Can water burn?

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We investigate the possibility of a spontaneous collapse of the nuclei constituting the water molecule. We show that, due to a practically exact agreement of the energy of the p + p + ^{16}O threshold and a resonance state of the ^{18}Ne nucleus, the probability of nuclear fusion involving p + p + ^{16}O → ^{18}Ne*(4.522, 1$^-$) in the rotationally excited H_2O molecule is significantly enhanced. The calculation of the fusion probability is performed using a scheme analogous to the linear combination of atomic orbitals (LCAO), well known in the theory of molecules.

Introduction

More than a century ago, the French writer Jules Verne wrote[1]:

> …I believe that water will one day be employed as fuel, that hydrogen and oxygen which constitute it, used singly or together, will furnish an inexhaustible source of heat and light, of an intensity of which coal is not capable.… I believe that when the deposits of coal are exhausted we shall heat and warm ourselves with water. Water will be the coal of the future.

In his science-fiction stories, Verne created many technological fantasies. Astonishingly, most of them, such as submarines or flight to the moon, have been realized in our time. The burning of water is one of his predictions that has not yet been realized. Meanwhile we are approaching the time he foresaw, when our consumption of fossil fuel will decline because we will exhaust our reserves of oil, gas and coal. The looming energy crisis forces us to look for alternative sources of energy. Undoubtedly, the most important of them is nuclear energy.

Nuclei can produce energy via two different types of reactions, namely, fission and fusion reactions. Fission is possible for heavy nuclei and fusion for very light nuclei. This is because any physical system tends to move into a state of minimum energy by getting rid of the energy excess. For light nuclei, this is achieved via fusion to form intermediate nuclei; for heavy nuclei, the energy is minimized when a nucleus splits into fragments of smaller masses. These fragments are more tightly bound and therefore occupy lower energy levels. This is because nucleons are most tightly bound in nuclei with $A \sim 56$, which corresponds to iron. When moving towards smaller or greater A in the periodic table of the elements, the binding energy per nucleon declines. Iron therefore is on the border separating light and heavy nuclei. The borderline nuclei are a kind of 'ultimate ashes' that cannot produce energy by either fusion or fission.

For a given mass of fuel, a fusion reaction yields several times more energy than a fission reaction. It is, therefore, a much more powerful source of energy. Moreover, it is environmentally clean because it does not produce radioactive waste. As soon as this was understood, attempts were made to fuse nuclei in laboratories. So far, they have succeeded only in producing uncontrollable fusion in the form of the hydrogen bomb. In such a bomb, fusion is achieved by the explosion of an ordinary (fission) plutonium bomb, which heats up the fuel to solar temperatures. In an attempt to make fusion controllable, most researchers have tried to do essentially the same. They have succeeded in producing high-temperature plasmas, but only for a relatively short time. In spite of such efforts and ingenious tricks, all such attempts till now have failed. This straightforward approach to controllable fusion is probably doomed.

The difficulty with fusion is that nuclei are positively charged and repel each other by the Coulomb force. As a result, at temperatures achievable in our laboratories, they keep apart. For a fusion event to occur, however, the nuclei must be close enough to feel the strong attraction. Nuclear fusion occurs when two or more light nuclei approach each other to a distance of a few fm (1 fm = 10^{-13} cm), where they then experience a strong attraction that overpowers the Coulomb repulsion. To approach each other within such a distance, they must have enough kinetic energy to overcome the Coulomb barrier (the energy hump between the strong attraction and the Coulomb repulsion). The height of the Coulomb barrier is approximately 1 MeV. The necessary kinetic energy is achieved at a temperature of ~10 billion degrees.The nuclei, however, need not vault the barrier as they can penetrate through it due to the quantum tunnel effect. In the Sun and other stars, for example, fusion occurs at 15 million degrees. Of course, the higher the temperature, the thinner the barrier is and the more easily a particle can penetrate it.

There is another way of forcing nuclei to fuse. Instead of lifting the particle against the barrier (which means increasing the temperature), we can try to make the barrier thinner or keep the particles close to the barrier for such a long time that even a low penetration probability would work. This can be done by placing the nuclei we want to fuse inside a molecule, where they can stay close to each other for a long time. Moreover, in a molecule the Coulomb barrier becomes thinner because of the electron screening. In this way, fusion may proceed even at room temperature. This notion of 'cold fusion' was originally (in 1947) discussed by F.C. Frank[2] and, in 1948, put forward by A.D. Sakharov.[3]

Cold fusion in molecules is not a purely theoretical idea. It has been performed in many laboratories via the formation of muonic molecules.[4] The muon is an elementary particle with the same characteristics as the electron. The only difference between them is that the muon is 200 times heavier. When an electron is replaced with the muon, a molecule becomes 200 times smaller, which makes the Coulomb barrier 200 times thinner and the nuclei 200 times closer to each other.

Although the fusion of hydrogen isotopes, catalysed by muons, has been observed by many experimental groups, unfortunately it cannot be used for energy production by industry. The obstacle is the negative efficiency, that is, to make muonic cold fusion we have to spend more energy than it produces. The reason is that muons do not exist like protons or electrons. We have to produce them in accelerators. Moreover, the muon is not a stable particle. Its lifetime is only ~10^{-6} s. This means that a muonic molecule cannot exist longer than 1 microsecond.

Research on muon-catalysed fusion was not in vain, however. From research over several decades, many theoretical and experimental methods were developed, and new features of

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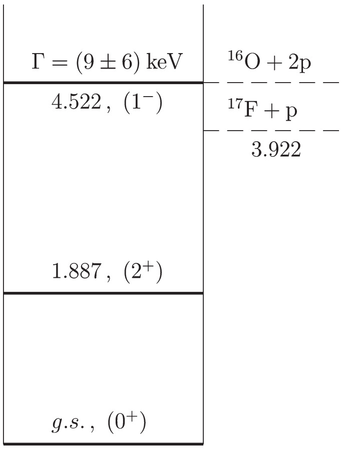

Fig. 1. Part of the ^{18}Ne spectrum (energies are given in MeV) and two break-up thresholds (dashed lines).

molecular systems were discovered and understood. For example, it was noticed[5–9] that for certain systems there is a possibility of resonant nuclear transitions that can significantly amplify the fusion probability. Studies of these resonant transitions in muonic molecules has led to the conclusion that under certain conditions, nuclear fusion can arise even in ordinary (electronic) molecules.[8] In particular, the ordinary water molecule possesses the properties that are necessary for the resonant fusion of its nuclei.[8,10]

If we fuse two protons and ^{16}O constituting a water molecule, H_2O, the resulting compound nucleus is ^{18}Ne. Among other levels, the spectrum of the ^{18}Ne nucleus has an excited state at 4.522 MeV with angular momentum 1 and negative parity[11] (see Fig. 1). The surprising fact about it is that the threshold for the break-up into two protons and oxygen is at the same level. This means that this excited state of neon is actually a three-body resonance of the system pp^{16}O with zero collision energy. In the molecule the nuclei are practically at rest relative to each other. Thanks to this resonance, therefore, they should be able to overcome the Coulomb barrier and undergo the transition

$$\mathrm{p} + \mathrm{p} + {}^{16}\mathrm{O} \longrightarrow {}^{18}\mathrm{Ne}^*(1^-) \tag{1}$$

much more easily than it would be in the absence of such a resonance. Thus, water molecules, in principle, can spontaneously collapse – that is, water can 'burn' via this nuclear reaction. If it is indeed so, a question then arises: Why do the oceans still exist? Why did they not 'burn out' during the billions of years of their existence?

The answer can be found if we look at total angular momentum and the parity of the resonance, given in brackets in Fig. 1. The transition is only possible if these quantum numbers are the same in the initial (molecule) and final (compound nucleus) states. The state of the water molecule with angular momentum 1 and negative parity is such that the molecule rotates around the axis through the oxygen nucleus, as shown in Fig. 2. For the fusion process to occur, therefore, the molecule of water must rotate. In ordinary water, however, there are no individual molecules. Our drinking water consists of small groups of molecules, the so-called clusters, in which several dozen molecules are tightly bound to each other. This prevents the rotation of individual molecules. A molecule can be liberated from a cluster if we warm water up to ~1000 degrees or higher.

What happens if we prepare steam at this temperature and force the molecules to rotate by exposing them to microwave radiation of the appropriate frequency? Will that lead to an explosion, a fire, smouldering, or just some rare fusion events? To answer this question, we need to know the rate of reaction (1). This is what we estimate in this paper. To calculate the reaction rate for the nuclear fusion inside a water molecule, we use a scheme analogous to the linear combination of atomic orbitals (LCAO) widely used in the theory of molecules.[12]

Reaction rate

Consider an ordinary water molecule. For the purpose of estimating the fusion rate, the oxygen nucleus can be treated as a structureless particle. We therefore have a system of 13 particles, which consists of two protons, one ^{16}O nucleus, and 10 electrons. There are many possible states for these 13 particles. We are interested, however, only in the transition between the two particular states both having total angular momentum 1 and negative parity. The initial state for this transition is the rotating water molecule and the final state is the ^{18}Ne atom with an excited nucleus, i.e.

$$\mathrm{H_2O}(1^-) \rightarrow {}^{18}\mathrm{Ne}^*(1^-) + 10\mathrm{e}\ . \tag{2}$$

The Hamiltonian of this system can be represented in two equivalent ways, namely,

$$H = H_1 + V^S \tag{3}$$

or

$$H = H_2 + H^e\ . \tag{4}$$

Here V^S is the sum

$$V^S = V^S_{p_1p_2} + V^S_{p_1O} + V^S_{p_2O} \tag{5}$$

of three strong potentials that describe nuclear interaction among the two protons and ^{16}O, and H^e is the total Hamiltonian of the electron subsystem (10 electrons). The representation (3) is convenient for treating the initial (molecular) state, where the strong forces are unimportant, while (4) is more natural for the final state, where the electrons moving around the compound nucleus ^{18}Ne do not affect its internal state. The main terms of these representations,

$$H_1 = H_0 + V^C_{p_1O} + V^C_{p_2O} + V^C_{p_1p_2} + H^e \tag{6}$$

and

$$H_2 = H_0 + V^C_{p_1O} + V^C_{p_2O} + V^C_{p_1p_2} + V^S\ , \tag{7}$$

include the kinetic energy operator H_0 of the nuclear subsystem and the Coulomb potentials $V^C_{p_1p_2}$ and $V^C_{p_iO}$ between the two protons and the oxygen nucleus. Let ψ_1 and ψ_2 be the eigenfunctions of H_1 and H_2, i.e.

$$H_i\psi_i = E_i\psi_i\ , \qquad i = 1, 2\ , \tag{8}$$

such that they describe the initial and final states, respectively. The terms V^S and H^e in Equations (3, 4) can be treated as perturbations for these states. Since E_1 practically coincides with E_2 (see

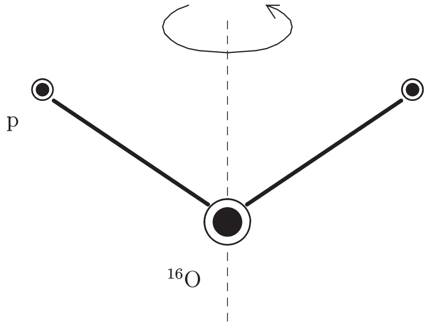

Fig. 2. Rotating water molecule in which the nuclei are in the state 1 .

Fig. 1), when these perturbations are taken into account the solution of the Schrödinger equation

$$H\psi = E\psi \tag{9}$$

can be found as a linear combination

$$\psi = C_1\psi_1 + C_2\psi_2 \tag{10}$$

of only these two states. This way of finding the solution is known as the linear combination of atomic orbitals (LCAO)[12] and is used in the theory of diatomic molecules to calculate wave functions of electrons having two centres of attraction. Substituting (10) into (9) and projecting onto ψ_1 and ψ_2, we derive the system of linear equations for C_1 and C_2:

$$C_1(H_{11} - E) + C_2(H_{12} - EI) \;=\; 0\,, \tag{11}$$

$$C_1(H_{21} - EI^*) + C_2(H_{22} - E) \;=\; 0\,, \tag{12}$$

where

$$H_{ij} \;=\; \langle\psi_i|H|\psi_j\rangle\,, \tag{13}$$

$$I \;=\; \langle\psi_1|\psi_2\rangle\,, \tag{14}$$

and we assume that both ψ_i are normalized, i.e. $\langle\psi_i|\psi_i\rangle = 1$. The homogeneous system of Equations (11) and (12) has non-trivial solutions if and only if its determinant is zero,

$$(H_{11} - E)(H_{22} - E) - (H_{21} - EI^*)(H_{12} - EI) = 0\,. \tag{15}$$

This quadratic equation determines the two 'perturbed' energy levels

$$E^{(+)} \;=\; E_1 + \Delta_1\,, \tag{16}$$

$$E^{(-)} \;=\; E_2 + \Delta_2\,, \tag{17}$$

that emerge from E_1 and E_2 as a result of mutual influence of the molecular and nuclear states. The Δ_1 and Δ_2 terms are small corrections to the corresponding energy levels. These corrections can be obtained by solving Equation (15) where, in accordance with Equation (8), the H_{ij} terms are expressed in terms of the matrix elements of the potentials,

$$H_{11} \;=\; E_1 + V^S_{11}\,, \tag{18}$$

$$H_{12} \;=\; E_1 I + V^S_{12}\,, \tag{19}$$

$$H_{21} \;=\; E_1 I^* + V^S_{21}\,, \tag{20}$$

$$H_{22} \;=\; E_2 + H^e_{22}\,. \tag{21}$$

Here H^e_{22} is just the energy (negative) of 10 electrons in the ^{18}Ne atom, i.e. the energy of its total ionization taken as a negative value. Thus, the corrections obtained,

$$\begin{aligned}\Delta_1 \;=\;& V^S_{11} + gH_{11} + (1+g)\Big[(\sqrt{1+s} - 1)(E_1 - E_2 \\ &+ V^S_{11} - H^e_{22}) - \mathrm{Re}\,(IH_{21})\Big]\,,\end{aligned} \tag{22}$$

and

$$\begin{aligned}\Delta_2 \;=\;& H^e_{22} + gH_{22} - (1+g)\Big[(\sqrt{1+s} - 1)(E_1 - E_2 \\ &+ V^S_{11} - H^e_{22}) + \mathrm{Re}\,(IH_{21})\Big]\,,\end{aligned} \tag{23}$$

where

$$g = \frac{1}{1 - |I|^2} - 1 = |I|^2 + |I|^4 + |I|^6 + \ldots \tag{24}$$

and

$$\begin{aligned}s \;=\;& \frac{4}{(E_1 - E_2 + V^S_{11} - H^e_{22})^2}\Big\{|I|^2 H_{11}H_{22} + |H_{21}|^2 \\ &-(H_{11} + H_{22})\mathrm{Re}\,(IH_{21}) + [\mathrm{Im}\,(IH_{21})]^2\Big\}\,,\end{aligned} \tag{25}$$

are different from what one would expect using the simple perturbation theory, namely, from $\Delta_1 \approx V^S_{11}$ and $\Delta_2 \approx H^e_{22}$. The difference is, however, small because of the smallness of the overlap integral (14).

Therefore the 'perturbed' wave function describing the initial state of the system, can be written as

$$\psi^{(+)} = C^{(+)}_1\psi_1 + C^{(+)}_2\psi_2\,, \tag{26}$$

where $C^{(+)}_1$ and $C^{(+)}_2$ are solutions of Equations (11) and (12), corresponding to the energy $E = E^{(+)}$. Then the probability P for the transition (2) is obtained by the projection

$$\begin{aligned}P \;&=\; |\langle\psi_2|\psi^{(+)}\rangle|^2 \\ &=\; \frac{|fI^* + 1|^2}{|f|^2 + fI^* + f * I + 1}\,,\end{aligned} \tag{27}$$

where

$$f = \frac{E^{(+)}I - H_{12}}{H_{11} - E^{(+)}} = \frac{\Delta_1 I - V^S_{12}}{V^S_{11} - \Delta_1}\,. \tag{28}$$

The reaction (2) can be viewed as the transition through a 'potential barrier'. The total wave function $\psi^{(+)}\exp(-iE^{(+)}t/\hbar)$ oscillates at such a barrier with the frequency $\nu = |E^{(+)}|/2\pi\hbar$. Hence, in order to obtain the reaction rate λ, the probability P should be multiplied by ν, which finally gives

$$\lambda = \frac{|E^{(+)}|}{2\pi\hbar}\,\frac{|fI^* + 1|^2}{|f|^2 + fI^* + f^*I + 1}\,. \tag{29}$$

Matrix elements

To obtain the reaction rate λ from Equations (29) and (28), we need to know the values of I, V^S_{11}, V^S_{12}, V^S_{21}, and H^e_{22}. As already mentioned, H^e_{22} is just the ionization energy of the atom ^{18}Ne. According to ref. 13, we therefore have $H^e_{22} \approx 962$ eV. The calculation of the other integrals, namely,

$$I = \int d\vec{x}\, d\vec{y}\, \psi^*_1(\vec{x},\vec{y})\psi_2(\vec{x},\vec{y}) \tag{30}$$

and

$$\begin{aligned}V^S_{ij} = \int d\vec{x}\, d\vec{y}\, &\left[V^S_{pO}\left(\vec{y} - \frac{\vec{x}}{2}\right) + V^S_{pO}\left(\vec{y} + \frac{\vec{x}}{2}\right) + V^S_{pp}(\vec{x})\right] \\ &\psi^*_i(\vec{x},\vec{y})\psi_j(\vec{x},\vec{y})\end{aligned} \tag{31}$$

requires knowledge of the wave functions $\psi_1(\vec{x},\vec{y})$ and $\psi_2(\vec{x},\vec{y})$ as well as the strong parts V^S_{pO} and V^S_{pp} of the proton-oxygen and proton-proton potentials. Here $\vec{x}$ and $\vec{y}$ are the Jacobi vectors representing spatial configuration of the nuclei as is shown in Fig. 3.

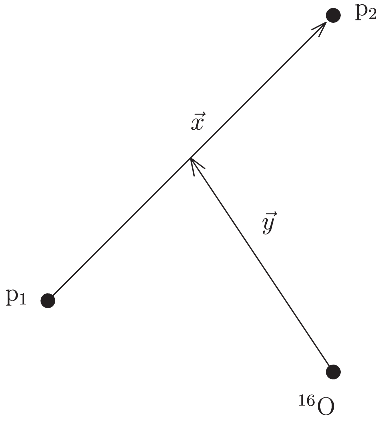

Fig. 3. Jacobi vectors representing spatial configuration of the three-body system pp^{16}O.

The $H_2O(1^-)$ wave function

An accurate evaluation of the three-body wave function ψ_1 describing relative motion of the nuclei in the rotating water molecule requires a separate cumbersome calculation. For the purpose of our estimate, however, it is sufficient to use an approximation that correctly reflects the behaviour of the wave function at short distances. An approximation of this kind was suggested in ref. 14, namely,

$$\psi_1^{JM}(\vec{x},\vec{y}) = N_1 \frac{F_{5/2}(\eta,\kappa\rho)}{\rho^{5/2}} e^{-\kappa\rho} \mathcal{Y}_{\ell\lambda}^{JM}(\hat{\vec{x}},\hat{\vec{y}}) \ , \qquad (32)$$

where F is the regular Coulomb wave function, $\rho = \sqrt{x^2+y^2}$ is the hyper-radius, $\kappa = \sqrt{2\mu|\varepsilon_{mol}|}$ represents the momentum corresponding to the binding energy $\varepsilon_{mol} \approx -10.087$ eV of the H_2O molecule[15] with the reduced mass $\mu = 16\, m_p/33$, $\eta = \mu e^2/\kappa$ is the Sommerfeld parameter, $\mathcal{Y}_{\ell\lambda}^{JM}$ is the eigenfunction of the total angular momentum $\vec{J} = (\vec{\ell}+\vec{\lambda}) + \vec{S}$ with $\vec{\ell}$ and $\vec{\lambda}$ being associated with $\vec{x}$ and $\vec{y}$, respectively, and S is the total spin of the *pp* pair. The normalization constant N_1 can be found via simple integration:

$$N_1^{-2} = \int_0^\infty dx \int_0^\infty dy \, \frac{x^2 y^2 e^{-2\kappa\sqrt{x^2+y^2}}}{(x^2+y^2)^{5/2}} \left| F_{5/2}\left(\eta, \kappa\sqrt{x^2+y^2}\right)\right|^2 \ .$$

The approximation (32) takes into account the Coulomb repulsion among the particles at short distances, as well as the geometric size of the water molecule. For the rotational 1^- state, we use it with $J = 1$. Since the protons are identical fermions, the wave function must be antisymmetric with respect to their permutations. If we assume that the rotation is associated with the coordinate $\vec{x}$, as is shown in Fig. 2, then $\ell = 1, \lambda = 0$, and $S = 1$. Therefore, the angular dependence in Equation (32) is given by

$$\mathcal{Y}_{10}^{1M}(\hat{\vec{x}},\hat{\vec{y}}) = \frac{1}{\sqrt{4\pi}} \sum_{\ell_z\sigma} C_{1\ell_z 1\sigma}^{1M} Y_{1\ell_z}(\hat{\vec{x}}) \chi_{1\sigma} \ ,$$

where $\chi_{1\sigma}$ is the spin function.

The ^{18}Ne*(1^-) wave function

Since ^{16}O is a closed-shell nucleus, it is reasonable to assume that the nucleus ^{18}Ne has the cluster structure ^{16}O+p+p. Considering the harmonic oscillator model, it is easy to show that in the ground state of ^{18}Ne both protons occupy the 2*s* state. Indeed, this immediately follows from comparison of the oscillator representation of the ground states of ^{16}O,

$$|^{16}\mathrm{O}\rangle = |(1s)^4(1p)^{12}\rangle \ ,$$

and ^{18}Ne,

$$|^{18}\mathrm{Ne}\rangle = |(1s)^4(1p)^{12}(2s)^2\rangle \ .$$

Therefore, the ground state wave function of ^{18}Ne is

$$\psi_{2(\mathrm{g.s.})}^{00}(\vec{x},\vec{y}) = \phi_{2s}\left(\vec{y}+\frac{\vec{x}}{2}\right)\phi_{2s}\left(\vec{y}-\frac{\vec{x}}{2}\right)\chi_{00} \ , \qquad (33)$$

where

$$\phi_{2s}(\vec{z}) = \frac{1}{\sqrt{4\pi}} \frac{\sqrt{8/3}}{\pi^{1/4} r_0^{3/2}} \left(\frac{|\vec{z}|^2}{r_0^2} - \frac{3}{2}\right) \exp\left(-\frac{|\vec{z}|^2}{2r_0^2}\right) \qquad (34)$$

is the standard harmonic oscillator function for the 2*s* state, and χ_{00} is the spin function of the two protons with total spin zero.The oscillator parameter $r_0 = \sqrt{\hbar/m_p\omega_0}$ is related to the frequency ω_0, which in turn is determined by the atomic number A as follows.[16]

$$\hbar\omega_0 \approx \frac{40\,\mathrm{MeV}}{A^{1/3}} \ .$$

To form the excited state ^{18}Ne(1^-), we can put one of the protons into the 2*p* state. The excited state has negative parity, which means that the spatial part of the corresponding wave function must be antisymmetric and, therefore, the spin part symmetric. Thus, for this state we obtain

$$\psi_2^{1M}(\vec{x},\vec{y}) = \sum_{\ell_z\sigma} \mathcal{A}\left\{\phi_{2s}\left(\vec{y}+\frac{\vec{x}}{2}\right)\phi_{2p}\left(\vec{y}-\frac{\vec{x}}{2},\ell_z\right)\right\} C_{1\ell_z 1\sigma}^{1M}\chi_{1\sigma} \ , \qquad (35)$$

where the (2*p*) function of the oscillator is given by

$$\phi_{2p}(\vec{z},\ell_z) = \frac{\sqrt{20/3}}{\pi^{1/4} r_0^{5/2}} |\vec{z}| \left(1 - \frac{2}{5}\frac{|\vec{z}|^2}{r_0^2}\right) \exp\left(-\frac{|\vec{z}|^2}{2r_0^2}\right) Y_{1\ell_z}(\hat{\vec{z}}) \ , \qquad (36)$$

and the antisymmetrizer $\mathcal{A}$ consists of the two permutation operators,

$$\mathcal{A} = \mathcal{P}(1,2) - \mathcal{P}(2,1) \ .$$

Therefore, for the wave function of the final state, we obtain

$$\begin{aligned} \psi_2^{1M}(\vec{x},\vec{y}) \ = \ & N_2 \sum_{\ell_z\sigma} \left[\phi_{2s}\left(\vec{y}+\frac{\vec{x}}{2}\right)\phi_{2p}\left(\vec{y}-\frac{\vec{x}}{2},\ell_z\right)\right. \qquad (37) \\ & \left. -\phi_{2s}\left(\vec{y}-\frac{\vec{x}}{2}\right)\phi_{2p}\left(\vec{y}+\frac{\vec{x}}{2},\ell_z\right)\right] C_{1\ell_z 1\sigma}^{1M}\chi_{1\sigma} \ , \end{aligned}$$

where N_2 is the normalization factor, which can be found by numerical integration, similarly to N_1.

The proton-proton potential

The total isospin of the *pp* pair is 1, which means that the strong forces between them are represented by an isotriplet nucleon-nucleon potential $V_{pp}^S(r) \equiv V_{NN}^{(1)}(r)$. In our calculations, we use the $N\,N$ potential constructed by Malfliet and Tjon.[17] Its isotriplet part is given by

$$V_{NN}^{(1)}(r) = \frac{\alpha}{r}\exp(-r/r_1) - \frac{\beta}{r}\exp(-r/r_2) \ ,$$

where $\alpha = 1438.72$ MeV·fm, $\beta = 626{\cdot}875$ MeV·fm, $1/r_1 = 3.11$ fm^{-1}, and $1/r_2 = 1.55$ fm^{-1}. Despite its simplicity, this potential proved to be very reliable in various calculations concerning scattering and nuclear structure problems.

The proton-oxygen potential

To describe strong proton-oxygen forces, we use the potential constructed in ref. 18. This potential is rather general. It describes the interaction between a nucleon and a spherical nucleus with arbitrary mass and charge. Omitting the spin-orbit forces (which are insignificant for our estimation), we obtain for the proton-oxygen case the following potential

$$V_{pO}^S(r) = \frac{V}{\{1+\exp[(r-R)/a]\}^\gamma}\left[1 + \frac{\delta}{1+\exp[-(r-R)/a]}\right] \ ,$$

where $V = -42.466183$ MeV, $R = 1.55766369$ fm, $a = 0.670758192$ fm, $\gamma = 0.577019974$, $\delta = 1.71551344$.

Results and discussion

The numerical evaluation of the multidimensional integrals for the potential matrix elements and the overlapping integral gave the following values:

$$\begin{aligned} V_{11}^S &= -5.35704941 \times 10^{-35}\,\mathrm{eV} \ , \\ V_{12}^S &= -9.82139868 \times 10^{-17}\,\mathrm{eV} \ , \\ I &= \ \ 2.49291260 \times 10^{-22} \ . \end{aligned}$$

Apart from these integrals, the reaction rate (29) critically depends also on the energies E_1 and E_2 of the initial and final states. Actually, λ strongly depends not on the values of these

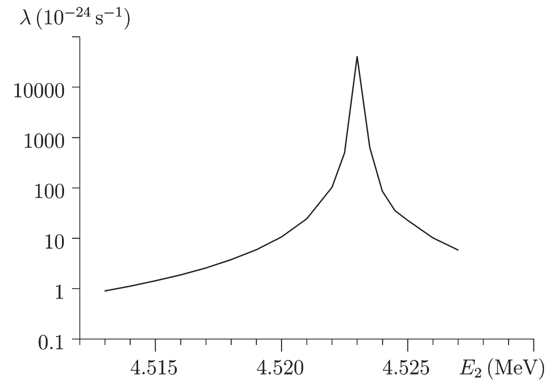

Fig. 4. The rate λ of reaction (2) as a function of the energy E_2 of the ^{18}Ne resonance within its interval of uncertainty.

energies but on their difference $\delta = E_1 - E_2$. From Fig. 1, one may guess that $E_1 = E_2$ and $\delta = 0$. This, however, should not be taken for granted. In fact, the energy E_2 of the excited state of ^{18}Ne is known with an uncertainty of ±8 keV. Besides this, it is a resonance with small but non-zero width $\Gamma = 15$ keV.

A resonance can be excited within the interval $\pm\Gamma$ around the central energy, and the relative probability $W(E)$ of its excitation is determined by the Breit-Wigner formula

$$W(E) = \frac{\Gamma/2}{(E-E_2)^2 + \Gamma^2/4}\ .$$

Assuming that the central energy of the resonance coincides with E_1 and making variations of E_2 around it, we can obtain different values $\lambda(\delta)$ depending on the variation in δ. The observable reaction rate is the average

$$\langle\lambda\rangle = \frac{\int W(E_1-\delta)\lambda(\delta)\,d\delta}{\int W(E_1-\delta)\,d\delta}\ . \qquad (38)$$

Although the virtual transitions are possible for any E_2, the real transitions, which we are interested in, are restricted to $E_2 \le E_1$ by the energy conservation law. The integration in Equation (38) is therefore run over positive δ.

The reaction rate λ for virtual transitions from E_1 to different E_2 around it is shown in Fig. 4. As expected, the dependence on δ is strong. The transition advances by several orders of magnitude when E_1 and E_2 are correlated. For the average (observable) reaction rate, we obtain

$$\langle\lambda\rangle = 2.1\times 10^{-23}\,\mathrm{s}^{-1}\ , \qquad (39)$$

which corresponds to the life-time of

$$T = 1/\langle\lambda\rangle = 1.5\times 10^{15}\,\mathrm{years}\ . \qquad (40)$$

Now, we can answer the question asked at the end of the Introduction. If we liberate water molecules from their clusters and force them to rotate, nothing catastrophic will happen: neither an explosion nor even a smouldering. The molecules will occasionally collapse, but only very seldom. If, for example, we take 18 grammes of water (containing $N_A = 6\times 10^{23}$ molecules) and manage to excite the necessary rotational state in 0.1% of them (which is extremely difficult to achieve), then every second only 0.001 $N_A\lambda = 0.012$ fusion events will occur, i.e. one event every 83 seconds.

From an academic point of view, reaction (2) is undoubtedly valid and occurs in real life. It was observed in the experiment[19] where the corresponding life-time T was estimated to be $\sim 7\times 10^{18}$ years.This value is even higher than our estimate. Its difference from the theoretical life-time (40) can be attributed either to the approximations in our calculations or to experimental challenges associated with the observation of extremely rare events. In the absence of independent calculations or experiments, it is impossible to decide which value is closer to reality. Both results clearly show, however, that the 'burning' of water is an extremely slow process, for all practical applications.

The impracticality of getting water to burn should not discourage further quests for molecular systems whose spectra are correlated with the spectra of their compound nuclei. The present calculation has proved our initial supposition that such correlation enhances the reaction probability by several orders of magnitude. The smallness of λ for water can be explained by the fact that the water molecule consists of three atoms, which makes the overlapping of the molecular and nuclear wave functions extremely small. What would it be in the case of a diatomic molecule? This is an open question, the answer to which requires further calculations and experiments.

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