Nuclear fusion rate enhancement in solid-state environments

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1. Introduction

The conceptual tools to model nuclear fusion emerged during the early part of the 20th century and have remained a trusted staple of physicists since (Gamow 1928, Bethe & Critchfield 1938). Their most important insight: for two nuclei two fuse, their electromagnetic repulsion needs to be overcome – which can be accomplished with high temperature or high pressure. The two physical parameters are thus major inputs to the famous Lawson Criterion, a figure of merit for nuclear fusion (Lawson 1955). The simplicity of this picture promised industrial applications of nuclear fusion within short reach – as soon as associated technical hurdles would be overcome. However, from today's perspective, the history of fusion has become a history of underestimated engineering challenges, resulting in the continued absence of fusion applications at the industrial scale.

This peculiar dynamic bore a regrettable side effect: because the perceived breakthrough was perennially within reach, taking a step back and revisiting the foundations of nuclear fusion seemed untimely. As a result, the trajectory of nuclear fusion development can be viewed as a case of technological and scientific lock-in (Cowan 1990; Perkins 2003), continuing incrementally along a fairly narrow path of relevant concepts. Even today, as truly much progress is being made on overcoming the engineering challenges of nuclear fusion, we propose that there is value in stepping back and re-examining – and possibly extending – our basic understanding of the underlying processes. That is the plan of this paper.

As will be laid out below, at the core of nuclear fusion lie physics that in their richness are not fully captured in the comparatively simple pictures of the first hour. Coincidentally, quantum tunneling – the key to modeling nuclear fusion – was first discovered in the context of nuclear physics (explanation of alpha-decay by Gurney and Condon 1928; Gamow 1928). However, in the decades that followed, much understanding about the intricacies of quantum tunneling was gained in other realms of physics -- most notably atomic, molecular, and optical (AMO) physics and condensed matter (CM) physics. In this paper, we will first identify major levers that affect fusion rates in the established model of nuclear fusion, the so-called Gamow model (Gamow 1928). We will then examine to which extent tunneling-enhancing mechanisms known from AMO and CM physics may be applicable at the nuclear scale and offer the potential of further enhancement.

In the absence of rate-enhancing factors, the fusion rates for deuterium-deuterium fusion at ambient temperatures and pressures are approximately 10^{-64}/s per pair of nuclei in hydrogen gas (Koonin and Nauenberg 1989) and 10^{-150}/s per pair in a metal hydride such as palladium (assuming the default interstitial site occupation at octahedral sites). In this paper, we present five mechanisms that offer the potential to enhance these rates – categorized into proximity-, screening- and resonance-based effects (see Fig. 1a). We also provide estimates for the magnitude of resulting rate enhancement from each mechanism (see Fig. 1b). Our considerations suggest that, when several rate enhancement mechanisms are combined, deuterium fusion rates of 10^{-30}/s and higher are conceivable at ambient temperatures and pressures. Nuclear fusion at such high rates would be expected to lead to macroscopically observable effects and could potentially be harnessed in applications. The presented mechanisms and rate estimates will be motivated and developed in the body of this paper.

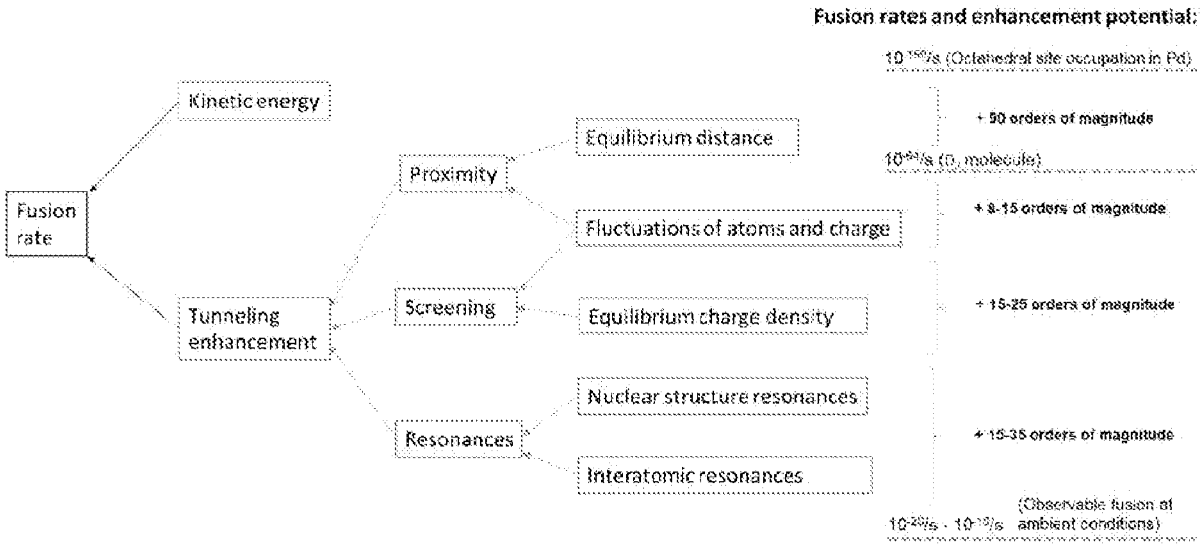


Fig. 1: Five levers for fusion rate enhancement, as identified in this paper. The three mechanisms associated with proximity and screening are largely established and fairly widely recognized. Collectively, they promise rate enhancements -- compared to molecular D_2 in gas phase -- of about 20-35 orders of magnitude. Here, the challenge lies in finding ways to superimpose multiple mechanisms in a single system. The two mechanisms associated with resonances -- while supported by some experimental data -- are more tentative. Each promises additional rate enhancement of about 15-35 orders of magnitude. More research is needed to confirm or reject proposed resonance-related effects.

2. Modeling nuclear fusion: quantum tunneling and the Gamow model

At the heart of modeling nuclear fusion lies the process of overcoming the so-called Coulomb barrier, the potential created by the repulsion of two positively charged nuclei. In a two-body potential between two nuclei, the Coulomb repulsion, given as[1]

$$V(r) = \frac{Z_1 Z_2\, q_c^2}{r} \qquad \text{(Eq. 1)}$$

dominates at distances between 0.01 and 50 pm (see Fig. 2b). At shorter distances <10 fm, the nuclear force dominates which is attractive among all nucleons (protons and neutrons) independent of their charge. The resulting nuclear potential is often expressed via the mean field expression given by Woods-Saxon (Fig. 2a; Woods & Saxon 1954). At far distances >50 pm, the exponentially decreasing Coulomb potential becomes comparatively weak and balanced by the attractive force of negatively charged electrons (Fig. 2c). The interaction of negative electrons and positive nuclei leads to a shallow well whose local minimum determines the spacing of atoms in molecules and lattices. Popular parametric versions of the interatomic potential are given by Jones (1924), Morse (1929), and Frost & Musulin (1954). In the example of Fig. 2 the three partial potentials are evaluated for the case of a deuterium molecule (D_2). A numerical equivalent is given by Kolos & Wolniewicz (1968). By overlaying individual potentials, a single potential can be generated across the distance from 0 to 200 pm and beyond.

[1] Like for other potentials given in this text, a constant factor K has been equated to unity here for the sake of simplicity (Gaussian units). To match SI units the expression should be scaled by $K = (4\pi\varepsilon_0)^{-1}$

In Fig. 2, note the differences in y-axis units: The nuclear potential exhibits a -28 MeV ground state of ^4He, the nucleus that results from D+D fusion. The highest point of the Coulomb potential, at around 5 fm, is approximately at energy 250 keV (see Fig. 3 for the peak that results from the superposition of the nuclear potential and the Coulomb potential). In the colloquialism of "overcoming the Coulomb barrier" this is the peak that is meant to be overcome. The well of the interatomic potential, at around 100 pm, has a depth of approximately 1 eV below 0 eV.

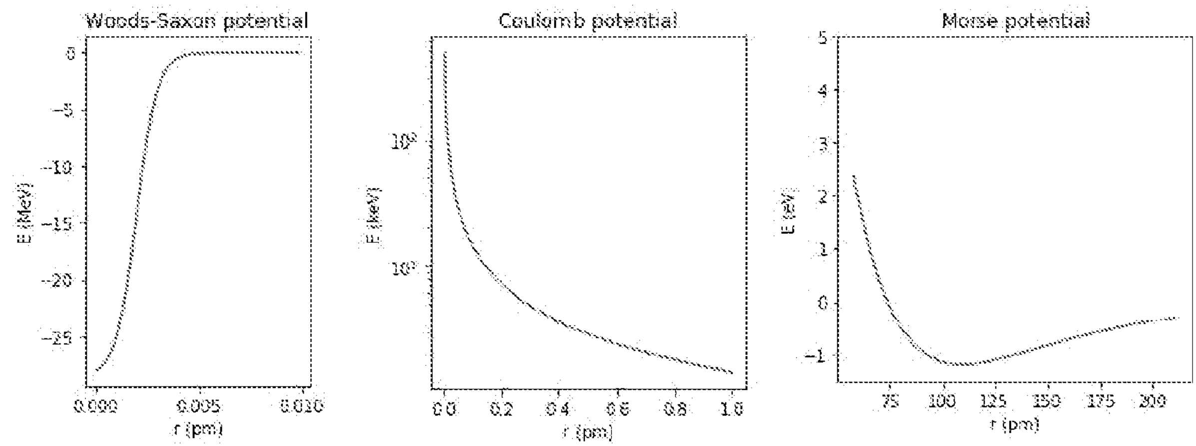


Fig. 2: Dominant components of the interatomic potential for a hydrogen molecule between 1 fm and 200 pm: (a) Nuclear potential (Woods-Saxon); (b) Coulomb potential; (c) Morse potential. Note differences in y-axis scaling. Potential sections can be superimposed to obtain a single continuous potential (see Fig. 3*). Numerically determined potentials offer greater accuracy over their parametrized counterparts. However, the potentials as given here are often sufficient in first approximation -- for instance, in fusion rate calculations.*

In plasma fusion of -- for instance – hydrogen, the concept of an interatomic potential well, as shown in Fig. 2c, does not apply since hydrogen atoms are stripped of their electrons and move around at great velocities, occasionally colliding. Consequently, such fast moving nuclei with large kinetic energy "attack" the Coulomb barriers formed with encountered nuclei at comparatively high attack points, typically on the order of tens of keV.

The kinetic energies of ions in a plasma can be obtained from the plasma temperature via the Boltzmann distribution. A temperature of 150M °C, as is common in many thermonuclear fusion setups, corresponds to a mean kinetic energy of around 20 keV with a small number of nuclei in the distribution tail on the order of 100 keV. Similarly, a temperature of 15M °C, as is common on the sun, corresponds to a mean kinetic energy of around 2 keV and a small number of nuclei on the order of 10 keV. Recalling the height of the D+D Coulomb barrier at about 250 keV, it becomes apparent that – even in thermonuclear fusion -- quantum tunneling must play a central role. In other words, the frequently used notion of "overcoming the Coulomb barrier" is more often than not "tunneling through the Coulomb barrier."

In classical mechanics, a particle cannot overcome a potential if its energy is below the potential height. In quantum mechanics, however, a particle has a nonzero chance of tunneling through a potential barrier even if the particle energy is below the barrier height. The possibility of tunneling follows from a basic principle of quantum mechanics, the Heisenberg uncertainty relation, that notes that for a wave-like particle at a given energy (and thus momentum), its position remains uncertain. Even finding a particle beyond a potential barrier then is a possibility. A quantitative estimate for observing the particle beyond the barrier can be obtained from solving the Schrödinger equation for said particle in the environment of the potential barrier (Griffiths and Schroeter 2018). Neglecting transient effects in the time-independent version of the problem, probability amplitudes can be obtained for both sides of the barrier. The ratio between the probability amplitudes on both sides of the barrier represents the transmission probability i.e. the tunneling probability. This is qualitatively illustrated in Fig. 3 where two probability amplitudes are given for a deuteron tunneling through a D_2 Coulomb barrier at an incoming kinetic energy of 150 keV.

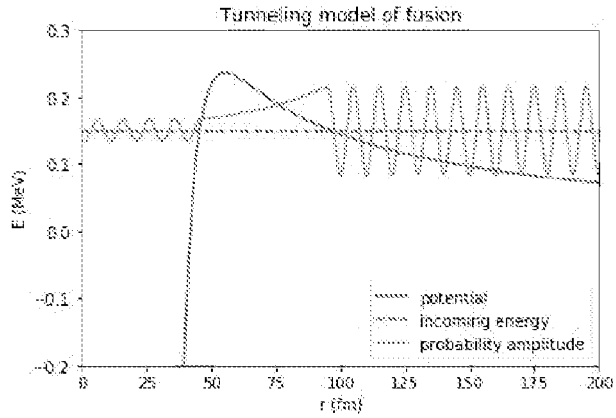


Fig. 3: Illustration of fusion via tunneling as assumed in the Gamow tunneling model. Two nuclei form a two-body potential of the form discussed above. An incoming nucleus (right) is located beyond the attractive well of the target nucleus (left). However, due to quantum tunneling, a small but nonzero probability exists for the incoming nucleus to be located beyond the well, after which fusion can take place.

A quantitative estimate of the tunneling probability can be obtained numerically via the following expression (derived from the WKB approximation to the Schrodinger equation, see Appendix A):

$$T(E) = e^{-2\int_{r_1}^{r_2} dr \sqrt{\frac{2m}{\hbar^2} V(r) - E}} \qquad \text{(Eq. 2)}$$

From the tunneling probability, fusion rates can be obtained when multiplying with the so-called trial frequency f i.e. the frequency of repeated tunneling attempts:

$$\Lambda_{fusion} = f A T \qquad \text{(Eq. 3)}$$

In thermonuclear fusion, the trial frequency f corresponds to the frequency at which nuclei collide. In a solid-state environment, the trial frequency has been attributed to zero-point fluctuations through which adjacent nuclei temporarily come closer to one another. Roepke and Baird (1989) consider a value of about 3 eV realistic for such fluctuations between a pair of deuterium atoms inside a Pd lattice. Here, 3 eV corresponds to a frequency of about 10^{15}/s. Horowitz 1989 provides a slightly smaller estimate of about 1 eV.

Another term in the fusion rate equation (3) is the correction factor *A* which accounts for features not captured in the simple Gamow model but suggested by experiment. The correction factor *A* is usually experimentally determined and then parametrized. Specifically, the Gamow model does not consider the environment surrounding the fusion reaction and potential impacts by that environment. It does also not consider the nuclear structure of the involved nuclei. Both aspects will be discussed in more detail in section 4 of this paper. For the D+D reaction at low energies, *A* is given as 1.5×10^{-16} cm^2/s (Fowler et al. 1967; Koonin and Nauenberg 1989).

To connect to the nomenclature in thermonuclear fusion, the product *A* x *T* is sometimes referred to as cross section σ which therefore represents an aggregate measure of the reaction probability. The cross section *σ* is expressed in units of area, representing the section around the target particle within which the particle responds to a corresponding scattering process. By comparing the fusion cross section of the particle to the actual area of the particle, the cross section can be turned into a dimensionless reaction probability – which makes it comparable to the tunneling probability *T*. The thermonuclear fusion equivalent to the trial frequency *f* is the product of particle density n and particle velocity *v* (which is a function of kinetic Energy *E* and therefore of temperature). Since the particle velocity is typically a distribution related to the Boltzmann temperature distribution, calculating an actual thermonuclear fusion rate requires integrating the fusion rate formula across all velocities.

The above considerations allow for connecting the general fusion rate (2) derived from basic considerations as in the Gamow model to the thermonuclear fusion rate (3) that forms the basis of the Lawson Criterion calculation (Lawson 1955):

$$\lambda_{thermonuclear fusion} = f\,(A\,T) = (v\,n)\,\sigma \qquad \text{(Eq. 4)}$$

In the case of thermonuclear fusion of hydrogen, the cross section of a 15 KeV deuterium nucleus impinging on another deuterium nucleus is about 10^{-32} m^2, which means a reaction probability of about 10^{-3} per collision (based on a deuteron charge radius of 2.127 fm and a corresponding area of 10^{-29} m^2). Given a density of xy target nuclei, we can expect xy collisions per second, and therefore an expected fusion rate of xy. Similarly, when the general fusion rate expression (2) is applied to D_2 molecules in deuterium gas, assuming zero-point fluctuations on the order of 3 eV, a reaction rate of about 10^{-64}/s is obtained (Koonin and Nauenberg 1989).

3. Enhancement potential within the Gamow tunneling model

This section will investigate how the fusion rate calculation (2) is affected by changes in the input parameters of the underlying Gamow model. We will focus on the expression (1) for tunneling probability *T* and its constituting components. The tunneling probability is often expressed only as a function of kinetic energy *T(E)* whereas larger kinetic energies *E* lead to larger tunneling probabilities *T* and therefore larger fusion rates[2]. However, a closer look at (1) suggests that *V(r)* – i.e. the shape and size of the interatomic potential -- also affects the tunneling probability *T*. It would therefore be more appropriate to express *T* as *T(E,V)*.

V(r) i.e. the shape of a pairwise interatomic potential is in turn affected by the proximity of the respective nuclei as well as the electron density of their immediate environment. These two parameters and their impact are discussed in this section.

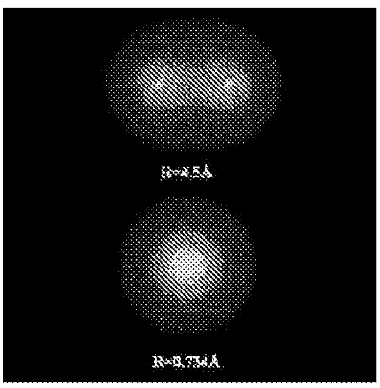
3.1. Proximity of nuclei

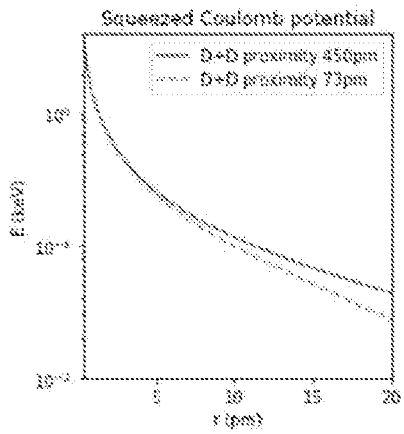
[2] In thermonuclear fusion, this relationship between kinetic energy E and tunneling probability is typically expressed via cross section graphs, as seen Fig. 7.

The distances between nuclei in molecules or solids are determined by the balance of electromagnetic repulsion and attraction between electrons and nuclei. Their interaction results in an interatomic potential as introduced in section 2 whose local minimum in the 50-500pm range determines the proximity between adjacent nuclei. If the shape of the potential is changed e.g. by increasing the surrounding electron density, the equilibrium proximity changes. Similarly, if the proximity between nuclei is changed e.g. through high gas pressure or constraints within a lattice, the shape of the potential changes. In this subsection we will focus on the impact of changes to the Coulomb potential that result from different equilibrium positions of nuclei in a lattice – and their impact on associated tunneling and fusion rates. Energy potentials are sometimes described as Born-Oppenheimer potentials, potential-energy profiles or potential-energy surfaces (if extended to more than one dimension as is often necessary in solids; see Mustroph 2016 for a discussion of these terms). For the purpose of determining fusion rates, the potential can be reduced to one dimension in that attention can be focused on the line between two nuclei that represents the minimum of a surrounding potential surface. Detailed modeling of interatomic potentials in lattices and the associated electron densities and interatomic distances are typically carried out through Density Functional Theory (DFT)- and molecular dynamics based approaches. Such approaches are discussed in more detail in Appendix C.

Fig. 4a shows the formation of a hydrogen molecule with the lower part depicting the equilibrium position of the gas phase molecule at approximately 73 pm. Since the Coulomb potential between the nuclei is given as a function of r (see eq. 1), an increase of proximity between the nuclei lowers the Coulomb potential as seen in Fig. 4b. It can be inferred that -- were the nuclei brought together even more closely e.g. through external force -- the Coulomb potential would lower further and thus the associated tunneling probability T in the Gamow model would increase. An overview of this relationship i.e. the fusion rate as a function of the proximity between two D nuclei is shown in Fig. 5b below.

Although a parametrized potential is used in our own calculations to obtain the estimates in Fig. 5b, these results are largely consistent with Koonin and Nauenberg 1989 who used a numerical potential based on Kolos & Wolniewicz (1968). Kooning and Nauenberg find that "the rate for d+d fusion is 3 x 10^{-64}/s, some 10 orders of magnitude faster than a previous estimate." At the same time, the authors caution: "These calculations [..] are only approximate. Screening by the electrons modifies the Born-Oppenheimer potential. Moreover, fluctuations present in many-body situations might significantly enhance fusion rates." We will follow their advice and discuss quantitative estimates for the effects of screening and fluctuations in the following two sections.





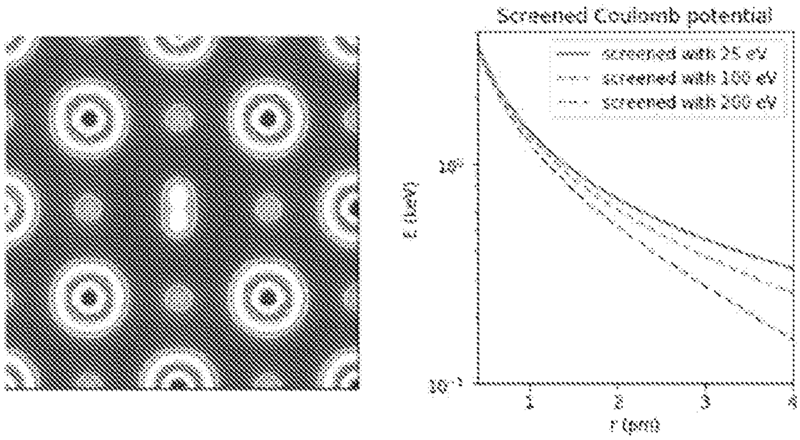


Fig. 4: (a) Illustrations of electron densities of hydrogen atoms in gas phase (TOP) and inside a metal lattice (BOTTOM). In the gas phase picture, two different proximities during molecule formation are shown. In the metal picture, Pd atoms are shown (red), individual hydrogen atoms in octahedral interstitial sites (white) and a hydrogen molecule near a vacancy (center). The distance between hydrogen atoms in octahedral interstitial sites is about 250 pm. Electron densities surrounding the molecule in the metal lattice are higher (100-200 eV) compared to the molecule in gas phase (25 eV). (b) On the right, different shapes of the Coulomb potential are shown, demonstrating the relative impacts of proximity (TOP) and screening (BOTTOM).

3.2. Electron screening

In the simple picture above, the impact of negatively charged electrons on the repulsion between the two positively charged nuclei is not yet considered. In the gas molecule, two electrons are involved; in a metal lattice the situation is more complicated since additional free electrons are available that the deuterons can attract. In any case, each electron contributes to the overall potential V(r) a negative electric component that is proportional to its charge and quadratically decreasing in radius in accordance with Coulomb's law. Therefore, depending on the proximity of the electrons, part of the positively charged repulsion of the nuclei is offset by the electrons. De facto this leads to closer proximity between adjacent nuclei (due to the shift in the potential well) and to a reduced tunneling length. This phenomenon is known as electron screening.

Assenbaum et al. 1987; Czerski et al. 2006; and Huke et al. 2008 provide detailed discussions on how electron screening can be modeled and quantified. Here, we will briefly summarize the main points. In first approximation, the effect of screening can be expressed by a factor $e^{-r/a}$ applied to the idealized unscreened Coulomb potential (as discussed in the previous section, see equation 1). This approach is based on the common assumption that free electrons in a metal can be treated as an electron gas (Fermi gas). Therefore, the semiclassical Thomas-Fermi model applies (Fetter & Walecka 1971) and the resulting screened potential is:

$$V(r) = \frac{Z_1 Z_2 q_e^2}{r} e^{\frac{-r}{a}} \qquad \text{(Eq. 5)}$$

where a is referred to as the screening length. The screening length a in turn consists of a constant multiplied by $n^{-1/6}$, the electron density surrounding the deuterons (the free electron density in Pd is given by Vaselli et al. 1989 as 6.8 x $10^{22}/cm^3$ and by Horowitz 1989 as $3.15/Å^3$). Following this approach for a D_2 molecule in Pd, Vaselli et al. 1989 find a screening length of 57 pm i.e. an effective increase of deuteron proximity when compared to the 74 pm for an unscreened D_2 molecule. More generally, electron screening in this picture can be interpreted as a shifting of the interatomic distance towards the screening length. Since the screening length a is typically much smaller than the typical interatomic distance to which r extends when modeling the potential, the multiplication by factor $e^{-r/a}$ in expression (5) can be simplified to a subtraction by a constant U_e where $U_e = e^{2/a}$. In other words, in first approximation, screening in a lattice can be expressed as the reduction of the Coulomb potential by a constant value, known as the screening potential energy U_e.

Targosz-Ślęczka et al. 2013 discuss further considerations such as the impact of positive ions on the screening potential as well as dynamic effects. These are further explained in Appendix D. For the purpose of this discussion, they can be considered comparatively small and we will proceed by examining the impact on fusion rates of a constant screening potential U_e, as introduced above.

In terms of concrete numbers, the two electrons in the case of the gas phase hydrogen molecule correspond to a screening potential U_e of approximately 25 eV (Raiola et al. 2002). The resulting new baseline for screened Coulomb potentials between molecular deuterons is shown in Fig. 4d (blue line). Following the approach laid out above, Huke et al. 2008 report theoretical screening energies U_e ranging from 50 to 150 eV for different metals (Li on the lower end and Pd and Ta on the upper end of the range). The impact of screening energies across this range on the effective Coulomb potential is shown in Fig. 4d (orange and green lines). The corresponding fusion rate enhancement is shown in Fig. 5a.

While the authors provide these theoretically predicted screening energies, they note that screening energies obtained by fitting observed fusion rates from experiment are higher. Experiments to determine screening energies have been carried out by multiple groups and typically involve low energy deuteron bombardment of different metal targets and measurement of resulting neutrons and charged particles. For the same materials where the theoretical screening energy range is given as 50 to 150 eV, the experimental screening energy range reported is 150 to 300 eV (Huke et al. 2008; Raiolla et al. 2004). In other words, the experimentally observed fusion rates are substantially higher than expected when considering proximity and screening alone within the Gamow model. Attempts to interpret such discrepancies and attempts to identify corresponding shortcomings in the Gamow model that may explain them are laid out in section 4 of this paper. Thus far the typical approach in the literature is to merely parameterize such discrepancies and include them in the phenomenological correction factor A without understanding them causally.

From the discussion above, we can see that proximity and screening can be interdependent. In the case of muon-catalyzed fusion for instance, an electron in a hydrogen molecule is substituted by a muon (Alvarez 1957; Iiyoshi et al. 2019). A muon corresponds to an electron with a mass increased by a factor of 207. The greater mass leads to a greater proximity of the electron to the nucleus by a factor of about 200 (corresponding to screening length a) and consequently, to a corresponding increased screening potential U_e and interatomic distance. Concretely, the interatomic distance between muonic deuterons has been estimated at <1 pm (citation needed). This in turn leads to an increase in tunneling probability and to a corresponding fusion rate enhancement of about 75 orders of magnitude (Szalewicz et al. 1989). Muon-catalyzed fusion is a widely accepted approach to fusion rate enhancement. However, from a practical point of view, the challenge with muon-catalyzed fusion has been the expense of producing muons and their short-lived nature (Kelly 2018). Muons can only be used for a small number of reactions before they recombine and need to be replaced, a process that remains very energy intensive.

Some authors proposed other hydrogen configurations with higher than ordinary proximity or charge density, somewhat analogous to muonic hydrogen. For instance, Holmlid (2013) proposes that clusters can form in Rydberg matter where the density of hydrogen nuclei is high. In such clusters Holmlid claims an interatomic distance between two adjacent deuterons of less than 3 pm (citation needed). Whereas the existence of Rydberg matter as an exotic phase of matter formed by Rydberg atoms was predicted by Manykin et al. in 1980 and appears to be well established today, Holmlid's proposed ultradense variants of Rydberg matter have not been corroborated to date. If such close distances were indeed possible, it can be seen from the considerations above and from Fig. 5 that such proximity would lead to very high fusion rates, analog to muon-catalyzed fusion. The question whether proposed dense regions exist in Rydberg matter can be pursued as a research question in its own right and does not need to be contingent on its potential for fusion rate enhancement.

We now discussed approaches such as muon-catalyzed fusion that aim to increase screening energies by getting negative point charges closer to nuclei; and we reviewed some cited estimates for theoretical screening energies based on averaged electron densities in metal hydrides. Alternative approaches involve the study of special sites in metal hydrides that allow for both high electron density and close proximity simultaneously. Such sites could comprise defects, interfaces or impurities. For instance, the formation of hydrogen molecules near point defects would allow for deuteron proximity on the order of 70 pm and for screening energies beyond 100 eV. Density functional theory (DFT) models by Nazarov et al. 2014 suggest that molecule formation is possible near defects in most metals. However, we are not aware of systematic efforts to use common computational techniques such as DFT for searches that simultaneously optimize for high proximity and high electron screening between hydrogen atoms inside metal lattices.

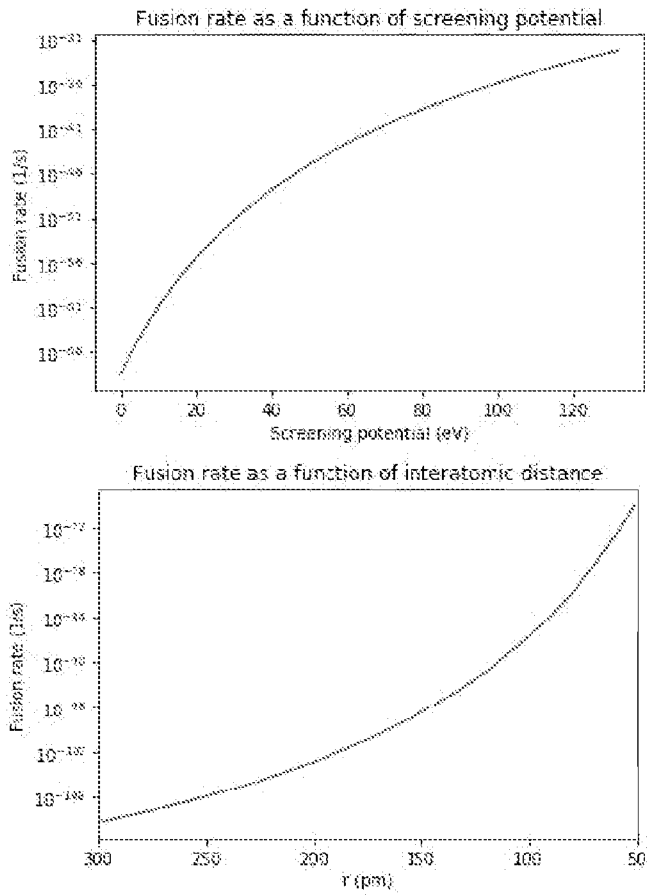


Fig. 5: Increase of predicted fusion rates within the Gamow model as a function of (b) interatomic distance (BOTTOM) and (a) screening potential (TOP)

3.3. Dynamic enhancement of proximity and electron screening

The discussions above on proximity and screening assumed that the system of interest was in equilibrium and essentially static. Fluctuations entered in the form of the trial frequency as the rate at which the tunneling probability needs to be compounded. However, some authors considered in more detail, how dynamic effects and associated temporary increases of proximity and local electron density may affect fusion rates. A key to that argument is that fusion reactions are expected to take place within a timescale of <1 fs whereas electron oscillations take place at a time scale of >1 fs. Therefore, even a short extremum in position and electron density might be "perceived" as long or effectively permanent from the perspective of two fusing nuclei. In other words, such dynamics would be adiabatic vis-a-vis fusion reactions.

Instead of considering the tunneling probability at a single given proximity between two nuclei, Koonin (1989) proposes to integrate across all the occurring proximities as nuclei fluctuate. Fluctuations of nuclei in a lattice can be caused by a number of factors. Koonin lists phonon motion (e.g. caused by heat or gas diffusion through a lattice) and flowing current as mechanisms to consider. Koonin's approach then exhibits parallels to the approach in thermonuclear fusion where fusion rate calculations are not based on just a single temperature (and thus a single kinetic energy) but rather integrate across the full distribution of expected temperatures. He argues that this approach suggests that "even relatively small fractional fluctuations [..] can produce enhancements [of fusion rates] of some 30 orders of magnitude." The question is what extent of fluctuations can be reasonably expected. Koonin suggests that, in first approximation, fluctuations on the order of 0.1 x the Bohr radius (i.e. about 5 pm) are conceivable which lead to an enhancement of the D+D fusion rate of about 8 orders of magnitude.

Yuki et al. 1998 attribute an observed D+D fusion rate in metal foil targets above theoretical predictions to deuterium diffusion in metal hydrides. They suggest that the materials dependence of their results could be attributed to differences in deuterium diffusivity across different metals. The enhancement would then be caused by "dynamic deuteron-deuteron screening" where the screening radius is temporarily increased during motion of the nuclei.

Fork et al. (2019) propose that electron density and thus fusion rate enhancement through screening can be dynamically increased by temporarily concentrating electrons near the nuclei to be fused. They propose that plasmon oscillations in target structures induced by electromagnetic radiation at frequencies above 1 THz will do exactly that (fast enough to prevent the material to changes its structure or disintegrate; slow enough that the faster fusion reactions are adiabatic with respect to the temporary enhancement of screening). They estimate temporary electron charge density increases of at least 10% and possibly up to a factor of 2 which would lead to increases in screening energy on the order of 40%. From Fig. xy can be seen that such screening increases would correspond to several orders of magnitude higher fusion rates.

3.4. Hypotheses and research questions

In the discussion above, we covered factors that increase fusion rates within the Gamow model. We found that proximity increases fusion rates. The D_2 molecule in the gas phase with a proximity of about 74 pm establishes a widely accepted reference case, as developed by Koonin and Nauenberg 1989, with a fusion rate of about 10^{-64}/s. However, in the case of the D_2 molecule in gas phase, the electron density of about 25 eV is low and therefore screening effects are limited.

Conversely, in a typical metal lattice such as palladium hydride, electron screening is much higher. However, typically deuterons are much farther apart: in an ideal palladium hydride lattice (perfect crystal), hydrogen atoms occupy octahedral interstitial sites resulting in a closest hydrogen proximity of only about 250 pm. This configuration sets the fusion rate back to about 10^{-150}/s since the higher screening values cannot offset the rate losses that result from the large distance between deuterons.

However, the formation of hydrogen molecules inside a lattice -- as suggested by He et al. 2012; Nazarov et al. 2014; and Fukumuro et al. 2020 -- would allow for fusion rate enhancement benefitting from both close proximity and high screening. The discussion above suggests that in such configurations, the reference rate of 10^{-64}/s for the molecule in gas phase could be increased by 15-25 orders of magnitude due to screening effects and another 8-15 orders of magnitude due to additional dynamic enhancement of proximity and screening. This reasoning explains the first three mechanisms for fusion rate enhancement in Fig. 1 and the corresponding rate and enhancement potential estimates.

Corresponding materials systems that can provide for simultaneous proximity (especially through molecule formation) and high electron density have been proposed by various authors and include defects in metal hydrides, interfaces between metals with lattice mismatch, and alloys (citation needed).

These considerations suggest to us the following research questions to be worthy of investigation:

- *How can screening effects be effectively modeled and included in state-of-the-art materials simulations?*
- *Which configurations in metal hydrides allow for the joint maximization of proximity and electron density? Can DFT models be adapted to optimize for both?*
- *What are supplier limits and what are practical implications for the temporary (dynamic) enhancement of distance and screening?*

4. Enhancement potential beyond the Gamow tunneling model

In the sections above, we found that already within the simple Gamow model, several levers can be identified that affect fusion rates and provide for the possibility of fusion rate enhancement. In this section, we will discuss where the Gamow model may fall short, given what we know today about factors affecting tunneling processes in other systems, and particularly in systems at the atomic and molecular level where quantum tunneling is widely employed and studied.

4.1. Appropriate system boundaries and levels of abstraction

The Gamow model makes certain assumptions and simplifications – for instance, it does not consider the energy levels of the nuclear well, thereby exogenizing the possibility of resonances which are central to tunneling processes at the atomic and molecular level. The Gamow model also treats the fusion reaction as a two-body process, independent of and unaffected by its environment. Such underlying assumptions can be justified if indeed the energy levels and structure of participating nuclei have no or only negligible impact on the resulting reaction rate; and if the surrounding environment in all relevant cases has no or only negligible impact.

Any physical model is necessarily abstraction, reduced to its essential features to avoid otherwise intractable complexity[3]. When modeling a cannon ball in air, friction can often be ignored when it is negligibly small compared to the magnitudes of interest. However, when modeling a cannon ball in water, friction may not be ignored as it may be significantly large compared to the magnitudes of interest. This example illustrates how for every physical model, questions arise such as: Where to draw system

[3] In 1929, Paul Dirac famously stated that it "becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation." The question is, of course, how to know which features are the main features without having full knowledge of the system a priori.

boundaries? What to model explicitly, what to neglect, and what to reduce to simple parameters? In other words: What level of abstraction is appropriate under what conditions? And how to justify these choices?

In gauging where to draw boundaries for a system to be modeled, it can be helpful to "zoom in" and "zoom out" and carefully investigate what factors may impact the outcome variables of interest at a greater level of detail or from a greater field of view. In the former case, the resolution of the model may increase, in the latter case the scope of the model may enlarge (see Fig. 6). In this section, we will consider both of these possibilities.

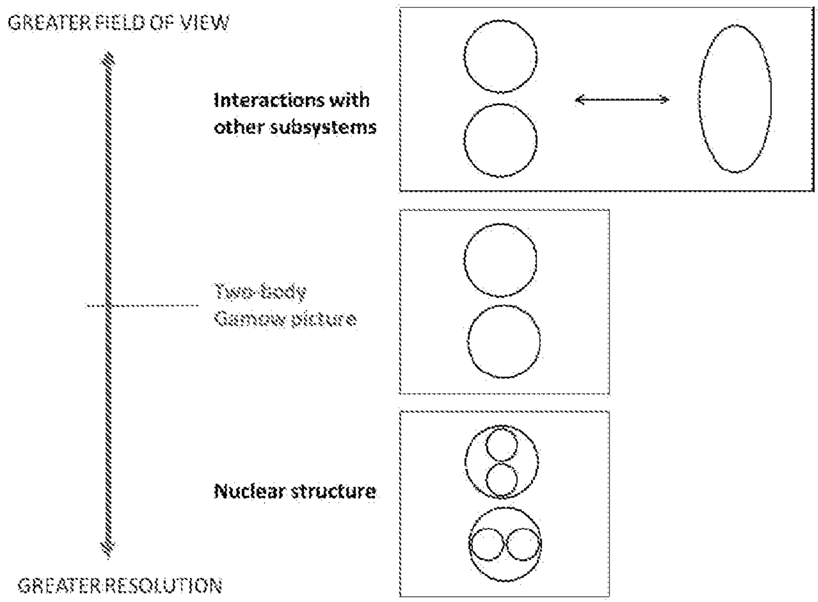


Fig. 6: Starting from the two-body Gamow picture, a simple model can be extended by increasing the field of view or by increasing the resolution with which the system is considered. In the case of nuclear fusion, the former corresponds to considering interactions with other subsystems and the latter corresponds to considering the role of nuclear structure.

We will zoom in to look at the nuclear system more closely. We will specifically focus on widely accepted discrepancies between experimental results and theoretical predictions and possible explanations at the nucleon scale. These discrepancies are typically attributed to nuclear structure which enter the Gamow model-based fusion rate calculation only vaguely through the empirical correction factor A, a parameter whose very name calls for some unpacking.

Conversely, we will zoom out and carefully consider the possible environments surrounding fusion reactions and the interactions that may arise in such environments. To which extent may other subsystems affect the two-body fusion process? If strong enough couplings to other subsystems exist, can the fusion process still be reduced to being treated as a two-body process? Where then to draw appropriate system boundaries?

The following two subsections will investigate such questions particularly in light of insights on quantum tunneling gained across recent decades from the study of systems at the atomic and molecular level. In that process, we will present for consideration a number of aspects that may require an extension of the Gamow model in order to accurately reflect nuclear fusion rates.

4.2. Zooming in: nuclear structure resonances

The concept of resonance is a central one in atomic, molecular, and optical physics and, particularly, in spectroscopy where it forms the foundation of the field. In general terms, resonance describes an oscillating system's increased response when intrinsic oscillating modes of said system – and therefore intrinsic energy levels – match with frequencies of an interacting system. In some circumstances, the oscillating system's intrinsic modes are fixed and given by the system's structure. In that case, resonances can only be achieved by adjusting the incoming stimulus to match intrinsic modes. In other systems, resonant modes can be tuned by adjusting variables such as the system's geometry or potential[4].

The concept of resonance applies both to observable amplitudes in classical systems and to probability amplitudes in quantum systems (which, in turn, determine a distribution of observable outcomes). In a quantum tunneling problem such as in the Gamow model, the probability amplitude beyond the barrier increases when the frequency of the incoming wave – e.g. the energy of an incoming deuteron -- matches an intrinsic mode of a nucleus that can result from the interaction. In other words, if the resulting nuclear structure can accommodate the total energy present in the interaction particularly well, then the corresponding reaction is more likely to occur. This is illustrated in general terms in Fig. 7a where an incident nucleus with energy $E_{incoming}$ is shown on the right and the intrinsic energy levels of the resulting nuclear structure (referred to as compound nucleus) are shown in the center. On the left, cross sections (i.e. tunneling probabilities) are shown as a function of energy. Peaks in tunneling probabilities are seen for incident nucleus energies that match the intrinsic energy levels of the compound nucleus. Such peaks are associated with the concept of resonance.

Whereas Fig. 7a is a cartoon, Fig. 7b shows actual cross sections for common fusion reactions obtained from experimental data. In the given energy range above 5 keV, the D+D fusion reaction exhibits no resonance peak. The D+T fusion reaction exhibits a broad resonance peak centered around 90 keV. The p+^{11}B fusion reaction exhibits narrower resonance peaks, for instance a particularly narrow one near 150 keV.

The theoretical explanation and prediction of such resonance peaks is complicated and the subject of much ongoing research in nuclear physics. As alluded to above, the peaks are ultimately a function of the nuclear structure that can form from the interaction of the incoming nucleus with the target nucleus (except if scattering is dominant, as is the case in some configurations). In the D+D case, the resulting structure comprises a four-nucleon system, in the D+T case a five-nucleon system, and in the p+^{11}B case, a twelve-nucleon system.

Common approaches to modeling such many-particle systems will be discussed in more detail below. First, we will make the explicit connection to the subject of this paper by introducing suggestions that different authors have put forth on how nuclear resonances may affect nuclear fusion rates.

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[4] (footnote on resonating tunneling diode and on quantum simulation where wells are tuned through lasers)

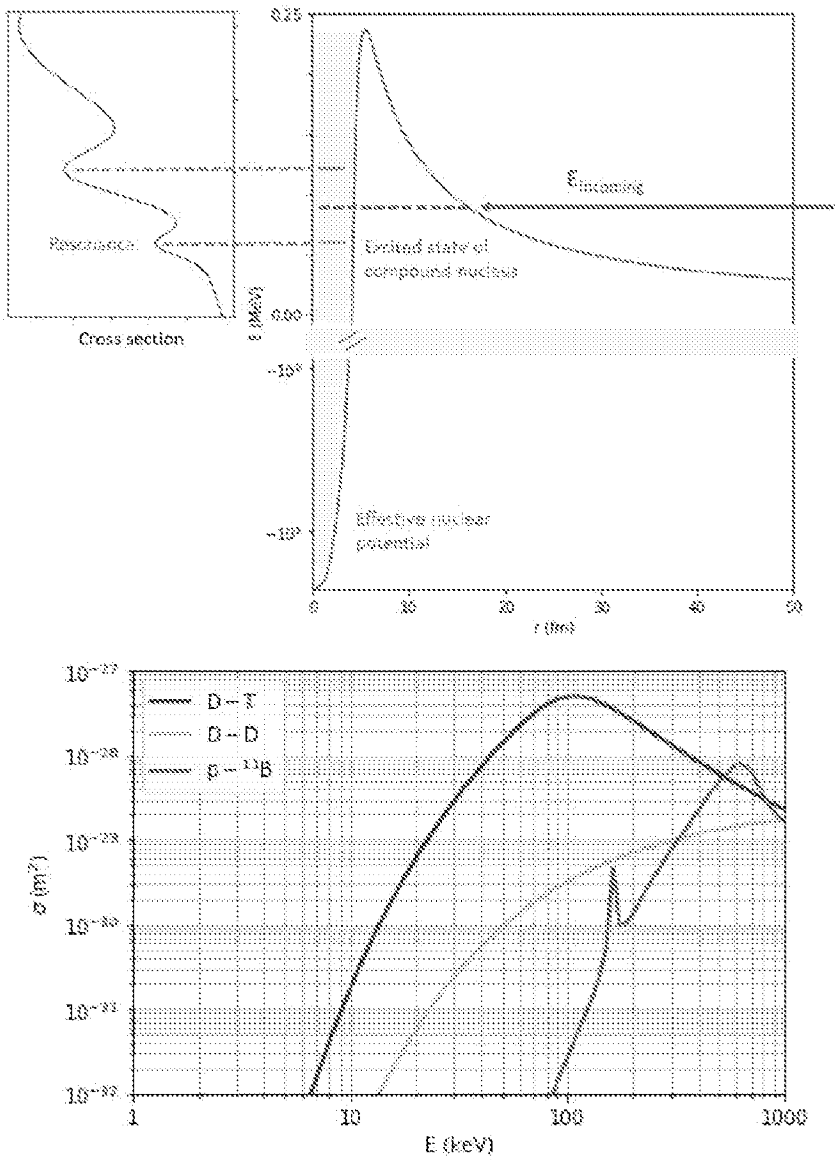

Fig. 7: (a) cartoon that illustrates the concept of nuclear fusion resonance and the relationship to energy levels of the compound nucleus; (b) experimentally obtained cross sections for common fusion reactions.

Fusion rate enhancement through nuclear resonances

In the literature on nuclear fusion, several mechanisms have been proposed that could enhance fusion rates at low energies. Typically, such proposals are motivated by discrepancies between experimentally observed fusion rates and predicted fusion rates. For discussions of such discrepancies, we refer to Shoppa et al. 1993; Czerski et al. 2001; Raiola et al. 2004; Spitaleri et al. 2016; and Berlinguette et al. 2019. In essence, all authors note fusion rates orders of magnitude higher than expected and do so in experiments that involve low energy hydrogen projectiles impinging on hydrided metal targets. Higher than expected here means after already having taken into account possible enhancements within the Gamow model such as proximity and screening, as discussed in section 3 of this paper. The remaining discrepancies prompted some researchers to consider possible rate enhancing factors beyond what is captured in the Gamow model. The focus here is on explanations that directly or indirectly propose an increase of resolution by turning to aspects of nuclear structure.

Czerski et al. 2016 argue that the experimentally observed enhancement ofis D+D fusion at low energies can be accounted for by a hypothetical resonance of the resulting ^{4}He nucleus. Such a resonance is proposed to be narrow and centered around 10 eV above the reaction threshold (which is at 23.84 MeV above the ^{4}He nuclear ground state and represents 0 eV in the two-particle interatomic potential of the Gamow model). Such a resonance is suggested to account for additional fusion rate enhancement on a comparable scale to the enhancement already provided by screening (see Fig. 9). Fig. 8 shows a diagram with an overview of presently known resonances in the four-nucleon system of ^{4}He (Tilley et al. 1992). The proposed resonance would correspond to a new nuclear excited state around 23.85 MeV, between the 23.64 MeV state and the 24.25 MeV state. The authors argue that a narrow resonance in that region might have not been noticed in previous experiments, especially if it was not explicitly looked for. Also note that in experiments, fusion rate data to establish a resonance could be only determined if other enhancements are already present such as discussed in section 3. Otherwise, even a substantial enhancement would still be insufficient to get above the noise threshold of measuring instruments. In other words, gas target experiments would likely not reveal such a resonance even if it were to exist. Consequently, dedicated experiments involving solid targets that allow for fusion rate enhancement through proximity and screening would need to be arranged. As an alternative to such solid target bombardment experiments, Kilic & Kustan 2019 suggest that the proposed resonance could also be tested for by exciting ^{4}He nuclei to higher excited states -- e.g. around 30 MeV -- and then observe whether corresponding gamma rays from relaxation to the proposed 23.85 MeV state can be measured.

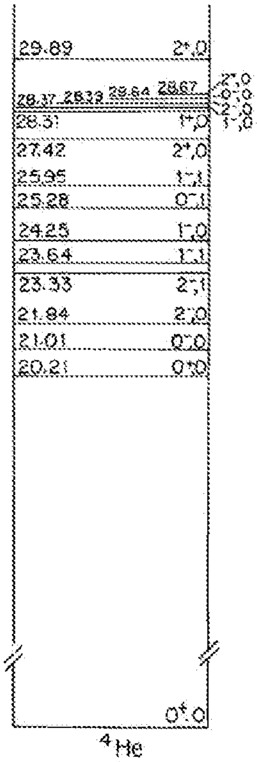

Fig. 8: Excited states of the ^{4}He nucleus as reported by Tilley et al. 1992.

Spitaleri et al. 2016 argue that for some nuclei, enhanced fusion rates observed in experiments can be explained by particular clustering configurations of nucleons in such nuclei. For instance, the six nucleons in ^{6}Li nuclei are believed to form 2-nucleon and 4-nucleon clusters whereas the nucleus as a whole can be thought of as a nuclear molecule of two clusters. In such a configuration, tunneling probabilities would be higher than suggested by the Gamow model which does not consider differences in nuclear structure across different nuclei.

Starting with Oppenheimer and Phillips (1935; see also Bethe 1938), a large number of authors have considered fusion enhancement through the polarization of nuclei (see Greife et al. 1995; Paetz gen. Schieck 2010; Bartalucci 2017; Benyo et al. 2018; Hupin et al. 2019). In proposed polarized fusion and different variants thereof, the spins or orientations of projectile and target nuclei are to be aligned, allowing for particular incidences of nucleons coming together in the fusion reaction and therefore different reaction rates and reaction products. For instance, in the case of a deuteron projectile, the incoming deuteron may approach the target nucleus with the "neutron end" which is less repulsive than the positively charged "proton end." At high energies such as in thermonuclear fusion, a main concern is whether polarization prevails in a plasma. At low temperatures such as in solid-state environments, some authors (Bencze and Chandler 1996) argue that polarization effects remain too small to become practically relevant (estimated <1% rate enhancement for low-energy fusion between light nuclei).

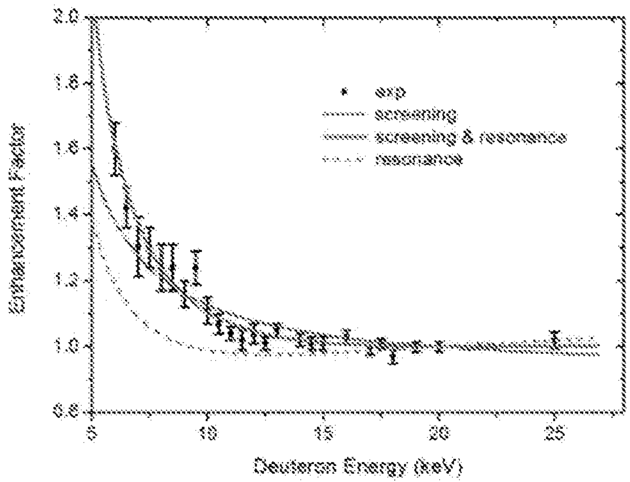

Fig. 9: Experimentally determined D+D cross sections at low energy (normalized to value at E = 20 keV) and theoretical predictions (Czerski et al. 2016). Considering screening alone (blue) cannot account for the observed fusion rate. Screening and an assumed resonance (red) would be able to account for the data.

Predicting nuclear resonances

An evaluation of hypotheses and proposals laid out above requires tools of nuclear physics. In nuclear physics, resonances have traditionally been determined phenomenologically, based on scattering experiments. Alongside such experimental efforts, models have been developed -- initially heavily reliant on experimental data -- and, more recently, also increasingly based on first principles approaches.

First principles modeling of nuclear reactions draws on nuclear structure models which in turn rely on appropriate nucleon-nucleon interaction models. Such models have been developed based on experimental data that allow for inferences about sizes and shapes of nuclei, energy levels and binding energies, scattering behavior, nuclear reactions and resonances. As in other areas of science, the initial top-down deconstruction of phenomenological data then informs the development of bottom-up models. These in turn can be used for predictions of new observations in experimentally inaccessible regimes. In this process of deconstruction and reconstruction, critical decisions need to be made as to what aspects to include in models and what reductions can be justified in order to keep resulting models mathematically and computationally tractable.

In first approximation toward the development of models and related intuition, nuclear excited states that cause resonances can be thought of as vibrational modes of nuclei: nuclei can "quiver, ring or even breathe" as Bertsch describes different dynamics of multi-nucleon systems (1983). Fig. 10a illustrates three common modes of nuclear excited states: nuclear monopole, dipole and quadrupole modes. The modes are caused by the interaction of nucleons as governed by nucleon-nucleon interactions between all nucleons and, to a lesser degree, by Coulomb interactions between the positively charged nucleons (i.e. the protons). Additionally, as alluded to above, nucleons can form molecule-like clusters which further impact the vibrational modes and thus the resulting excited states and resonances. Specifically, the ^4He compound nucleus that results from D+D fusion is expected to be able to exist in several different 2-2 and 3-1 cluster configurations. Instabilities in the excited states of nuclei lead to different reaction products (decay channels) and angular distributions of reaction products – which can be measured experimentally. For instance, the 20.21 MeV state of ^4He (as seen in Fig. 8) is believed to have a 3-1 structure, where the individual nucleon can be either a proton or a neutron (Aoyama and Baye 2018).

Nuclear excited states are typically short-lived and excitation occurs in the context of nuclear reactions. Incoming projectiles can transfer energy as well as additional nucleons to the target system. Fig. 10b shows a cartoon that illustrates how an incoming projectile – e.g. a photon, neutron, or deuteron – brushes over a target nucleus as a particle wave. If the projectile energy and structure resonate with the target, certain nuclear reactions such as absorption can occur (instead of scattering). This would manifest as resonance peaks in cross section diagrams such as the exemplary photon absorption peaks seen in Fig. 10c. The case of deuteron absorption i.e. nuclear fusion is analogous. Such absorptions then typically lead to an excited state in a resulting compound nucleus and subsequent breakup into reaction products. This is, in essence, the system that needs to be modeled to predict nuclear resonances.

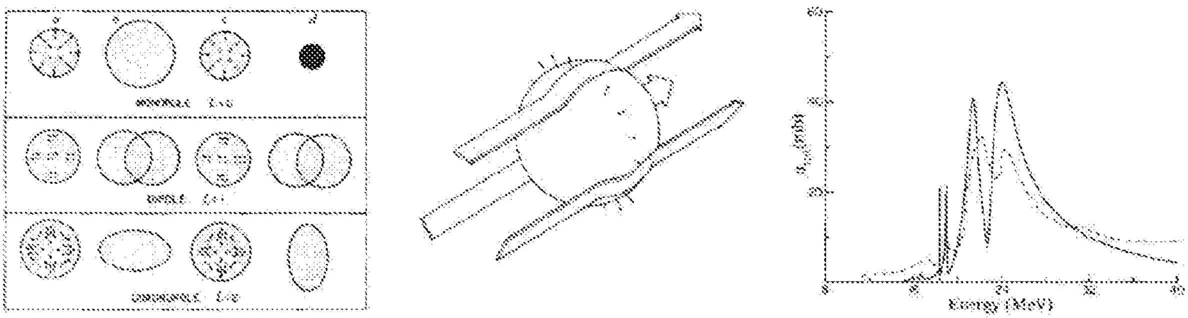

Fig. 10: (a) Three common types of oscillations corresponding to nuclear excited states: monopole, dipole, and quadrupole oscillation; (b) interaction of an incoming particle wave (shown as arrows) with a target nucleus; (c) example of a photon absorption spectrum (in this case for ^{16}O) -- the solid line corresponds to predictions from theory and the dashed line to experimental observations. All images from Bertsch 1979.

The underlying nucleon-nucleon interaction – also known as the nuclear force or strong force -- exhibits a number of features that make it particularly difficult to model: it exhibits three-nucleon effects in addition to two-nucleon effects; it can saturate based on the number of affected nucleons; it is short-range yet strongly attractive at <2 fm and strongly repulsive at <1 fm; and it is not organized around a center as in the case of electrons around a nucleus. A central question has been whether nucleon-nucleon interactions could only be explained based on even more fundamental quantum chromodynamics (QCD) models that consider detailed quark interactions of which nucleons are composed, or whether it could be sufficiently simplified and parameterized (see Paetz gen. Schieck 2010 for background). In recent years, a wide consensus emerged around chiral effective field theory-based models of the nucleon-nucleon interaction which assume that the interaction is mediated by the exchange of virtual mesons, analog to how the electromagnetic interaction at the atomic scale can be understood as being mediated by the exchange of virtual photons (Machleidt 2011). This approach does exhibit the advantage of representing nucleon-nucleon interactions comparatively accurately without requiring the full QCD treatment.

Turning to concrete modeling approaches, a basic nuclear structure model is the nuclear shell model. The shell model emerges from solving the Schrödinger equation in a mean field nuclear potential such as the Woods-Saxon potential seen in section 1, Fig. 1a. In this context, "mean field potential" means a potential where all nucleons are assumed to be equally affected by the nucleon-nucleon interaction. As can be seen from the listing of characteristics of the nucleon-nucleon interaction in the previous paragraph, this assumption will likely leave out some dynamics among nucleons. Nevertheless, this approach leads to a simple quantum mechanical model -- not unlike the harmonic oscillator model for excited states in atoms -- that can be solved and that leads to a range of nuclear excited states. Over time, the nuclear shell model evolved to make better use of insights gained about nucleon-nucleon interactions. A recent first principles variant of the shell model is the so-called no-core shell model (NCSM) which includes an explicit treatment of three-nucleon interactions (Barrett et al. 2013). This allows for an integration of the previously discussed chiral effective field theory-based models of the nucleon-nucleon interaction with higher level nuclear structure models. Overviews of recent first principles unification efforts in that direction are given by Bacca 2016 and Quaglioni 2018.

In addition to non-relativistic models such as the nuclear shell models, relativistic models of the nucleus have been developed. In different variants of the nuclear shell model, nucleons are typically treated as non-relativistic particles based on the argument that they are comparatively heavy and slow. This allows for the use of the nonrelativistic Schrödinger equation instead of the relativistic Dirac equation and keeps models from growing even more complex. However, this modeling choice comes at the price of not being able to account for some experimentally observed phenomena such as the nuclear spin-orbit interaction. The nuclear spin-orbit interaction follows intrinsically from relativistic nuclear models but needs to be added phenomenologically through correction terms in nonrelativistic models (Goeppert Mayer 1950) – a circumstance that will be picked up again in the next section of this paper when interactions between nuclei are discussed.

Alternative nuclear models include density functional theory (DFT)-based models which seek to transfer DFT-based approaches from the atomic scale to the nuclear scale -- therefore trading off computational expense with approximations. Introductions to nuclear DFT are given by Dobaczewski 2010; Stoitsov 2010; Colo 2018. Nuclear DFT models can specifically provide important qualitative insights into the structure and behavior of some nuclei. However, quantitative predictions from DFT often fall short substantially when compared with experiment. An advantage of DFT-based methods is their ability to scale well even to medium- and large-sized nuclei where most first principles approaches become computationally overwhelming. Fig. 11a shows simulations of deuterons in two different substates which were generated from nuclear DFT-based methods. The figures provide some intuition for the polarized fusion arguments cited above which suggest that the relative orientation of two nuclei (such as two deuterons as seen here) matter for predicting their nuclear reaction dynamics and outcomes. A computational alternative is the Quantum Monte Carlo method of which recent overviews are given by Carlson et al. 2015 and Lynn et al. 2019.

Another conceptual approach to modeling nuclear structure, which recently received a surge of attention, is the skyrmion model (Skyrme 1954; Naya & Sutcliffe 2018). In this approach, some of the intricacies of the nucleon-nucleon interaction are captured by treating nuclei as quantum fields with so-called skyrmions – quasi-particles that can be described as knots or twists in quantum fields. Similar to nuclear DFT, skyrmion-based models allow for the prediction of nucleon density. Additionally, more recent skyrmion models can predict nuclear binding energies in reasonable agreement with experimental values. Fig. 11b shows predicted nucleon densities for nuclei from A = 1 to A = 8. Predicted clustering can be seen clearly.

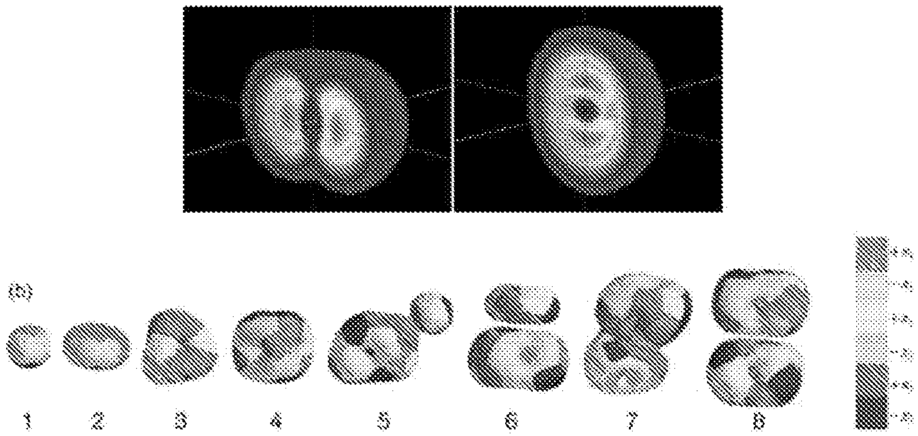

Fig. 11.: Representations of atomic nuclei from nuclear structure models: (a) deuteron densities in M = 0 and M = 1 magnetic substates. Highest densities are in red, lowest in blue. Image from Garcon & Van Orden 2001. (b) Baryon density isosurfaces that represent shapes of nuclei up to mass number 8. Image from Naya & Sutcliffe 2018..

Thus far, the discussion centered on models for predicting nuclear structure. From the considerations at the beginning of this section, one could deduce that nuclear structure models and nuclear reaction models ought to be closely related. While recent efforts toward the integration of nuclear structure and nuclear reaction models are indeed underway, historically this was not always the case. Traditionally, nuclear reaction models were not constructed from first principles but heavily phenomenological and thus dependent on experimental input. Meissner (2014) summarizes the process of predicting fusion cross sections: "typically, scientists perform experiments at the lowest energy at which fusion reactions can be observed—from thousands down to hundreds of kiloelectronvolts—and then make theoretical extrapolations to lower energies of interest. However, the resulting estimated low-energy data may be unreliable because nucleon dynamics are disregarded in those calculations."

A common method to that end is the phenomenological R-matrix method (Peierls & Kapur 1938; Wigner & Eisenbud 1947) which provides a framework for fitting experimental data and deriving parameterized cross section estimates. However, even this process is not purely deterministic and requires some judgment, and in some cases "arbitrary" parameter choices (Descouvermont & Baye 2010). At the heart of the R-matrix method lies a separation of the configuration space into an outer region where short-range forces are ignored and an inner region which is considered confined. This approach allows for the calculation of both scattering states (outer region) and bound states (inner region). The R-matrix method has been evolved into a variant known as the computational R-matrix method which is attributed the advantage “that narrow resonances which can escape a purely numerical treatment are easily studied” (Descouvermont & Baye 2010). In either case, once an R-matrix is calculated for a given nuclear system, then the so-called S-matrix (scattering matrix) can be derived from it. The S-matrix relates initial states to final states and some of its poles are indicative of resonances (and others of bound states). Many of the cross section plots for fusion reactions, as shown in Fig. 7b, are determined this way -- some relying more on experimental data and others more on computational estimation.

The concept of the S-matrix was first introduced by Wheeler (1937) in the context of developing the Resonating Group Method (RGM). The RGM represents early efforts to link nuclear reaction properties to nuclear structure properties explicitly and is also still used today. Originally devised for describing resonant transfer of groups of electrons in scattering processes, the approach was later extended to also apply to groups of nucleons in scattering processes (Nielsen 2016). While the original RGM approach does not consider the structure of nuclei in as much detail as most of the nuclear structure models discussed above, it does consider different clusters of nucleons and the interactions among them. Recent efforts seek to integrate RGM approaches to nuclear reaction modeling and advanced shell model approaches to nuclear structure modeling such as NCSM (see Quaglioni et al. 2012 for a discussion of such efforts). Since NCSM already represents an integration between nucleon-nucleon interaction models and nuclear structure models, such efforts promise to provide a unified picture connecting nucleon interactions to nuclear structure theory as well as nuclear reaction theory.

Returning to the concrete case of the D+D ⍰ ^{4}He reaction for which discrepancies between experimental data and theoretical predictions exist, Czerski et al. 2016 ground their proposal for a new resonance near a hypothetical 23.85 MeV excited state of the ^{4}He compound nucleus on RGM calculations. Specifically, they refer to Kanada et al. 1986 who suggest that a resonance “very close to the threshold of the d+d channel” may exist. At the same time, the authors imply – like others (Aoyama & Baye 2018) -- that the four-nucleon system is complicated and that certain assumptions are required to make such calculations. It appears that more research is necessary to assert or reject theoretical predictions of proposed near-threshold resonances in the ^{4}He system.

Challenges with predicting nuclear resonances

A number of points need to be considered in the evaluation of previous research and in view of future research in this area:

First, because of the complexity of the nuclear system, all of the modeling approaches introduced face a common challenge: a tradeoff between theoretical comprehensiveness and computational tractability. This compromise is expressed by Quaglioni, an expert in NCSM techniques, as follows (Meissner 2014): “Our model can often contain billions of terms. While more terms improve the accuracy of the model, they also make solving the Schrödinger equation more difficult.” Consequently, “these results cannot be considered conclusive until more accurate calculations using a complete nuclear interaction [...] are performed.” Similarly, Al Hassid (2020) comments on nuclear DFT approaches: "Density functional theory (DFT) is unique in providing a global theory of nuclei. However, it can miss important correlations beyond the mean field."

Second, nuclear reaction and resonance prediction is often very sensitive to small changes in corresponding models. During the modeling process, often assumptions and fairly arbitrary choices need to be made by researchers that can result in large differences in predicted outcomes. Quaglioni emphasizes predicted resonances are "extremely sensitive to higher-order effects in the nuclear interaction, such as three-nucleon force (not yet included in the calculation) and missing isospin-breaking effects in the integration kernels." Given this background, it is maybe not surprising that more resonances continue to be predicted -- whereas some of them end up being experimentally confirmed and others not (see Shirokov et al. 2016; Hupin et al. 2019 for recent predictions of new resonances).

Hypotheses and research questions

In this section, we considered under what circumstances the Gamow model may need to be extended to endogenize underlying nuclear physics to more fully capture mechanisms that could potentially affect outcome variables of interest.

We started out by noting that -- as is common in tunneling applications in AMO and CM physics -- resonances can enhance tunneling probabilities and rates. With respect to nuclear resonances, several groups have proposed mechanisms that suggest fusion rate enhancement ranging from several to tens of orders of magnitude. Proposed enhancement mechanisms based on polarized fusion, nucleon clustering, and near-threshold resonances are conceivable and can be motivated by the established literature. The hypotheses of fusion rate enhancement from polarized fusion in solid-state environments would benefit from further modeling and quantification. As discussed, some preliminary estimates suggest that enhancement from polarized fusion-related mechanisms may remain below 1%. However, to date, modeling and experimental efforts remain limited and far from being exhaustive. As for near-threshold resonances, Czerski et al. 2016 propose that an additional fusion rate enhancement on the same order as screening-based rate enhancement -- i.e. about 15-25 orders of magnitude – could be explained this way. If such a resonance were to exist -- which is conceivable but not confirmed -- then such estimates appear plausible.

However, we also found that the prediction of nuclear resonances is a difficult and still an emerging field. To increase the reliability of nuclear structure predictions what is likely needed is a combination of unified nuclear models that integrate models for nucleon-nucleon interactions, nuclear structure, and nuclear reactions; ample computing resources; and dedicated, targeted experiments designed to investigate specific resonance-related hypotheses.

To test and either confirm or reject hypotheses discussed in this section, we consider the following research questions worthy of further investigation:

- *How can nuclear reaction resonances be identified from theoretical first principles models?*
- *How can the reliability of such predictions be improved and quantified?*
- *What dedicated experiments would be suitable to test for predicted resonances of interest?*

4.3. Zooming out: interatomic resonances from interactions with other subsystems

A central question in many AMO and CM physics problems is the choice of system boundary, as reflected in the distinction between open quantum systems and closed quantum systems. The Gamow model assumes a two-body process where released energy is emitted into an environment incoherently: the fusion products can take on a very large number of different configurations of position and momentum which makes the process irreversible -- akin to the emission of heat into a bath in a classical system. This incoherent dissipation of energy makes the Gamow model correspond to an open quantum system. The question arises whether other significant channels of energy redistribution might exist. If couplings to other subsystems in the environment are sufficiently strong, released energy might also be accommodated in alternative ways, for instance via the excitation of nearby nuclei -- a process with the potential of being coherent i.e. reversible. If the latter process were dominant, the system could be viewed, in first approximation, as a closed quantum system where energy gets redistributed internally.

This distinction is important for fusion rate calculations because the available energy channels and their characteristics impact reaction probabilities. Note, for instance, that the Fermi Golden Rule calculation of transition rates only applies to energy transfer to a continuum of states i.e. to incoherent processes[5]. As will be seen from several examples discussed below, tunneling and other forms of energy transfer can occur at faster rates in a resonant and closed quantum system compared to a nonresonant and open quantum system. The distinction between one and the other – and therefore also the determination of system boundaries -- is given by the strengths of couplings that exist between the system of interest and potential subsystems in the environment. Consequently, special attention will be given to relevant couplings and coupling strengths later in this section.

Nuclear fusion as a two-state quantum system

A central feature of Quantum Electrodynamics (QED) is its ability to account for complex energy conversions and state changes (Feynman 1985; Andrews et al. 2020). A well-known example is the explanation of spontaneous emission – a quantum system's transition from an excited state to its ground state – by exchanging energy with a quantized field in the environment (such as a photon field populating the vacuum or a phonon field populating the surrounding atomic lattice). Such dynamics are typically explored in the simplest version of the problem constituting a field and a two-state system[6] (see Jaynes & Cummings 1963; Cohen-Tannoudji et al. 1973). The corresponding model is sometimes described as a *dissipative two-state system*.

A tunneling problem such as in the case of fusion in the Gamow model can also be modeled as a two-state system. Here, the first state describes the system before tunneling and the second state describes the system after tunneling. If the potential takes the form of a symmetric double well, both states can be degenerate i.e. at the same energy levels and highly resonant. If the potential takes the form of an asymmetric potential, the higher state can be viewed as an excited state and the lower state as a ground

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[5] As will become clear below, the Gamow model can be reframed such that the incoherent tunneling rate can be calculated via Fermi's Golden Rule (see Raju 2014 for a concrete example).

[6] In quantum information science a two-state system is typically described as a qubit. In biophysics this could be a fluorescing molecule with excited and ground state. In semiconductor research this could be a quantum dot.

state. In either case, the barrier between the two wells is inversely proportional to what can be thought of as the coupling between the two states. In other words, a large tunneling barrier corresponds to a weak coupling between excited state and ground state -- and thus a long decay time.

From this perspective, a system of two close deuterons such as discussed in section 2 can be viewed as a highly excited (as well as highly clustered and highly metastable) state of a four-nucleon system. This framing was proposed by Julian Schwinger in 1990: "two deuterons in close proximity can be thought of as an excited state of He-4." Lending more physicality to this picture, Walker and Dracoulis in a 1999 paper on nuclear structure propose the existence of "secondary energy minimum at large elongation of the nucleus" -- although the nucleon systems they consider still exhibit much smaller scales at the sub-picometer level. In the two-state picture of nuclear fusion, the state transition would then correspond to a decay to a more stable, and thus energetically preferred, lower state -- in the case of D+D ⍰ ^{4}He fusion, from the four-nucleon configuration at greater distance to the four-nucleon configuration at greater proximity. The two states can be expressed as $|D_2\rangle$ and $|^4He\rangle$. As seen in Fig. 12, the excited state can be associated with energy -4 MeV (the sum of the binding energies of the two nucleon pairs) and the ground state with energy -28 MeV (the binding energy of the integrated four-nucleon system). The energy transition of 24 MeV corresponds to the energy released in the exothermic decay and thus the mass difference between D_2 and ^{4}He. In summary, the two nucleon pairs in the D_2 molecule are viewed as a highly clustered four-nucleon system with a state transition coupling that is greatly weakened by the barrier between the two constituting parts. The fusion rate then corresponds to the transition rate of the two-state system from the $|D_2\rangle$ state with lower binding energy -- and thus higher excitation energy -- to the energetically favored $|^4He\rangle$ state. Spontaneous emission in the two-state picture would correspond to tunneling in the Gamow picture with a decay rate equivalent to the fusion rate i.e. 10^{-64}/s for the unscreened D_2 molecule.

This framing of the fusion problem so far remains fully compatible with the Gamow model. However, in this framing, the full might of the modern QED toolbox and associated literatures can be brought to bear. We can already take note of the fact that, in other contexts, the QED perspective applied to equivalent two-state systems offers various ways of transition rate enhancement. We will first introduce known mechanisms of such decay acceleration at the atomic and molecular level, then discuss whether and under what circumstances those may extend to the nuclear level.

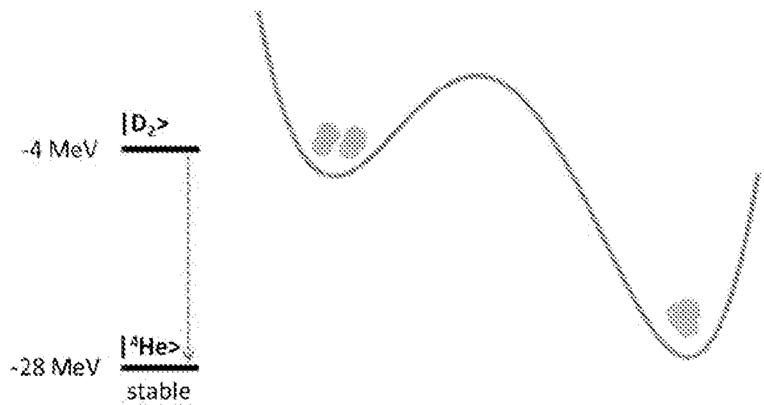

Fig. 12: The $D_2 \rightarrow {}^4He$ tunneling problem in the Gamow picture (right) and the equivalent representation as a two-state system (left).

Two-state transition rate enhancement at the atomic and molecular level

In the dissipative two-state system introduced above, a single two-state system is coupled to a field such as a photon or phonon bath. The resulting dynamics depend greatly on the parameters involved: If the coupling to the field is large compared to the transition energy of the two-state system, then direct energy exchange is possible e.g. excitation of an atom by a photon or deexcitation of a molecule by emission of phonons. If said coupling is weak compared to the transition energy – which would almost certainly be the case if comparatively large nuclear transitions were involved – then other dynamics may be dominant as direct energy exchange becomes very unlikely (Andrews 2009). An alternative dynamic frequently observed in systems with comparatively weak couplings is known as resonance energy transfer (RET; see Jones & Bradshaw for a recent overview). RET occurs when a shared field does not itself absorb or emit the full quantum of energy in the transition of a (single) two-state system but instead mediates simultaneous deexcitation and excitation between (multiple) nearby two-state systems. An excited system with state |a*> and a stable system with state |b> coupled to the same field can no longer be treated separately and will form the entangled state |a*b> (or, more precisely, the state |a*b,n> where n keeps track of the number of photons or phonons in the field i.e. the field's energy). Excitation transfer can then be described as the state change |a*b> → |ab*> whereas the transfer rate is a function of the coupling matrix element in the corresponding mixed state Hamiltonian that links the two states.

In such configurations of coupled two-state systems, transfer of excitation can occur even in the case of very weak couplings, particularly if the donor and receiver states are resonant i.e. exhibit matching energy levels. This can be confirmed through evolving the respective Hamiltonians, as discussed in the literature (DeLosh & Grant 1970; Andrews 2009), as well as by classical analogs of coupled oscillators[7] (see Fig. 13).

[7] Besides the examples given below, a famous analog is Huygens' 17th century observation that, after some time, wall clocks can end up with synchronized fingers due to the weak coupling provided by the shared wall – a phenomena that is still the subject of much interest and ongoing research (see Oliveira & Melo 2015).

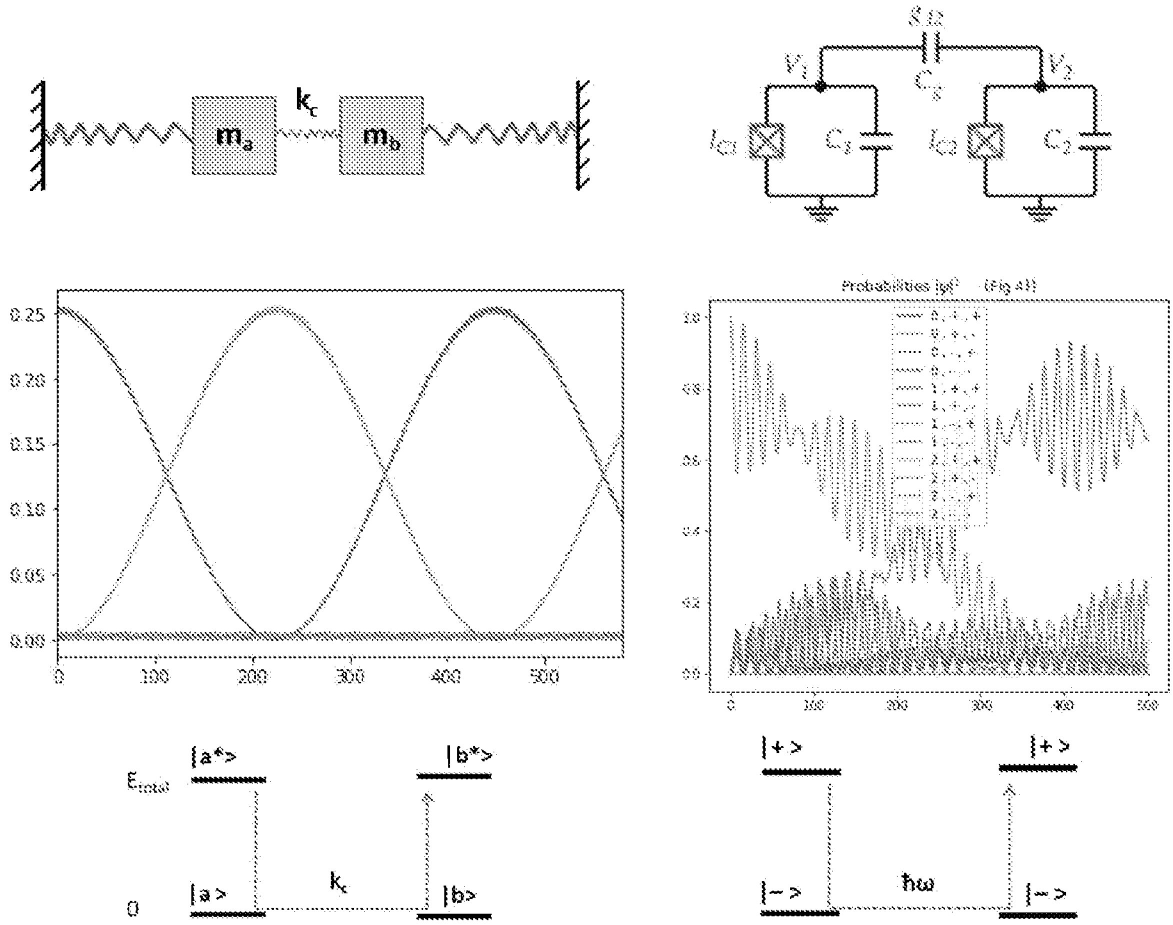

Fig. 13: Classical and quantum versions of coupled systems with weak coupling: (a) LEFT: two simple harmonic oscillators with a weak coupling in the form of spring k_c. The plot below shows the total energy (kinetic and potential) each oscillator holds. Energy on the order of 0.25 units moves back and forth between the two oscillators even though the coupling energy is about two orders of magnitude smaller. (b) RIGHT: a corresponding quantum version of the problem -- two qubits coupled by g_{12}. Shown in the plot are not the energies of each qubit (which are discrete) but instead their probability amplitudes (which are continuous). The weak coupling facilitates oscillation in the probability amplitudes between the two qubits, leading to state transitions during decoherence. Image from Lilley et al. 2020.

A concrete example for RET is provided by Kaur et. al. 2018 where state transition rates at the atomic level are accelerated. The authors use Rb atoms in Rydberg states which are long-lived outer excited states of atoms. In the experiments, a pair of such Rb atoms is prepared, one in an upper state |60p> and another in a lower state |60s>. The upper state is considered metastable with a natural decay time on the order of 500 s. A coupling exists naturally between nearby atoms due to a transition dipole moment associated with the excited states. The researchers then observe repeated excitation transfer across atoms – in other words, simultaneous deexcitation and excitation -- with a rate on the order of 1 us (see Fig. 14). The central point here is that in such a system, studying the two states |60s> and |60p> of individual Rb atoms independently (i.e. without considering the dynamics introduced by couplings to other subsystems) would lead to an underestimation of the transition rate amounting to about 8 orders of magnitude. If similar mechanisms can affect atomic nuclei under circumstances where couplings to other subsystems exist, then the fusion rates predicted by the Gamow model would fall short of actual rates.

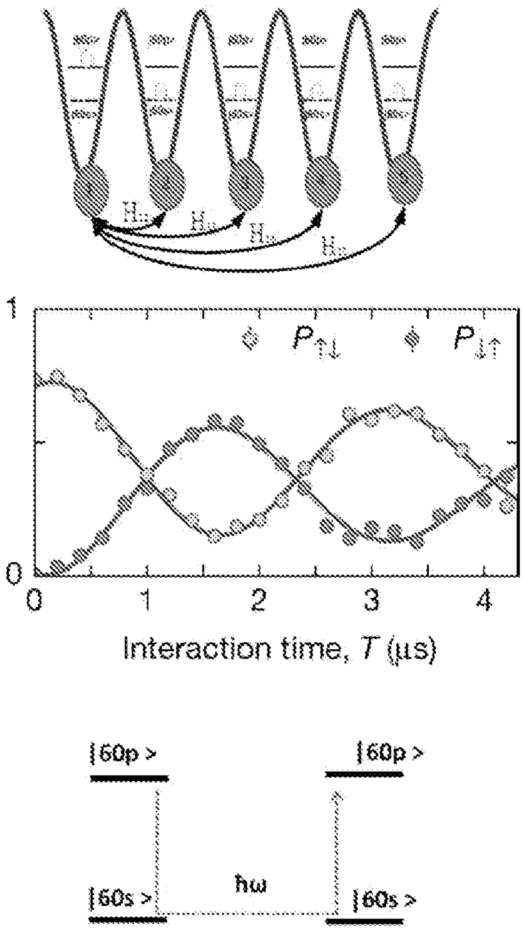

Fig. 14: (a) An example for a chain of donor and receiver atoms participating in RET. Here, the first atom is in the upper state |60p> and all other atoms are in the lower state |60s>. The atoms are coupled via the dipole coupling matrix elements H_{ij}. Due to matching energy levels, the system is already resonant and energy will redistribute in this closed quantum system in an oscillatory manner. Image from Kaur et al. 2018. (b) The oscillatory behavior of state probability amplitudes during excitation transfer, as measured in a RET experiment with two Rydberg atoms going back and forth between |60p> and |60s> states. Compare the observed behavior with the numerical results in Fig. 13. *Image from Barredo et al. 2018.*

An observer might argue that deexcitation in the context of excitation transfer should not be viewed as an acceleration of decay since an equivalent state is similarly excited. However, the RET literature suggests that excitation transfer can be combined with downconversion (also known as quantum cutting), a process where excitation gets resonantly transferred to two or more matching states – which, after decoherence, can further decay and thus move energy from the closed quantum system to the environment (see Fig. 15 and de la Mora et al. 2017; Andrews 2009).

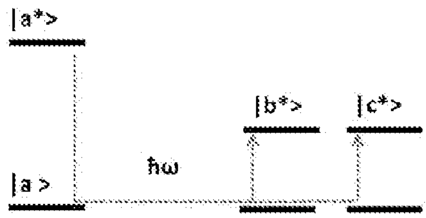

Fig. 15: Excitation transfer in combination with downconversion (quantum cutting). In a coupled system, energy can transfer resonantly to multiple donors as long as the receivers can accommodate the total donor energy. During coherence, energy is expected to oscillate back and forth between donors and receivers -- a process that can be cut short by decoherence and subsequent decay.

The quantification of coupling strengths and commensurate transition rates is the subject of much ongoing research. Generally, the larger the coupling strength, the faster the transition rate. Calculations of coupling strengths will be discussed in the next subsection. It should be noted, however, that many authors observe transition rates that are substantially faster than predicted based on calculated coupling strengths. Such authors then considered what mechanisms might cause an amplification. The quantum coherent phenomenon of superradiance offers an explanation for the enhancement of coupling strengths observed in some RET experiments. Superradiance theory predicts that, if a large number of quantum states is coherently excited, then deexcitation occurs much faster than if only a small number is excited. Bang et al. 2019 show that – analog to other systems where superradiant effects occur -- an enhancement of the RET transfer rate by a factor up to N^2 can be expected due to superradiance (where N corresponds to the number of two-state systems participating in the resonant process). Brekke 2009 reports on RET experiments with Rydberg atoms where an enhancement of the transition rate by an order of magnitude is attributed to superradiance. Newman et al. 2018 report on RET experiments with transfer rate enhancements of about two orders of magnitude. Scheibner et al. 2007 report "superradiant lifetime changes" i.e. accelerated decay from excited states in quantum dots. Wang et al. 2007 report on Rydberg atoms with a "decrease of the radiative excited state lifetimes" of two orders of magnitude.

Two-state transition rate enhancement at the nuclear level

The previous section discussed transition rate enhancement with examples on the atomic scale. The insights gained are relevant to nuclear fusion rates if similar enhancements can be expected to be applicable – and ideally experimentally observed – at the nuclear scale. Here we present two examples that suggest this may be the case.

Chumakov et al. 2018 report on experiments with a sample comprising ^{57}Fe nuclei which are excited to the 14.4 keV nuclear state by a X-ray Free Electron Laser. The documented lifetime of the 14.4 keV nuclear state is about 100 ns. However, the authors observe an acceleration of decay as the number of simultaneously excited nuclei is increased. They attribute this accelerated state transition to superradiance at the nuclear scale which "leads to enhancement of emission and strong 'speed-up' of the collective response." Fig. 16 shows experimental data that exhibit the relationship between the number of excited nuclei and the acceleration factor obtained. For N=20 nuclei, an enhancement of the nuclear transition rate by a factor of 15 is observed.

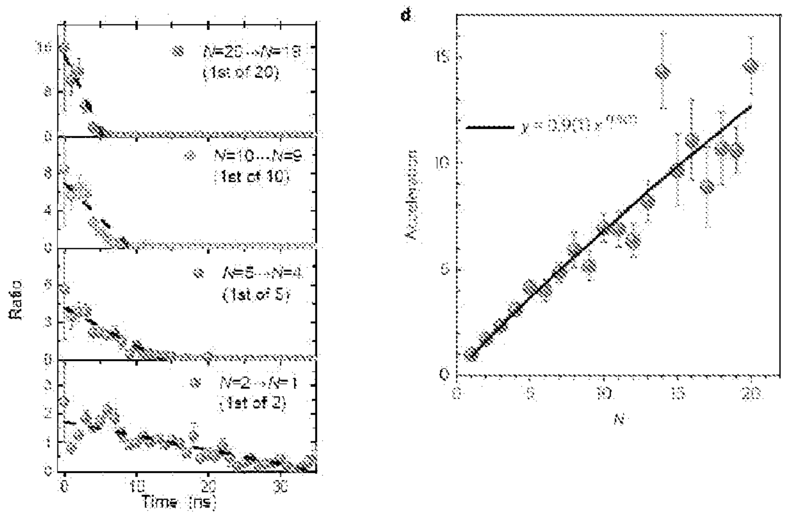

Fig. 16: (a) Decay times in ns of the first gamma out of a group of N nuclei where N=20, N=10, N=5, N=2 from top to bottom (normalized by the average decay time of the group). (b) Acceleration of gamma decay as a function of group size of excited nuclei. Images from Chumakov et al. 2018.

In experiments with samples constituting ^{57}Fe nuclei in ground state and $^{57}Fe^*$ nuclei in excited state (continuously populated by decaying ^{57}Co nuclei), Metzler et al. 2020 report a delocalization of 14.4 keV gamma emission on the order of 1 mm during the application of mechanical stress. In interpreting these results, the authors suggest that the observed emission change may be caused by repeated phonon-mediated excitation transfer (see Fig. 17) with a step size on the order of a typical THz phonon length (10 nm). A transfer range of 1 mm would then correspond to a total of 10^5 transfers within the 100 ns state lifetime, and thus an estimated transfer time of about 1 ps for deexcitation of the donor and excitation of the receiver. If these experiments can be further validated, they would represent an enhancement of the nuclear transition rate by a factor of 10^5.

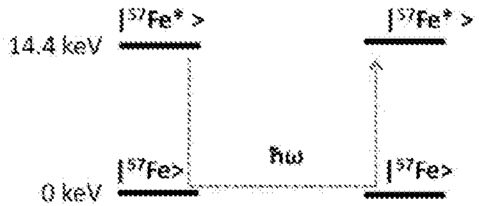

Fig. 17: Excitation transfer of 14.4 keV nuclear excitation from excited state donor to ground state receiver nuclei suggested to account for delocalization of gamma emission reported by Metzler et al. 2020.

Common couplings between molecules, atoms, and nuclei

In most RET applications at the atomic and molecular level, the coupling that mediates excitation transfer between donors and receivers is a form of electromagnetic dipole coupling. In the example of Rydberg atoms discussed above, transition dipole moments are induced by the excited states. These dipole moments determine the coupling matrix element μ_{fi} (connecting final and initial states in a transfer) that enters the equation for the resulting coupling strength between donor and receiver:

$$V = \frac{\mu_{fi}\,\kappa}{r^3} \qquad \text{(Eq. 6)}$$

Here μ_{fi} comprises components of atomic wave functions too extensive to reproduce here (see Šibalić 2020), *r* represents the distance between the interacting particles, and *κ* a geometric orientation factor which is sometimes ignored when the particles are randomly oriented. *V* itself represents an interaction term in the system Hamiltonian that can be evolved to obtain the overall system dynamics. It can be seen from the equation that this coupling is strongly distance-dependent. Even more so, the transition rate is proportional to the square of the coupling strength. Consequently, this kind of coupling is typically assumed to become vanishingly small beyond a narrow range. As already discussed above, in some RET experiments, an enhancement of the coupling due to superradiance is possible. Moreover, in some RET experiments, another type of enhancement is obtained by applying an electric or magnetic field. This leads to a splitting of energy levels (Stark and Zeeman effects) and can thus lead to an enhancement of the coupling strength (Andrews & Bittner 1993; Bohlouli-Zanjani et al. 2007; Grimmel et al. 2015). In first approximation, this can be viewed as a correction term added to the coupling *V*:

$$V_{correction} = \mu_{fi}\,\boldsymbol{D} \qquad \text{(Eq. 7)}$$

Here ***D*** is the electric displacement of the applied electric field. Varying the electric displacement -- i.e. the electric field -- therefore allows for some tunability of the coupling strength and level shifts.

Next, we will present some concrete values for coupling strengths commonly observed in experiments. In Rydberg atoms at interatomic distances, the coupling strength can be on the order of 1-10 ueV (Šibalić 2020; Barredo et al. 2018). For comparison, transition energies between Rydberg states such as the |60p> and |60s> state are about 70 ueV. This results in a comparatively large ratio of about negative one order of magnitude between coupling strength and transition energy -- which is one of the reasons why Rydberg atoms are often used to study RET phenomena. However, not all states used in RET experiments exhibit such strong coupling strengths and such large coupling-to-transition-energy ratios. Ditzhuijzen 2009 lists interaction strengths below 1 neV for some Rydberg states used in excitation transfer experiments. Scholes et al. 1995 list a coupling strength on the order of 1 meV for single-digit eV level states at a distance of about 0.4 um. These values are consistent with what is reported in Kim et al. 2016. Overall, this suggests a coupling-to-transition-energy-ratio of negative 3-4 orders of magnitude.

In contrast to atoms, nuclear electric dipole moments offer no suitable coupling with the environment. That is because properties of nuclear structure prevent the existence of substantial dipole moments. Electric quadrupole moments do exist for nuclei, however, the coupling they might offer is vanishingly small. Alder & Steffen 1964 report nuclear level splitting from electric quadrupole interaction on the order of 10^{-19} eV resulting from the application of an electric field of about 10 kV/cm^2. In comparison, the energy level splitting from the application of a magnetic field of 20,000 Gauss is given as 10^{-7} eV. This is consistent with common measurements in Nuclear Magnetic Resonance (NMR) applications, where nuclear level splittings on the order of 10^{-12} eV or lower are observed. Practitioners of solid-state NMR concern themselves with further interactions between nuclei and their environment such as with nearby electrons and phonons. Such interactions are sometimes summarized as nuclear spin interactions and come in different flavors (see Fig. 18). However such interactions are generally on a similar order as the small magnetic interactions employed in NMR, or below. Comparing some of the larger coupling strengths identified in this paragraph with one of the lower nuclear transitions such as the 14.4 keV transition of ^{57}Fe, still yields a coupling-to-transition-energy ratio of about negative 12 orders of magnitude (compare to the negative one order of magnitude in the Rydberg atoms experiments).

The numbers resulting from such considerations suggest that couplings commonly considered at the atomic and molecular level are too weak to interact with atomic nuclei; and that based on such couplings, resonance transfer effects as discussed above would not be expected to manifest at the nuclear level on a relevant timescale. This would imply that the Gamow model's assumption of two-body fusion as an independent process would be justified. However, before gaining confidence in such a conclusion, other possible couplings between nuclei need to be considered. This will be done in the following section.

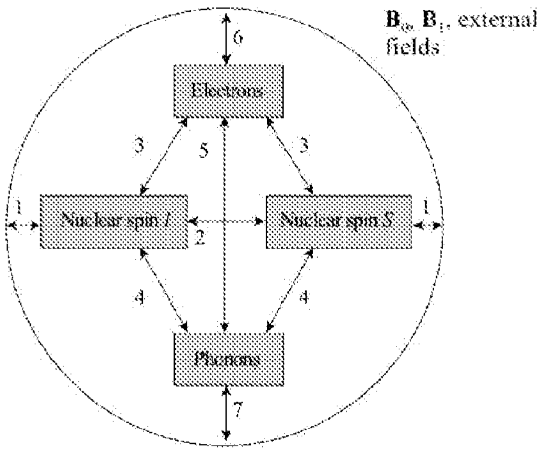

Fig. 18: Common types of nuclear spin interactions are typically below 10^{-7} eV. Listed here are: 1 Zeeman interaction of spins. 2 Direct spin interaction. 3 Nuclear spin-electron interaction and indirect spin interaction. 4 Direct spin-lattice interaction. 3-5 Indirect spin lattice interaction via electrons. 3-6 Shielding and polarization of nuclear spins by electrons. 4-7 Coupling of nuclear spins to sound fields (Mehring 1983)

Other couplings between nuclei

The discussion in the previous section yielded that common couplings at the atomic level -- such as electric dipole-dipole coupling -- are much less relevant at the nuclear level. This is especially the case for two reasons: compared to the atomic level, electromagnetic interactions tend to be much weaker at the nuclear level, and nuclear transitions much larger – both circumstances owed to the specific properties of the nuclear system.

This suggests that it may be worthwhile to consider whether some of the specific properties of the nuclear system may work the other way i.e. whether some nuclear properties cause other couplings to be larger than what would be expected when coming from the atomic level. In particular, it is well known that the spin-orbit coupling and the resulting level splitting is much larger in the case of nuclei compared to atoms (sometimes splitting on the MeV level instead of the meV level – see Mitra & Narasimham 1960). In fact, even the comparatively stronger magnetic interaction -- as made use of in NMR -- has its origins in the prominent role of the nuclear spin. To build on this observation, it may be helpful to consider the principles that underlie spin-orbit coupling. Spin-orbit coupling, as both at the atomic and at the nuclear level, is a relativistic effect: according to special relativity, a moving particle such as an electron can be viewed as contracted compared to said particle at rest. The resulting contraction impacts the configuration and structure of the atom -- and therefore its excited states. The resulting energy level splitting is thus a function of the assumed velocity of the electron, compared to the speed of light. The same principle applies to the moving nucleons and excited states of nuclei (see Fig. 19b for an illustration of nuclear level splitting due to relativistic treatment of nucleons). This is, for instance, expressed by Alder & Steffen 1964 ("the nuclear forces are velocity dependent") and by Dommelen 2012 ("scattering data suggests that the [nuclear] potential also depends on the motion of the nucleons"). Fig. 19a illustrates the effect of nucleon motion, as encapsulated in spin-orbit coupling, on the mean field nuclear potential (and thus on predicted excited states).

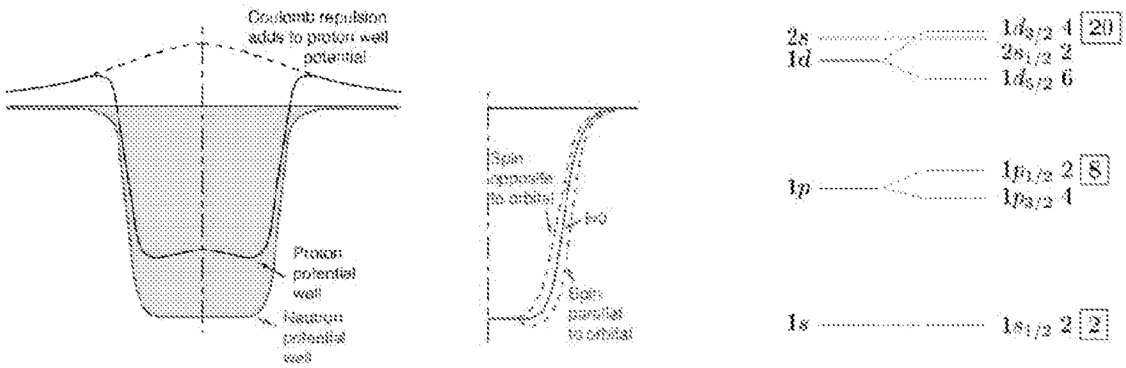

Fig. 19: (a) LEFT: Woods-Saxon mean field potential with proton and neutron contributions. (b) CENTER: impact of momentum dependence as represented by spin-orbit coupling on nuclear potential; (c) RIGHT: resulting energy splittings for excited states in the nuclear shell model.

For the purposes of modeling spin-orbit coupling, the velocity of a fermion such as the electron is given by the fermi velocity which, for instance in the case of electron movement in graphene, is estimated as 10^6 m/s (Li et al. 2017) i.e. a fraction of the speed of light on the order of 10^{-3}. In comparison, the fermi velocity of moving nucleons is given by Negele 1985 as about 6 x 10^7 m/s i.e. a fraction of the speed of light on the order of 10^{-1}. It should be noted that in both atomic and nuclear cases, this relativistic effect cannot be cancelled by simply transforming from the rest frame to the moving frame as both electron and nucleon motion is expected to be not constant but changing due to the nature of orbitals.

The considerations summarized above establish a widely recognized dependence between momentum and excited states in both atoms and nuclei. As would be expected, this momentum dependence is also captured by relativistic models of the nucleus (Breit 1937; Elliott & Skyrme 1955; Kurasawa & Suzuki 2002) as well as by comprehensive models of the nucleon-nucleon interaction (Machleidt 2014). In nonrelativistic models, the momentum dependence is introduced explicitly in the form of an added term, as motivated by the experimentally observed level splittings attributed to spin-orbit coupling (Goeppert-Mayer 1950).

Given this momentum dependence of nuclear states, one may naturally inquire about the impact that any additional momentum imparted on nucleons might have. In most calculations of spin-orbit coupling, only the relative momentum of nucleons (inside the nucleus) is considered. However, this momentum would be boosted (in the relativistic sense) if the nucleus as a whole were moved -- akin to a person walking on a train where the absolute momentum of the person includes a center-of-mass contribution from the train. Similarly, the center-of-mass momentum of the nucleus adds an additional contribution to the overall nucleon velocity, and therefore to the level splitting expected from the momentum dependence of the nuclear state. A relevant type of motion, comparable – albeit at a lower intensity -- to the orbital oscillatory motion of nucleons, is the oscillatory center of mass motion of nuclei. This kind of motion is of course known as phonons.

The central question then becomes how much of an impact on nuclear states, quantitatively, would the phonon contribution to nucleon motion represent. Before entering into calculations, it can be noted that a typical phonon velocity of 100 m/s would correspond to a fraction of the speed of light on the order of 10^{-6} (compare to the values 10^{-3} and 10^{-1} above). From these considerations it is clear that the contribution would be weaker than the main form of spin-orbit coupling from relative nucleon motion. As for calculations, ideally a corresponding estimate is obtained from a first principles relativistic model of the nucleus that pays particular attention to this aspect, as developed in Hagelstein 2016. A simpler approach that can serve as a first approximation is to use the spin-orbit coupling term introduced by Goeppert-Mayer (1950) and evaluate it for the momentum contribution expected from typical phonon motion. The regular spin-orbit coupling term is given as (Jackson 2007):

$$V = \frac{1}{2M^2c^2}\frac{dU}{dr}\boldsymbol{S}\cdot\boldsymbol{P_{relative}} \qquad \text{(Eq. 8)}$$

This term only takes into account the relative momentum of nucleons $\boldsymbol{P_{relative}}$. Therefore, a correction term is added that takes into account the additional center-of-mass momentum $\boldsymbol{P_{com}}$ contributed to the absolute momentum of each nucleon A by the motion of the nucleus:

$$V_{correction} = \frac{1}{2M^2c^2}\frac{dU}{dr}\boldsymbol{S}\cdot\frac{\boldsymbol{P_{com}}}{A} \qquad \text{(Eq. 9)}$$

Here U is a mean field nuclear potential such as the Woods-Saxon potential; and $\boldsymbol{P_{com}} = M\,\boldsymbol{v} = M\,\omega\,u$ contains the frequency and amplitude of the lattice vibrations. Note how varying the center-of-mass momentum (through phonon frequency and amplitude) would also allow for some tunability of this proposed coupling strength, analogous to the effect of adding an enhancing electric field in the above-discussed case of atomic dipole-dipole coupling (eq. 7).

For THz phonons and in the exemplary case of a ^{181}Ta nucleus, Hagelstein (2018) and Metzler (2019) show evaluations of this expression to yield a coupling strength estimate of about 5 meV. It can be seen that this coupling strength, if confirmed, would be much larger than the nuclear-scale dipole-dipole coupling considered in the previous subsection.

Nevertheless, such a phonon-induced coupling would still be rather weak, especially when compared to nuclear transition energies. Following the comparisons above, the coupling-to-transition-energy ratio is about negative 6 orders of magnitude in case of the 6 keV transition of ^{181}Ta. The form of this coupling does, however, imply important differences to the dipole-dipole coupling widely used in RET at the atomic and molecular level. First, the phonon-induced coupling does not exhibit the $1/R^3$ dependence of the dipole-dipole coupling. In other words, the interaction is equally strong across the phonon coherence domain and can grow as the coherence domain grows (i.e. the number of nuclei N participating in the phonon mode). Note that extremely large, macroscopic phonon coherence domains have been reported in the context of phonon lasers (see Pettit et al. 2019 for a review). Second, a large number of nuclei N in a coherent phonon mode would be expected to exhibit superradiance effects (as discussed above), leading to possible amplification of the coupling up to a factor of N^2. Note also that the number of nuclei N(r) grows to the power of 3 of the radius that spans the coherence domain. This implies that simply doubling the phonon coherence length could lead to an increase of coupling strength by as much as about $2^6 = 64$. In summary, even though the suggested phonon-induced coupling appears comparatively weak, it may be subject to several enhancement mechanisms and therefore may manifest as substantially stronger in environments where such enhancement mechanisms can be activated (especially by providing a large phonon coherence domain).

Implications for nuclear fusion rates

This section began with a reframing of the fusion problem as a two-state system with a highly metastable excited state and, correspondingly, a long spontaneous emission decay time. This framing allowed us to consider mechanisms for accelerating state transition rates that are well-known in atomic, molecular, and optical physics as well as condensed matter physics. Of particular interest is the resonance energy transfer (RET) mechanism where even comparatively weak couplings allow for accelerated deexcitation of two-state systems if the corresponding energy quantum can be moved within the coupled system resonantly. We found that conventional electromagnetic dipole-dipole couplings would likely be too weak to make this mechanism relevant to the nuclear level. However, the momentum dependence of nuclear states suggests the possibility of phonon-mediated couplings and transfers. While still comparatively weak, we pointed at potential enhancement mechanisms such as superradiance which have been demonstrated experimentally, including at the nuclear scale.

Returning to the case of D+D fusion as illustrated in Fig. 12, fusion rate enhancement based on the principles above is conceivable if a receiver state were available that would be well-matched to the D_2 donor state -- and therefore allow for resonant coupling between the two systems. A perfect match would be a ^4He nucleus, as it would be able to accommodate the exact same amount of energy released by the D_2 ⍰ ^4He transition by undergoing the reverse ^4He ⍰ D_2 transition. This process is conceivable if a ^4He nucleus is present as an impurity in a lattice near a D_2 molecule and both subsystems were coupled (see Fig. 20a). Hagelstein 2013 estimates the coupling matrix element and the transfer rate for this process to be on the order of 10^{-35} – which would be a substantial enhancement over the D_2 ⍰ ^4He spontaneous emission rate i.e. the tunneling probability in the Gamow model, corresponding to a fusion rate enhancement of about 30 orders of magnitude (note that in this picture, screening is not yet considered and would be expected to lead to additional rate enhancements as discussed in section 3).

However, while exhibiting the strongest resonance possible due to perfect level matching, such a system would be less interesting from an application and from an experimental point of view. That is because it would be difficult to observe or harness the enhanced reaction since energy merely coherently rearranges within a short-range, closed system at the nanoscale. Similar concerns were discussed above, in anticipation of the objection that deexcitation of one subsystem with simultaneous excitation of an equivalent subsystem ought not to be viewed as accelerated decay. The response to such potential concerns consisted of reference to the experimental and theoretical literature on downconversion (also known as quantum cutting). Applying the equivalent argument here would suggest the possibility of resonant transfer not to just one matching receiver nucleus that can resonantly accommodate the 24 MeV released from a D_2 ⍰ ^{4}He transition, but to several receiver nuclei that can accommodate the 24 MeV together such as 2 x 12 MeV, or 3 x 8 MeV, etc. (see Fig. 20b). Many nuclei typically present in metal lattices exhibit a dense number of excited states at such energy ranges and could thus become receiver candidates in such a process. Excitation of nuclei at such energy levels would likely lead to quick disintegration of said receiver nuclei e.g. through alpha, proton or neutron emission – unless further resonant transfer of the energy takes place if enabled by the existing couplings and by the donor and receiver configurations. The result of such a process, first alluded to in Hagelstein 2000, would be both a substantial enhancement of fusion rates and also a de facto change of reaction products (which would then depend on the excited state decay channels of the receiver nuclei).

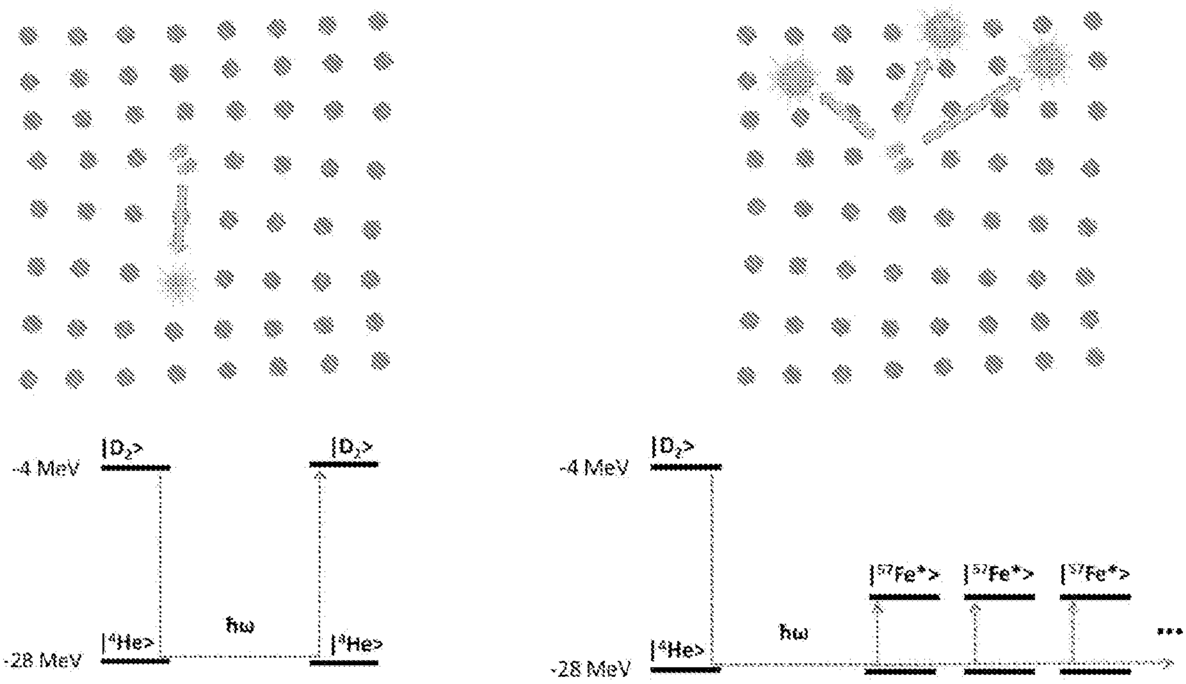

Fig. 20: Proposed resonant energy transfer between coupled nearby nuclei in the presence of strong enough interactions. Variant (a) exhibits perfect resonance due to equivalent and thus well-matched energy levels, but shows no observable effects. Variant (b) involves downconversion to matching states of nearby nuclei. During decoherence, energy would leave the system incoherently, for instance via gamma, alpha, proton or neutron emission. Here, ^{57}Fe nuclei are shown as receiver systems to make the connection to the ^{57}Fe experiments discussed above (Metzler et al. 2020). However, a wide range of receiver nuclei are conceivable and many may be better suited based on their energy levels, state lifetimes, and reaction cross sections.

Hypotheses and research questions

In this section we considered -- informed by coupling-induced energy transfer phenomena at the atomic and molecular scale -- under what circumstances the system boundaries in the Gamow model may need to be extended beyond the two-body perspective to more fully capture mechanisms that could potentially affect outcome variables of interest.

We reframed the fusion problem as a two-state problem, a prototypical framing in quantum electrodynamics. We presented different literatures, both theoretical and experimental, that suggest and report substantial transition rate enhancement in two-state problems. Many of these mechanisms hinge on the presence of couplings that connect a two-state system of interest to other subsystems. Consequently, we spent some time investigating what couplings and with what coupling strengths may affect atomic nuclei as in the nuclear fusion problem. We concluded that the momentum dependence of nuclear states may offer a coupling to other nuclei that may be strong enough (especially when considering amplification mechanisms) to affect outcome variables in the Gamow model.

How much of a handle the momentum dependence of nuclear states actually provides for coupling to other nuclei is still the subject of ongoing research. As for continued investigation of this subject, an important advantage is the ability to focus piecewise on individual aspects of the overall argument presented here. Such research does not necessarily need to be centered around the presumably more complicated problem of fusion. Instead, hypotheses can be formulated and experiments developed that focus rather narrowly on pieces of the argument such as the further quantification of coupling strengths and the applicability of RET at the nuclear level.

The application potential of an efficient short-range coupling and related energy transfer mechanism between nuclei would extend beyond fusion rate enhancement. If further confirmed and evolved, it could potentially lead to a host of use cases that involve more deliberate excitation and deexcitation of atomic nuclei.

If further validated, then -- from the perspective of maximizing fusion rates -- an ideal system drawing on such mechanisms would contain a suitable match of donor and receiver nuclei (that exhibit large coupling matrix elements as can be modelled, long state lifetimes, and matching fractional energy levels) as well as strong couplings from highly excited phonon modes with a large coherence domain. A high D_2 concentration would be considered helpful to enable superradiant amplifications.

To test and either confirm or reject hypotheses discussed in this section, we consider the following research questions worthy of further investigation:

- *Under what circumstances can nuclear states of nearby atomic nuclei become significantly coupled? What is a realistic upper limit for respective coupling strengths?*
- *Under what circumstances can couplings between nuclei increase nuclear transition rates?*
- *Can resonant transition rate increases cause fusion rate enhancements and if so, to what extent?*

5. Discussion and conclusions

In this paper, we considered the potential for fusion rate enhancement within the established Gamow model and beyond. Because the Gamow model dates back to 1928, we placed particular emphasis on novel insights gained about quantum tunneling from all areas of physics since then. Many such insights come from areas other than nuclear physics which is why some parts of this paper can be viewed as a consolidation and integration effort on what can be said about quantum tunneling in nuclear fusion – an effort that may well be overdue. We found potentially fruitful cross-connections particularly to condensed matter physics and materials science; atomic, molecular and optical physics; biophysics; and even quantum information science. In this process of exploration and consolidation, we came across a wide range of mostly well-known mechanisms that may impact fusion rates but have not been widely considered in this context. We believe that such mechanisms are deserving of further investigation. This assessment is consistent with the perspectives of some well-known nuclear physicists who have long described the Gamow model as “naive” (Koonin 1989). Nevertheless, simple conclusions derived from the Gamow model continue to remain authoritative among many members of the physics community as to what is and what is not possible in nuclear fusion. That is not to say that the Gamow model is to be rejected. We also found the Gamow model helpful in developing basic insights about the fusion problem and as a reference point for establishing a baseline in our fusion rates calculations. However, as with most models, it is important to remain aware of its underlying assumptions and limitations. We encourage other physicists and engineers to join us in the debate on how the Gamow model, as a fundamental model of nuclear fusion, can be – and maybe must be – extended and evolved.

Referring back to Fig. 1, we identified three major areas – proximity, screening, and resonances – and five corresponding mechanisms that could potentially cause substantial fusion rate enhancements. Some of these mechanisms are clearly more established and others more exploratory. Nevertheless, they all are anchored in modern physics and can be derived from and motivated by related literatures. And they are certainly all in need of further research and clarification. If multiple of such mechanisms can be further confirmed and possibly superimposed, then fusion rate enhancement to the extent of observable fusion at ambient temperatures and pressures is conceivable. Consider that one cubic centimeter of hydrogen loaded palladium can contain as many as 10^{32} deuteron pairs. Therefore, a fusion rate of 10^{-30}/s -- an enhancement of 34 orders of magnitude from the 10^{-64}/s rate of gas phase molecular deuterium given by Koonin and Nauenberg 1989 -- would amount to 100 fusion events per second. Such a fusion rate would become accessible to experiment. Moreover, if enhancement on this order can be achieved, further enhancement along similar lines is easily conceivable.

Our framework for thinking about fusion rate enhancement can be turned into a research roadmap. Whereas from an application’s point of view, the simultaneous superposition of as many enhancement mechanisms as possible -- i.e. the overall maximization of fusion rates -- is desirable, this is not necessarily the case in research. We advocate for research into all five mechanisms separately with crossover points where necessary. Electron densities and hydrogen site occupation in metal hydrides can be studied computationally and experimentally. The same is true for dynamic enhancements of the same. Refined nuclear structure models can increase the reliability of predicted resonances which allows for the development of dedicated experiments to test for them. Couplings between nuclei can be investigated and quantified from first principles models and tested with slight modifications to already existing experiments (such as Chumakov et al. 2018). The potential of superradiant enhancement of nuclear transition rates is of interest to a large audience and will inevitably see more activity in coming years. Research on resonance energy transfer (RET) is already carried out by a large community of researchers who may recognize transferability of their insights to the nuclear scale. Such modularization can make the complicated problem of fusion rate enhancement more tractable. It goes without saying that each module should be, to paraphrase Einstein, “as simple as possible, but not simpler” (Sessions 1950).

We suggest that research on fusion rate enhancement -- with the goal of achieving nuclear fusion at ambient conditions -- should not be viewed as competition to research on thermonuclear fusion, but rather as a complement. Both in terms of relevant knowledge domains and in terms of potential applications, the differences are substantial. Whereas thermonuclear fusion is dominated by plasma science, research on solid-state rate-enhanced fusion is more closely related to nano and quantum sciences. Thermonuclear fusion aims for large, centralized power stations whereas solid-state fusion bears the potential of small-scale, integrated devices (which ideally are aneutronic).

Fusion rate enhancement has been considered since the early days of nuclear engineering. However, as laid out in the introduction, this approach has hitherto not become a prominent branch of nuclear fusion research. In part, this can be understood from the explanation given above: thermonuclear fusion was perennially considered "around the corner" and alternatives, potentially more complicated ones, were beyond the bandwidth of many researchers and institutions. A second factor was a sort of polarization that took place in the wake of an announcement by electrochemists Fleischmann and Pons in 1989: Fleischmann and Pons claimed that fusion at ambient conditions ("cold fusion") had been achieved – and that it could be reduced to practice in short order. As we know today, the latter was certainly not the case – and the former claim remains contested. Nevertheless, a very real consequence of this announcement, and the dynamics that ensued, was a bifurcation among researchers, with a large majority steering clear of this area and only a small minority remaining engaged. What followed was much focus on individual experiments and the interpretation of claimed results, the credibility and accountability of various researchers, and debates over scientific and institutional best practices -- with little systematic attention to theoretical considerations as to what is and what is not possible when it comes to fusion in solid-state environments. Julian Schwinger echoed this sentiment by stating in 1991: "I have asked myself not whether Pons and Fleischmann are right – but whether a mechanism can be identified that will produce nuclear energy by manipulations at the atomic -- the chemical -- level."

As a result of these dynamics, research on fusion rate enhancement remained scattered, often inconsistent, and for most parts not cumulative. In a paper on the "advent and development of eight scientific fields from their inception to maturity," Bettencourt et al. 2009 study the evolution of networks of scientific collaboration. The authors find that emerging scientific fields typically undergo a transition from small disconnected pockets of ideas and researchers to larger, more integrated networks of collaboration (see Fig. 21). The scientific fields that the authors investigate include, among others, carbon nanotubes, quantum computing, superstring theory – and cold fusion. They find that, except for cold fusion, all fields eventually underwent "a process of cognitive and social unification out of many initially separate efforts." We attribute this hitherto absence of such a transition in the field of cold fusion on the one hand to a lack of contributors with advanced credentials and familiarity with academic best practices, and on the other hand to a lack of a cognitive organizing framework and a shared language.

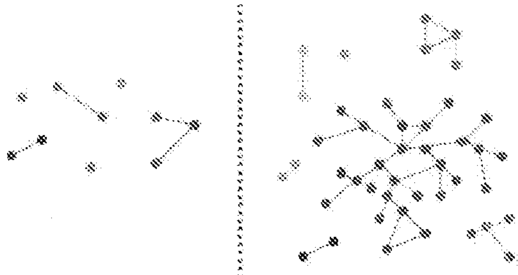

Fig. 21: Idealized representation of collaboration networks in emerging scientific fields before (LEFT) and after (RIGHT) convergence around accepted cognitive frameworks and subsequent consolidation and maturation. Image from Bettencourt et al. 2009.

This paper seeks to address the latter point, ideally with positive spillovers on the former. We present this framework – using the Gamow model as a starting and reference point and then expanding from it in depth and scope – as a way to anchor the conversations around fusion rate enhancement. We invite researchers with an interest in this subject to provide feedback and criticism, suggestions and questions. We also invite researchers with similar research interests to locate their own efforts and ideas with respect to this framework, and particularly in view of the five potential mechanisms of fusion rate enhancement that we identified (see Fig. 1). Which mechanisms does their research speak to? In what ways would it represent an advance over the existing literature? Which points raised in this paper can be confirmed or refuted? And if new hypotheses are not congruent with any of the mechanisms presented here: What is missing in this framework and on what basis can additional mechanisms of fusion rate enhancement be justified?

The timing for integration and harmonization of research in this area could not be better. In its 2020 appropriations to the National Science Foundation (NSF), US Congress called for more research to "evaluate the various theories, experiments, and scientific literature surrounding the field of LENR [low energy nuclear reactions]" and directed NSF to "provide a set of recommendations as to whether future federal investment into LENR research would be prudent, and if so, a plan for how that investment would be best utilized." In March 2020, the research agencies of [STILL CONFIDENTIAL] granted support to a new program with a budget of about $7M for research on enhanced fusion in metal hydrides. These developments coincide with a greater sense of urgency vis-a-vis climate change and a greater recognition of the importance of calculated risk-taking in the funding of basic research.

The insights presented in this paper suggest that such scientific endeavors are justifiable and well appropriate. Given the number of promising candidate mechanisms for fusion rate enhancement, the existing gaps of knowledge, and the potential impact of corresponding advances, we consider further research in this area highly prudent. Based on the mechanisms we identified and the rate enhancements they promise, we conclude that fusion at ambient conditions is conceivable – the last word, of course, will be with Nature and more research will either confirm or refute some of the claims and arguments presented here.

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From the text above follows the usefulness and the importance of modeling materials systems in such ways where chemical and nuclear properties of constituting nuclei are both included in the modeling process process in order to arrive at systems that are best suited for a range of desired applications. In other words, in such a process, modeling and design techniques that traditionally consider chemical properties of atoms and modeling techniques that traditionally consider nuclear properties of atoms (related to nuclear excited states) are combined.
Such applications can include the generation of heat or electricity or radiation such as photons from nuclear reactions – and specifically from nuclear reactions where reaction rates are enhanced beyond presently conventionally accepted rates; or where reaction products are changed beyond presently conventionally accepted products.
It can also involve optimizing across a number of different desired output parameters or combinations thereof, including but not limited to: maximization of output energy, minimization of cost, reduction of hazardousness, minimization of weight.

Specifically, the modeling and design process and resulting software and tools comprise:

- chemical data including but not limited to: behavior in a lattice, lattice structure, electron density.
- nuclear data including but not limited to: nuclear excited states, nuclear reaction resonances and cross section data, photonuclear cross sections

The modeling and design process and resulting software and tools can include:

- modeling the proximity and the electron screening configurations possible in different lattice configurations, including finding a desired combination between proximity and screening
- modeling resulting nuclear reactions and reaction products (and if applicable excitation transfer chains) given different material and lattice configurations
- modeling coupling strengths between nuclei in different lattice configurations including phonon-nuclear coupling strengths (that enable nuclear excitation transfer), as affected by phonon modes and phonon energies in the lattice, possible superradiant amplification, phonon coherence domains and lifetimes, and the nuclear transitions of involved (coupled) nuclei.

Claims

1. Claimed is a process for modeling or designing lattice configurations, which involves chemical and nuclear data of constituting atoms and which results in a system that involves a lattice whose configuration is informed by such models or designs.
2. The claim of 1 where nuclear excitation transfer processes are modeled or designed, and their key parameters are determined (as described in the text above).
3. The claim of 2 where the resulting system's desired output and performance parameters of are optimized according to the designer's preferences.
4. The claim of 1 where enhancement of nuclear reaction rates beyond the presently published and widely accepted rates are achieved in the system.
5. The claim of 4 where the nuclear reactions comprise one of nuclear fusion, nuclear fission, or nuclear decay.
6. The claim of 1 where in the resulting system a change of conventionally expected nuclear reaction products is achieved.