton is negligible). Recall that E is the CoM system kinetic energy of the two incident protons (i.e. twice the energy of one proton in the CoM system). Using (X3) the pp capture cross section is tabulated below for our three different g values:-

E (MeV)	cross-sections, barns		
	$g = x1.2$	$g = x1.3$	$g = x1.4$
0.0005	6.5E-23	1.12E-22	8.2E-23
0.001	3.81E-19	6.56E-19	4.82E-19
0.002	1.7E-16	2.92E-16	2.15E-16
0.005	4.27E-14	7.26E-14	5.31E-14
0.01	8.4E-13	1.41E-12	1.03E-12
0.02	9.07E-12	1.47E-11	1.08E-11
0.05	1.1E-10	1.64E-10	1.21E-10
0.075	2.89E-10	4.07E-10	3E-10
0.1	5.66E-10	7.53E-10	5.59E-10
0.25	4.19E-09	4.55E-09	3.46E-09
0.5	1.39E-08	1.47E-08	1.18E-08
1	2.63E-08	3.97E-08	3.52E-08
2	5.42E-08	8.95E-08	9.14E-08
5	1.04E-07	1.86E-07	2.53E-07
10	1.24E-07	2.62E-07	4.59E-07



Curiously, we see that, for energies of 1 MeV and below, the cross section appears to reach a maximum for an increase in the strong nuclear force of $\sim 30\%$ (in g). It is not clear why this should be so. This behaviour is not evident from the zero-range, non-Coulomb analytic result of Equ.(X2), and so is surmised to be a result of the non-zero range and/or the Coulomb interaction.

Finally, as expected, the pp capture cross section is far smaller than the np capture cross section as shown below,



Thus, at energies typical during big bang nucleosynthesis (0.05 – 0.1 MeV), the pp capture cross section is 5 or 6 orders of magnitude smaller than the np capture cross section. At energies typical of the centre of solar mass stars (~0.0012 MeV), the pp capture cross section is 14 or 15 orders of magnitude smaller than the np capture cross section. The implications of this are addressed in Chapter 9C of the “Cosmic Coincidences” part of this web site.

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