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NUMERICAL EXAMPLES FOR HYDROGEN ISOTOPE FUSION REACTIVITY UNDER THE MAXWELL-BOLTZMANN ASSUMPTION

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Abstract

Examples with numerical values reflecting hydrogen isotope reactions are given. These exercises are intended as an aid, or companion paper to **Calculation of the First Moment of Energy Using D-T Reactivity Formalisms Under the Maxwell-Boltzmann Distribution—Parts I and II**, [1, 2] by the same authors.

Example 1. Mass Energy Equivalents for Calculating Speeds, and Distinguishing Between $(v^2)_{av}$ and $(v_{av})^2$

We will be using the energy-mass equivalent for hydrogen-isotope nuclei, 931.5 MeV proton, 1875.6 MeV deuteron, and 2808.9 MeV triton, to find the average root-mean-square (*rms*) speed at 273 degrees Kelvin (=0.0235 eV=2.35e-8 MeV). We will use for the value of the speed of light, c , 3.00e08 meters per second. We will use the product of Boltzmann's constant, k_B (k), and T^o in Kelvin to express temperature in units of energy.

$$(v^2)_{av} = \left(\frac{3k_B T^o}{mc^2} \right) c^2 = \frac{0.0705 \text{ eV}}{931.5 \text{ MeV}} \cdot 9.00 \text{e}16 \left(\frac{m}{\text{sec}} \right)^2 = 6.81 \text{e}6 \left(\frac{m}{\text{sec}} \right)^2 \quad (\text{C1})$$

$$v_{\text{root-mean-square}} = \sqrt{(v^2)_{av}} = 2.61 \text{ km/sec} \quad (\text{C2})$$

Care must be taken to ensure the difference between $(v^2)_{av}$ and $(v_{av})^2$. The value $(v^2)_{av}$ comes from consideration of the kinetic energy, a quantity involving the square of the velocity, and is developed using (C7) below.

The $(v_{av})^2$ is the average speed quantity squared. The average speed, v_{av} , comes from the expected value (first moment) of the Maxwell-Boltzmann (MB) velocity distribution, which is:

$$v_{av} = \sqrt{\frac{8k_B T^o}{\pi m}}$$
$$(v_{av})^2 = \frac{8k_B T^o}{\pi m}.$$

Using the energy-mass equivalent for the hydrogen nucleus to be the same as that for hydrogen atom, 931.5 MeV, find the average speed at 273 degrees Kelvin (0.0235 eV=2.35e-8 MeV). The value for the speed of light, c , is 3.00e08 meters per second.

$$(v^2)_{av} = \left(\frac{8k_B T^0}{\pi m c^2} \right) c^2 = \frac{0.188 \text{ eV}}{3.14159 \cdot 931.5 \text{ MeV}} \cdot 9.00 \text{e}16 \left(\frac{m}{\text{sec}} \right)^2 = 5.78 \text{e}6 \left(\frac{m}{\text{sec}} \right)^2$$

$$v_{av} = 2.40 \text{ km/sec.}$$

Example 2. Equations for pressure, volume, density, temperature under the assumption of the MB distribution

Equations for pressure, volume, density, temperature under the assumption of the MB distribution can be used to derive the expressions in (C1) and (C2). Equation (C1) results from noting that pressure P (ideal gas law) is

$$P = \frac{1}{3} \rho (v^2)_{av} \quad (\text{C3})$$

$$\rho = Nm/V \quad (\text{C4})$$

where N is the number of atoms (molecules) mass m , in volume V , and ρ is the density defined in (C4).

One may ask from where the fraction 1/3 in the gas law in (C3) comes. Pressure can be derived from consideration of the impact force of a single particle, perfectly elastic (conserving kinetic energy) during the collision with a container wall. The rate of change of one component of a momentum vector normal to a container wall is the force considered. Two momentum components, parallel to the face of a containing wall are unaltered, they do not change; only the component of momentum normal to the wall is altered: it is reversed. Note that the magnitude of the momentum vector is proportional to the magnitude of the velocity vector. Averaging of the tri-component, or tri-directional squared speed gives:

$$(v^2)_{av} = (v_x^2)_{av} + (v_y^2)_{av} + (v_z^2)_{av}$$

where $(v_x^2)_{av} = (v_y^2)_{av} = (v_z^2)_{av} = 1/3 (v^2)_{av}$. This is an assumption with no external forces acting. The fraction of 1/3 is evident in the gas law in (C3).

This has been a simplified explanation. It assumes for the pressure of N particles, each particle has the same speed and behaves the same way. N gas particles will be moving in all directions with equal likelihood $v_x^2 = v_y^2 = v_z^2$ with the result that $v_x^2 = 1/3 v^2$. In the paper (by the authors) *Calculation of the First Moment of Energy Using D-T Reactivity Formalisms Under the Maxwell-Boltzmann Distribution—Part I*, [1], v is defined:

$$v = \sqrt{v_x^2 + v_y^2 + v_z^2}.$$

The energy-dependent MB distribution is used below in (C12), and produces the resulting equation in (C3). A general result shown in classical statistical mechanics is the “equipartition theorem”.¹ It states that the mean value of each *independent, quadratic* term in the energy is equal to $\frac{1}{2} kT$.² There are three independent velocity terms considered here. The equipartition theorem is valid only in classical statistical mechanics. Real-gas components interact, and are treated quantum mechanically.³

Returning to the ideal gas law discussion, and using the density in (C4), the expression in (C3) becomes:

$$PV = \frac{1}{3} Nm(v^2)_{av} . \quad (C5)$$

The following is also a version of the ideal gas law, using Boltzmann’s constant and T^o in Kelvin:

$$PV = Nk_B T^o. \quad (C6)$$

The translational kinetic energy (*K.E.*) of an object mass m is

$$K.E. = \frac{1}{2} mv^2.$$

Taking the averages of both sides produces the necessary expression defining $(v^2)_{av}$

$$(K.E.)_{av} = \frac{1}{2} m(v^2)_{av} . \quad (C7)$$

Combining PV expressions in (C5) and (C6) gives:

$$Nk_B T^o = \frac{1}{3} Nm(v^2)_{av}, \quad (C8)$$

¹ See for example, F. Reif’s book [3].

² The equipartition theorem is a generalization, not without controversy. E. Hecht [4] states: “The idea [equipartition hypothesis] was proposed by J.J. Waterston when considering a mix of two different gases held at the same temperature in a chamber. He suggested that each gas would have the same average translational KE [kinetic energy].” An implication is that relatively massive particles in a mixture of gases travel slower than relatively lighter particles.

³ Real-gas has energy at lowest, “absolute zero” temperature, known as “zero-point” energy. This is not in accordance with the equations offered herein. In the correct quantum mechanical description, the spacing between possible discrete energy levels can be large compared to the absolute energy. See for example, F. Reif’s book [3]. At higher temperatures, presently considered, the spacing between possible quantum energy levels decreases. The fact that there exist discrete energy levels is not important at higher temperature considered here, leading to the equations given herein. Note that this implies that temperature and energy are not strictly equivalent. Temperature is a fundamental quantity, not expressible in terms of other fundamental dimensions: “... like length, time and mass, [temperature] is not expressible in terms of other quantities,” E. Hecht [4, p. 504].

and replacing $m(v^2)_{av}$ using (C7) gives an expression useful later on:

$$Nk_B T^o = \frac{2}{3} N(K.E.)_{av}. \quad (C9)$$

Returning to (C8) and solving for $(v^2)_{av}$, gives the expression used in (C1):

$$(v^2)_{av} = \frac{3k_B T^o}{m}. \quad (C10)$$

The full expression in (C1) uses the mass-energy equivalence, mc^2 , to match the energy units of $k_B T^o$ (e.g., eV) by dividing both sides by c^2 :

$$\frac{(v^2)_{av}}{c^2} = \left(\frac{3k_B T^o}{mc^2} \right).$$

The root-mean-square speed is found by taking the square root of $(v^2)_{av}$ in (C10):

$$v_{root-mean-square} = v_{rms} = \sqrt{(v^2)_{av}} = \sqrt{\frac{3k_B T^o}{m}}. \quad (C11)$$

Equation (C1) can also be found by using the MB energy distribution,

$$g(E) = 2 \left(\frac{E}{\pi} \right)^{1/2} \left(\frac{1}{k_B T^o} \right)^{3/2} \exp \left(-\frac{E}{k_B T^o} \right),$$

whose average (mean) is $3k_B T^o/2$. That is to say, from $g(E)$, shown to be a gamma distribution [1, p. 3], the mean E is E_{av} :

$$E_{av} = \frac{3}{2} k_B T^o. \quad (C12)$$

Again the average translational kinetic energy of an object mass m , reproduces (C7):

$$E_{av} = av \left[\frac{1}{2} m v^2 \right] = \frac{1}{2} m (v^2)_{av}.$$

As expected, (C7) with (C12) produces (C1):

$$(v^2)_{av} = \left(\frac{3k_B T^o}{m} \right),$$

$$\frac{(v^2)_{av}}{c^2} = \left(\frac{3k_B T^o}{mc^2} \right).$$

Example 3. Velocity of Hydrogen Isotopes as a Percentage of the Speed of Light

It is interesting to find speeds using a standard scale because we use the mass-energy equivalent for calculating speed. A standard of speed is the speed of light in vacuum. This also gives us a basis to consider nuclear reaction rates in addition to D-T fusion. G.R. Caughlan and W.A. Fowler [5] provide analytic expressions for the reaction rates of astrophysically important reactions of low-mass nuclei. The formulation in [5] is given for many reactions of interest in astrophysics. The reaction rate (RR) is:

$$RR = N_A f(T9)$$

where N_A is Avogadro's number, temperature $T9$ is in units of a billion degrees Kelvin, and f is their reactivity formulation in terms of $T9$. Interesting nuclear-reaction rates occur in the temperature range 10^6 - 10^{10} Kelvin, or equivalently about $10^{-1} \text{ keV} \leq T9 (\cong T/10^9 \text{ Kelvin}) \leq 10 \text{ MeV}$. The rates are expressed as $N_A \cdot \langle \sigma v \rangle$; Avogadro's number times the average of the cross-section σ , times the relative velocity, v , of the reactants taken over the Maxwell-Boltzmann distribution as a function of temperature. Interesting astrophysical nuclear reactions take place over a large dynamic range, about four or five decades in energy, beginning at about 10^2 eV . When atomic reactions are included, interesting reactions range over at least $10^{-7} T9 \leq T9 (\cong T/10^9 \text{ Kelvin}) \leq 10^{-3} T9$, ($273 \text{ degrees Kelvin} = 0.0235 \text{ eV}$).

Take one billion degrees Kelvin, $T9$ to be the equivalent energy of 86 keV. For the hydrogen nucleus H, using (C10), a measure of speed compared to light at 86 keV is:

$$\begin{aligned} \frac{v_{av-H}^2}{c^2} &= \left(\frac{3T}{mc^2} \right) = \frac{3 \cdot 86 \text{ keV}}{931.5 \text{ MeV}} \\ \frac{v_{av-H}}{c} &= 0.0166 = 1.666\% . \end{aligned} \quad (C13)$$

For hydrogen isotopes deuterium (subscript D) and tritium (subscript T) the relationship is:

$$\frac{v_{av-H}}{c} = \sqrt{2} \frac{v_{av-D}}{c} = \sqrt{3} \frac{v_{av-T}}{c}. \quad (C14)$$

The square roots of 2 and 3 in (C14) are due to the deuterium mass, roughly, twice that of hydrogen and tritium's mass being three times, respectively. **Example 4** below demonstrates this scaling for all the central measures of speed. The root-mean-square of velocity at $T9$, 86 keV, for deuterium is 1.2% c , and for tritium is 0.96% c . At room temperature, these velocities are of the order of 10^{-5} the speed of light.

Example 4. Comparing Central Measures of Speed from the MB Distribution

The speeds of particles of isotopes go as the inverse square root of the mass, as shown in **Example 2**. The MB distribution has several statistics or measures that represent the central characteristic of that distribution. The mean, or average, is the most commonly used;

however, others include the mode (aka the most probable value), the median (the middle value), and the root-mean-square from **Example 1**.

What is the difference between the most probable speed v_p ; the mean speed, v_{av} or $\langle v \rangle$; and the root-mean-square speed, v_{rms} , given that the appropriate distribution assumption is the MB distribution?

The MB distribution is also recognized as the chi pdf with 3 degrees of freedom, and as such is not a symmetric distribution, which results in these central measures being non-identical. Wikipedia® [6] gives the formulae for these measures and some of the following development:

$$v_p = \sqrt{\frac{2kT^\circ}{m}} \quad v_{av} = \langle v \rangle = \sqrt{\frac{8kT^\circ}{\pi m}} \quad v_{rms} = \sqrt{(v^2)_{av}} = \sqrt{\frac{3kT^\circ}{m}}$$

$$\frac{v_p}{c} = \sqrt{2} \sqrt{\frac{kT^\circ}{mc^2}} = 1.41 \sqrt{\frac{kT^\circ}{mc^2}}, \quad (C15)$$

$$\frac{v_{av}}{c} = \frac{\langle v \rangle}{c} = \sqrt{\frac{8kT^\circ}{\pi \cdot mc^2}} = 1.60 \sqrt{\frac{kT^\circ}{mc^2}}, \quad (C16)$$

$$\frac{v_{rms}}{c} = \frac{\sqrt{v^2_{av}}}{c} = \sqrt{\frac{3kT^\circ}{mc^2}} = 1.73 \sqrt{\frac{kT^\circ}{mc^2}}. \quad (C17)$$

Notice the relative relationship among the central measures in (C15) - (C17) is:

$$v_p < v_{av} < v_{rms}.$$

The result for the speed of sound, v_s , in a gas is:

$$v_s = \sqrt{\frac{\gamma}{3}} v_{rms},$$

where γ is the adiabatic index,

$$\gamma = 1 + \frac{2}{d},$$

and d is the number of degrees of freedom, 3, in this application. The answer becomes:

$$v_s = \sqrt{\frac{\gamma}{3}} v_{rms} = .745 v_{rms} = 1.29 \sqrt{\frac{kT^\circ}{mc^2}}. \quad (C18)$$

According to (C18), the speed of sound, v_s , is the smallest in comparison to the central measures:

$$v_s < v_p < v_{av} < v_{rms}.$$

Example 4. Average Relative Velocity and Comparison of MB Distributions

Wikipedia® [6] also gives average relative velocity:

$$v_{rel} = \langle |\vec{v}_1 - \vec{v}_2| \rangle = \int d^3_{v_1} d^3_{v_2} |\vec{v}_1 - \vec{v}_2| f(\vec{v}_1) f(\vec{v}_2),$$

$$v_{rel} = \frac{4}{\sqrt{\pi}} \sqrt{\frac{kT^\circ}{m}} = \sqrt{2} \langle v \rangle, \quad (C19)$$

where the three-dimensional MB velocity distribution is:

$$g(\vec{v}) \equiv \left(\frac{m}{2\pi kT^\circ} \right)^{3/2} \exp \left(\frac{-m\vec{v}^2}{2kT^\circ} \right). \quad (C20)$$

The *rms* speed derived from the average (mean) energy differs from the average speed computed by deriving the first moment $\langle v \rangle$. The comparisons of central measures of speed in **Example 3** indicate that the ratio the *rms* speed to $\langle v \rangle$ is:

$$\frac{v_{rms}}{\langle v \rangle} = \frac{\sqrt{\frac{3kT^\circ}{m}}}{\sqrt{\frac{8kT^\circ}{\pi m}}} = \sqrt{\frac{3\pi}{8}} = 1.085 = \frac{\sqrt{2}v_{rms}}{v_{rel}}. \quad (C21)$$

Inserting (C16) into (C21):

$$\frac{v_{rel}}{c} = \sqrt{2} \cdot 1.60 \sqrt{\frac{kT^\circ}{mc^2}} = \frac{\sqrt{2}v_{rms}}{c} = 2.26 \sqrt{\frac{kT^\circ}{mc^2}}. \quad (C22)$$

The comparison to the central measures of speed is:

$$v_s < v_p < v_{av} < v_{rms} < v_{rel}.$$

The expression for v_{rms} in (C11) holds whether it is derived from the mean energy from the MB energy distribution, $g(E)$, or from the mean speed from the MB velocity distribution, $g(v)$, given below in (C24). This is because $g(E)$ is derived from $g(v)$ using the transformation $E = \left(\frac{1}{2}\right)mv^2$. The transformation of the MB velocity distribution to an MB energy distribution required an additional factor of speed, v , from the Jacobian of the transformation [1, p. 37]. The formulation in energy space amounts to averaging the squares of velocity. The average energy corresponds to the energy at the mean of the square of speed, proportional to $\langle v^2 \rangle$.

The integral for fusion reactivity, f , given the MB velocity distribution is:

$$f = \langle \sigma v \rangle = \int_0^\infty \sigma(v) v g(v) dv = \int_0^\infty \sigma(v) v 4\pi \left(\frac{m}{2\pi kT^\circ} \right)^{1.5} v^2 \exp \left(\frac{-mv^2}{2kT^\circ} \right) dv. \quad (C23)$$

In this integral, the speed is cubed, v^3 . If one ignores the dependence of the cross-section, σ , on speed, then f is expressed as the average over the MB speed distribution, $g(v)$, with constant cross-section, σ ,

$$f = \sigma \langle v \rangle = \sigma \int_0^\infty v g(v) dv = \sigma \int_0^\infty 4\pi \left(\frac{m}{2\pi k T^\circ} \right)^{1.5} v^3 \exp\left(\frac{-mv^2}{2k T^\circ} \right) dv \quad (\text{C24})$$

where the MB velocity probability density function (pdf) is:

$$g(v)dv = 4\pi \left(\frac{m}{2\pi k T^\circ} \right)^{1.5} v^2 \exp\left(\frac{-mv^2}{2k T^\circ} \right) dv \quad . \quad (\text{C25})$$

Example 5. The Mean-Free-Path Under the MB Approximation

As a comparison, the mean-free-path, λ , according the kinetic theory, does not depend directly on mass (see for example John F. O'Halon's book [7]):

$$\lambda = \frac{1}{\sqrt{2}\pi d_o^2 n} \quad , \quad (\text{C26})$$

where d_o is the molecular diameter and n the gas density. The mean-free-path is pressure dependent. *The mean-free path does not, in these approximations, depend on particle mass.*

Example 6. Center-of-Mass and Lab Frame Energies

The transformation from nuclear physics lab frame to center-of-mass (cm) frame is as follows. In the nuclear physics experiment, if particle A of mass m_A , strikes stationary target particle B of mass m_B , then energy E_A in the lab is:

$$E_A = \frac{E_{cm}(m_A+m_B)}{m_B} \quad , \quad (\text{C27})$$

where E_{cm} is the center-of-mass energy. Center-of-mass energy is equation (3) in [1] and is:

$$E_{cm} = \left(\frac{1}{2} \right) \left(\frac{m_A m_B}{m_A + m_B} \right) v^2 \quad .$$

Example 7. Tunneling Function

The Coulomb repulsion between two nuclei in a fusion reaction is generally greater than the energy available in the center-of-mass, for typical applications. Fusion reactions are

possible because of the tunneling effect, also known as the tunneling function. The cross-section for fusion is proportional ($\sim$) to the tunneling function:

$$\sigma \sim \exp(-\sqrt{E_C/E_{cm}}), \quad (\text{C28})$$

where E_{cm} is the center-of-mass energy and E_C is the energy characterizing the magnitude of the Coulomb barrier, [1, p. 17].

Compare the cross-section in (C28) to equation (53) in [1]:

$$\sigma(E) = \frac{S(E)}{E} \exp(-\sqrt{E_C/E}),$$

where $S(E)$ is the astrophysical S-factor in **Example 8**. This factorization is also equation (4) in Bosch & Hale [8, p. 612], with $B_G = \sqrt{E_C} = 34.3827$ for $D(t,n)_4^4\text{He}$.⁴

The tunneling function in (C28) is plotted in Figure 1.

Figure 1. Tunneling function for D-T. The scale for the x-axis is in keV.

By inspection of Figure 1, note that the tunneling value appears to become appreciable starting above ~ 30 keV.

⁴Bosch & Hale state [8, p. 613]: “Strictly speaking, the factorization of the cross-section given by Eq. (4) holds only at energies for which the nuclear reaction is dominated by incident S-wave transitions. Furthermore, the Gamov penetrability form used [tunneling function] is appropriate only as long as the energy of the particles is much smaller than the barrier potential [...]. (The Coulomb barrier is ≈ 210 keV for the d+d reaction, ≈ 280 keV for d+t and ≈ 580 keV for d+ ^3He , calculated using the channel radii from the R-matrix calculations.) [...] We regard the factorization simply as a mathematical normalization [...]”

Example 8. Tunneling Function and the Geometric Factor in the Definition of $S(E)$

In addition to the Coulomb repulsion between two nuclei, modeled using the tunneling function in **Example 7**, quantum mechanics includes a geometric factor proportional to the inverse of E_{cm} and also proportional to the de Broglie wavelength, λ :

$$\text{Geometric Factor} \sim \frac{1}{E_{cm}} \sim \pi \lambda^2.$$

The product of the tunneling function and the geometric factor carries the energy dependence for non-resonant reactions. The proportionality of these factors with cross-section is the astrophysical S-factor, $S(E)$. The tunneling function cross-section in **Example 7**, (C28), can be specified using the center-of-mass energy and the astrophysical S-factor as:

$$\sigma = \frac{S(E_{cm})}{E_{cm}} \exp(-\sqrt{E_c/E_{cm}}) \quad . \quad (\text{C29})$$

The product of the geometric function with the tunneling function is plotted in Figure 2.

Figure 2. Product function of tunneling with the geometrical factor for D-T. The scale for the x-axis is in keV.

By inspection of Figure 2, it appears that this product function begins to become appreciable at about 20 keV, and the shape is changed in comparison to Figure 1.

Example 9. Three Dominant Energy-Dependent Factors

Fusion reactivity involves the Coulomb repulsion between two nuclei, the energy dependence of the reactants due to the temperature, and the astrophysical S-factor or cross-section. These three are represented by:

1. penetrability (which is the tunneling function, **Exercise 7**),
2. the MB energy distribution (which is temperature dependent [1, p. 3]), and,
3. the astrophysical S-factor (which relates to the intrinsic nuclear physics of the reaction cross-section).

The MB energy distribution was developed in [1] from the MB velocity distribution and was given as equation (7):

$$g(E) = 2 \left(\frac{E}{\pi} \right)^{1/2} \left(\frac{1}{T} \right)^{3/2} \exp \left(-\frac{E}{T} \right).$$

The energy dependence of the reactants due to the temperature, is captured by $g(E)$.

The geometric factor, Figure 2 in **Example 8**, and tunneling function, Figure 1 in **Example 7**, represent the Coulomb repulsion. These are two dominant factors determining the cross-section, as shown in (C28) and (C29). The latter involves the astrophysical S-factor as a function of energy.

Equation (C29) gives the cross-section as a function of energy as the product of:

$$\sigma = \frac{S(E_{cm})}{E_{cm}} \exp(-\sqrt{E_c/E_{cm}})$$

cross-section = S-factor · geometric factor · tunneling function.

As concluded in [1] and [2], determining the D-T cross-section as a function of energy is important for properly formulating reactivity. The physics represented in (C29) is one of the reasons why cross-section should not be constant over a range of energy values.

The product of the tunneling function and the MB energy distribution carries the energy dependence for non-resonant reactions. In the case of DT fusion, the astrophysical S-factor also carries a strong energy dependence, which varies by a factor of 25 from 1 keV to 200 keV. This reactivity f is described in (C30).

$$\begin{aligned} f &= \int_0^\infty \sigma(v) \cdot v \cdot g(v) dv = \int_0^\infty \sigma(E) \sqrt{\frac{2E_{cm}}{m}} \cdot g(E) dE \\ f &= \int_0^\infty \sqrt{\frac{2}{E_{cm}m}} \cdot g(E) \cdot \exp \left(-\sqrt{\frac{E_c}{E_{cm}}} \right) \cdot S(E) dE, \\ f &= \left(\frac{1}{\pi m} \right)^{1/2} (2)^{3/2} \int_0^\infty \left(\frac{1}{T} \right)^{3/2} \exp \left(-\frac{E_{cm}}{T} \right) \cdot \exp \left(-\sqrt{\frac{E_c}{E_{cm}}} \right) \cdot S(E) dE, \end{aligned} \quad (C30)$$

where E_{cm} is the center-of-mass energy. The first line in (C30) is the first line of equation (9) in [1]. The second line in (C30) substitutes the expression in (C29) for $\sigma(E)$. The third

line substitutes the MB energy distribution as $g(E)$. Notice that the geometric factor originally was included for $\sigma(E)$; however, it was combined with the existing $\sqrt{E_{cm}}$ term. The integral contains the dominating factors for the three listed factors above:

1. $\exp\left(-\sqrt{\frac{E_c}{E_{cm}}}\right)$ tunneling function (penetrability)
2. $\exp\left(-\frac{E_{cm}}{T}\right)$ MB energy distribution, and
3. $S(E)$ S-factor

These are compared in the following figures:

- The D-T astrophysical $S(E)$ factor from A. J. Peres [9] is shown in Figure 3.
- The D-T astrophysical $S(E)$ factor from Bosch and Hale [8] is shown in Figure 4.
- Using the Peres $S(E)$ [9] in Figure 3 and applying equation (C29), the D-T fusion cross-section is in Figure 5.
- The D-T penetrability and MB energy function for $T=10$ keV is shown in Figure 6.

Figure 3. Astrophysical $S(E)$ factor for D-T from Peres [9]. The scale for the x-axis is in keV. The scale for the y-axis is keV-millibarns.

The S -functions in Figures 3 and 4 vary by a factor of about 25 over the energy range shown. While not visually obvious from Figures 3 and 4, the Bosch and Hale $S(E)$ values are always larger than those from Peres. For example, the Bosch and Hale maximum $S(E)$ value is $2.728\text{e}07$ and Peres' is $2.645\text{e}07$, both occurring about 50 keV as shown in Figures 3 and 4. A plot of their difference, $\text{B\&H } S(E) - S^*(E)$, is shown in Figure 7.

Figure 4. Astrophysical $S(E)$ factor for D-T from Bosch and Hale [8]. The scale for the x-axis is in keV. The scale for the y-axis is keV-millibarns.

Figure 5. Fusion cross-section in center-of-mass frame for D-T from A. J. Peres [9]. The scale for the x-axis is in keV. The scale for the y-axis is millibarns.

Figure 6. Two functions are shown that determine much of the energy dependence of nuclear fusion: the plasma temperature (10 keV MB energy distribution is plotted, red) and the tunneling function, which depends on the reactants. D-T tunneling function is plotted in blue. The scale for the x-axis is in keV.

Figure 7. The difference between B&H $S(E)$ [8] and Peres $S^*(E)$ [9] over the energy range below 200 keV varies nonlinearly with E . The scale for the y-axis is keV-millibarns. The x-axis has units of keV. This relative difference amounts to about 19% of the value of $S^*(E)$ at low energies and 3% on-resonance.⁵

⁵ This difference is acknowledged briefly in the caption of Figure 3 of [8, p. 615]: “S-values from the measurements of Katsurov [10] in 1962 (also published by Kobzev *et al.* [11] in 1966) and from Conner *et al.* [12] in 1952. [...] These data agree very well with the parametrization of Duane and of Peres, and they are a little lower than the R-matrix evaluation [8].” The quantitative difference between Peres [9] and B&H [8] due to the experimental work performed at Los Alamos in the 1980’s, [13] and [14], is presently

The cross-section varies by orders of magnitude, due in part to the strong energy dependence of the Coulomb barrier.

Peres [9] calculates $S(E)$ based upon a Pade' expansion:

$$S^*(E) = \frac{A_1 + E(A_2 + E(A_3 + EA_4))}{1 + E(B_1 + E(B_2 + E(B_3 + EB_4)))}, \quad (C31)$$

where his A and B coefficients, in Table I, were obtained by fitting experimental data. Bosch and Hale adopted the same approach, fitting their data set separately. Coefficients for both references are listed in Table I.

TABLE I. Coefficients from Bosch and Hale [8]; and Peres [9], for determining $S^*(E)$.

Numerator Coefficients, A		Denominator Coefficients, B	
Bosch & Hale	Peres	Bosch & Hale	Peres
6.927 e04	9.599811 e06	6.38 e01	-2.532427 e-02
7.454 e08	1.956029 e04	-9.95 e-1	2.679938 e-04
2.050 e06	4.146769 e01	6.981 e-5	0
5.2002 e04	0	1.728 e-4	0

Cross-section, $\sigma(E)$, is determined using equation (53) in [1] listed above Figure 1:

$$\sigma(E) = \frac{S^*(E)}{E} \exp(-\sqrt{E_C/E}),$$

where $\sqrt{E_C} = 34.3827$ for $D(t,n)_4^4He$, as before.

The product of these two factors, $\exp\left(-\frac{E_{cm}}{T}\right) \cdot \exp\left(-\sqrt{\frac{E_C}{E_{cm}}}\right)$, is shown in Figure 8 as the yellow curve. The maximum (mode) of this produce is known as the Gamow peak energy. In Figure 7, that peak is about 35 keV.

The three curves in Figure 8 are often found and referred to in the literature with the vertical axis designated as probability. Statistically speaking those exponential functions do not produce probabilities; however, it is desired that they convey a notion of them. Cross-sections have the same interpretation, even though their values look nothing like probabilities. We suggest the same probabilistic notion can be represented using the designation of likelihood for the functional outputs on the vertical axes. A likelihood

unknown to the authors. However, the inclusion of the data [13, 14] into the evaluation of [8] is known to be true.

function can be any functional output without requiring adherence to the laws of probability and yet it conveys relative comparisons and weighted occurrences of outputs.

Figure 8. Two functions are shown that determine much of the energy dependence of nuclear fusion: the plasma temperature (10 keV energy distribution is plotted, red) and the tunneling function, which depends on the reactants (D-T, blue). The product function (Gamow, yellow) is multiplied by 1000 for comparison purposes.

The rescaled (multiplied by 10^{12}) Gamow product and $S(E)$ are shown together in Figure 9, using the Bosch and Hale [8] $S(E)$ function from Figure 4.

Figure 9. The product function (Gamow) times 10^{12} is shown in red (10 keV). The Bosch and Hale [8] $S(E)$ function is shown in blue. The units for the blue curve on the y-axis are keV-millibarns.

Multiplying together the two curves in Figure 9 completes the integrand for reactivity in (C30). In order to preserve a common scale, this is multiplied by 10^5 as shown in Figure 10 in yellow. Notice, that the maximum of about 35 for the Gamow product (orange) combined with the maximum of about 50 for the $S(E)$ (blue) results in a maximum of about 40 in yellow.

Figure 10. The product of $S(E)$ and Gamow function, times 10^5 , is shown in yellow (for a temperature of 10 keV). The Bosch and Hale $S(E)$ [8] function is shown in blue. The Gamow product function at 10 keV for D-T fusion, times 10^{12} , is shown in red. The blue and red are the same as in Figure 9. The yellow curve peaks at 40 keV, corresponding closely to the average energy of D-T fusion reactants in a 10 keV plasma. The scale for $S(E)$ is keV-millibarns (blue curve).

Example 10. Average Energy of D-T Fusion Reactants

Given a plasma gas burning in equilibrium at 10 keV, what is the average (or central measure of) energy of the fusion reactants? To provide answers, Table II is reproduced from [1] below. The central measures of E in Table II are:

$\langle E \rangle$	first moment numerical values provided by G.M. Hale [15]
$\langle K_{soln} \rangle$	Brysk's solution [16], a function of the ratio of reactivity T derivative to reactivity, equation (47) in [1]. Bosch & Hale reactivity [8] and Caughlan & Fowler reactivity [5] used
$\langle E^* \rangle$	average E (the first moment) for constant cross-section
$\langle E_{avg} \rangle$	average E (the first moment) determined in [1].

Note that the central measures of E of the reactions comprising the fusion are much greater than the temperature given for the plasma gas (except for the constant cross-section case). This is the result of the changing energy dependence for fusion over the width of the energy distribution due to temperature, the MB energy distribution. For example, the first moment

of energy at $T = 10$ keV is about 40 keV. This is the example illustrated in **Example 9**. Figure 10 shows the product of $S(E)$ and Gamow function in yellow (for a MB plasma temperature of 10 keV). The yellow curve peaks at 40 keV, corresponding closely to the average energy of D-T fusion reactants in a 10 keV plasma. This can be seen in Table II, below.

TABLE II. Selected Values of D-T for the Three Cases: $\langle E^* \rangle$, $\langle E_{avg} \rangle$, and $\langle K_{soln} \rangle$

T (keV)	Hale [15] $\langle E \rangle$	$\langle K_{soln} \rangle$ from B&H	$\langle K_{soln} \rangle$ from C&F	$\langle E^* \rangle = T$	$\langle E_{avg} \rangle$
0.5	4.6	4.6	4.7	0.5	4.6
1	7.6	7.6	7.6	1	7.7
2	12.6	12.6	12.5	2	13.0
5	25.3	25.3	26.3	5	25.1
10	40.1	40.0	41.9	10	40.2
20	57.2	57.1	53.8	20	60.9
50	86.9	87.1	86.8	50	108
100	123	123	128	100	160
200	192	193	211	200	242
500	447	482	463	500	502
800	788	838	707	800	819
1000	1062	1112	878	1000	1031

Example 11. Separated Reactants

This example is meant to introduce an analogy of a plasma-physics experiment with a nuclear-physics laboratory experiment. Consider that in a nuclear physics experiment, there exists a particle-beam (deuterium accelerated to 5 keV in the lab, for this example, considered to be quasi-monoenergetic), and the deuterium beam is incident on a stationary target (tritium in this example).

The transformation from nuclear physics lab frame to center-of-mass (gas) frame is as follows. In the nuclear physics experiment, if particle A of mass m_A strikes stationary target particle B of mass m_B , then (C27) becomes:

$$E_A = \frac{E_{cm}(m_A + m_B)}{m_B},$$

where E_{cm} is the center-of-mass energy. The 5 keV deuterium beam represents a D-T reaction in the cm-frame with an energy in the center-of-mass of 3 keV. A calculation of the reaction rate would use $\sigma(E_{cm} = 3 \text{ keV})$.

Now, consider a tritium beam with energy 5 keV. If it were to strike a stationary wall of deuterium, the energy in the D-T reaction cm-frame is 2 keV. A calculation of the reaction rate would use $\sigma(E_{cm} = 2 \text{ keV})$. Note that the D-T cross-section $\sigma(E_{cm} = 3 \text{ keV})$ is greater than at $\sigma(E_{cm} = 2 \text{ keV})$.

Consider now the case of a plasma burning in equilibrium. Reaction rates are based on the equilibrium temperature of the plasma. For example, the thermal reactivities, f , for D(t,n) α , (a D-T plasma) could be used based on Bosch & Hale [8], with units of cc/s. These are tabulated in the cm-frame. Below are a few examples of reactivity at temperatures:

$$\begin{aligned} 2 \text{ keV } f &= 3.0\text{e-}19; \\ 3 \text{ keV } f &= 1.9\text{e-}18; \\ 5 \text{ keV } f &= 1.4\text{e-}17. \end{aligned}$$

Therefore, the ratios of reactivities, without consideration of the particle density, are
1 : 6.3 : 47.

We deduce that from kinematic considerations alone, the D-T reaction-rate could be a sensitive measure of the experimental conditions, for example, in the case that the reactants are initially separated (plasma versus wall). If the plasma gas were tritium, and the “wall” of the container is initially deuterium “at rest”, the yield is “low”. [The tritium-ion plasma is the slowest-moving ion of this example, because its mass is the highest in this example.] If the plasma gas is deuterium, and the “wall” of the container is initially tritium “at rest”, the yield is “medium”. If the gas is DT, and the container has no role in the fusion reaction, the yield is “high”. The yields are in the ratios of

$$\begin{array}{ccccc} 1 & : & 6.3 & : & 47 \\ \text{low yield} & & \text{medium yield} & & \text{high yield.} \end{array}$$

This example is contrived, and assumes that the reactant number densities and “geometry” play no role in the yield. The reactivities were chosen at 2, 3 and 5 keV. This is meant to make the qualitative comparison with the quasi-monoenergetic case of a nuclear-physics particle accelerator at 2, 3 and 5 keV. The temperature-distributed reactivity formulation is appropriate for a plasma in equilibrium under the assumption of Maxwell-Boltzmann statistics. Because nuclear-physics accelerator experiments are very difficult at low energies, nuclear physicists are turning to plasma experiments to determine cross-sections and branching ratios. In a DT plasma burning at 5 keV, the average E (the first moment) determined in [1] is about 25 keV, see Table II in **Example 10**.

This example assumes that the dynamic considerations that produce a plasma of 5 keV temperature, is reproducible for deuterium, tritium, and DT gas. A better comparison would have been to use the cross-section for D-T fusion at 2, 3 and 5 keV complete with number

densities. One would then adhere to the relevant “geometry” for each case. In lieu of such information, which is complicated and inherently dynamical in reality, we point out that the cross-section information is experimentally uncertain in both accelerator and plasma reactivity formalisms.

The point of this Example 11 is to imagine different experimental configurations that could be used to illuminate dynamics, the difference of speeds. The lab frame is used when one of the reactants is stationary. For this reason, this thought exercise is “separated reactants,” meaning one gas interacting with a stationary “wall.” One can thereby see how considerations due to mix are confounded with efforts to determine cross sections using inertial or magnetic confinement.

Example 12. Model-form Uncertainty of the Choice of Astrophysical S-factor

Sensitivity related to differences in the astrophysical S-factor of Peres [9] and Bosch and Hale [8] can be estimated using the ratio of S-factors as:

$$Ratio = \frac{S(E_{cm})}{S^*(E_{cm})} , \quad (C32)$$

where $S(E_{cm})$ is from [8] and $S^*(E_{cm})$ is from [9], defined in (C31) and Table I. The difference was illustrated in Figure 7, and the ratio is illustrated in Figure 11. The ratio of cross-sections is equal to the ratio of astrophysical S-factors, as can be seen by substituting equation (53) of reference [1] into (C32):

$$Ratio = \frac{\sigma_{[8]}(E)}{\sigma_{[9]}(E)} . \quad (C33)$$

Figure 11. The ratio of astrophysical S-factors and cross-sections as defined in (C32) and (C33). The y-axis is dimensionless and the x-axis is in keV. The peak ratio value is 1.19 at 1.1 keV. The value of the ratio at 5 keV is 1.10.

For example, a plasma burning at 1 keV has the average E (the first moment) determined in [1] to be ~ 7 keV, (**Example 10**). Therefore, fusion reactants at the average energy for a 1 keV plasma are subject to this model-form choice sensitivity of 10%. To estimate this 10% at 1 keV, note that the value of the ratio at 5 keV is 1.10. Below 5 keV, the model-choice difference is higher, and above 5 keV, the model-choice difference is lower. Reactivity involves the integral of the energy-dependent factors. The reactivity values are given in [8]. Producing and studying reactivities based on Peres [9] is a subject for future work. When reactivities based on Peres [9] are extant in the data bases of the authors, then a simple ratio of the reactivities will serve as a measure of this model-form uncertainty.

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