Screened Coulomb potentials for astrophysical nuclear fusion reactions

T.E. Liolios[a]

European Center for Theoretical Studies in Nuclear Physics and Related Areas, Villa Tambosi, I-38050 Villazzano (TN), Italy
University of Thessaloniki, Department of Theoretical Physics, Thessaloniki 54006, Greece [b]
Hellenic War College, BST 903, Greece

Abstract. The electron-screening acceleration of laboratory fusion reactions at astrophysical energies is an unsolved problem of great importance to astrophysics. That effect is modeled here by considering the fusion of hydrogen-like atoms whose electron probability density is used in Poisson's equation in order to derive the corresponding screened Coulomb potential energy. That way atomic excitations and deformations of the fusing atoms can be taken into account. Those potentials are then treated semiclassically in order to obtain the screening (accelerating) factor of the reaction. By means of the proposed model the effect of a superstrong magnetic field on laboratory hydrogen fusion reactions is investigated here for the first time showing that, despite the considerable increase in the cross-section of the dd reaction, the pp reaction is still too slow to justify experimentation. The proposed model is finally applied on the $H^2 (d, p) H^3$ fusion reaction describing satisfactorily the experimental data although some ambiguity remains regarding the molecular nature of the deuteron target. Notably, the present method gives a sufficiently high screening energy for hydrogen fusion reactions so that the take-away energy of the spectator nucleus can also be taken into account.

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1 Introduction

At astrophysical energies of a few keV corresponding to stellar temperatures of several millions degrees kelvin the cross-section $\sigma(E)$ of the predominant s-wave fusion reactions is given by

$$\sigma(E) = \frac{S(E)}{E} P(E), \qquad (1)$$

where the astrophysical factor $S(E)$ embodies all the nuclear effects of the reaction and for non-resonant cases is a slowly varying function of the center-of-mass energy E. On the other hand, the penetrability factor $P(E)$ embodies all atomic effects of the reaction and when the electron cloud around the fusing nuclei is ignored it is given by $P(E) = \exp(-2\pi n)$, where n is the Sommerfeld parameter.

As the astrophysical factor varies slowly with energy we usually replace it with a truncated Taylor series which will be studied extensively in the present paper:

$$S(E) = S(0) + S'(0) E + 0.5 S''(0) E^2. \qquad (2)$$

[a] e-mail: `theoliol@physics.auth.gr`
[b] *Correspondence address.*

Any error in the zero-energy astrophysical factor $S(0)$ is actually an error in the corresponding reaction rate in the stellar plasma, which in turn reflects linearly on the energy production rate.

In the past years there have been exhaustive efforts to extend measurements of the $S(E)$ towards even lower energies [1, 2] in order to obtain a reliable value for $S(0)$. This is necessary as extrapolating higher-energy data to zero energies introduces an inevitable numerical error. However, at such low energies, the electron cloud that screens the fusing nuclei enhances the fusion reaction by lowering the Coulomb barrier. Consequently, disregarding its presence leads to an overestimation of $S(0)$. Unfortunately, even very recent experiments [3] cannot explain the screening enhancement which exceeds all the available theoretical predictions as was recently admitted [4, 5] .

Various authors have studied the influence of the atomic cloud on the cross-section of low-energy nuclear reaction. A qualitative study [6], which parametrized various atomic processes such as molecular formation, excitation and ionization, yielded a fair approximation for the possible contributions of the electronic degrees of freedom in the nuclear collision experiment. Moreover, by assuming a constant charge density around the target nucleus, a subsequent model [7] predicted a screening shift which

was compatible with the experimental data. However that assumption is an oversimplification which will be amended in the present paper. The most sophisticated approach has been a few-body treatment [8] which established a lower (sudden) and a higher (adiabatic) limit for the screening energy transferred into the relative nuclear motion. Although more studies followed [9,10], which also extended the calculations to molecular fusion reactions [11], despite their mathematical rigor they could not explain the discrepancy between experimental and theoretical screening energies.

In this work there is presented a mean-field model for the study of screened nuclear reactions at astrophysical energies in the laboratory [12]. That model agrees well with the available experimental data, thus enabling us to improve the accuracy of the associated astrophysical factor. Moreover, by means of the proposed model the effect of a superstrong magnetic field on laboratory hydrogen fusion reactions is also investigated for the first time, yielding the associated magnetic accelerating factor. Notably, the present method gives a sufficiently high screening energy for hydrogen fusion reactions so that the spectator nucleus take-away energy can also be taken into account.

2 Screened Coulomb potentials

After the pioneering work [6] that established the importance of atomic effects in low-energy nuclear reactions various authors have tried to create models that account for the observed enhancement. A simple model [7], suggested at an early stage, assumed that the electronic charge density around the target nucleus is constant, thus predicting for the nucleus-atom reaction between the atomic target $Z_1 e$ and the projectile $Z_2 e$ a screening energy $U_e = (3/2) Z_1 Z_2 e^2 a^{-1}$. In order to take into account the dependence of the screening radius on the charge state of the reaction participants, that model used a screening radius taken from scattering experiments [13] so that

$$a = 0.8853 a_0 \left(Z_1^{2/3} + Z_2^{2/3} \right)^{-1/2} , \qquad (3)$$

where a_0 the Bohr radius. Although that screening energy is larger than the one predicted by the simple formula [6] $U_e = Z_1 Z_2 e^2 \left(a_0/Z_1 \right)^{-1}$ it has some very obvious defects. The assumption that the charge density is constant leads to an unnaturally sharp cut-off at a distance $r = a$ from the center of the target nuclei, which is not born out either by theory or experiment. Moreover, atomic excitations and deformations of the target atom are totally disregarded. On the other hand, normalizing the charge distribution so that the total charge is $-Z_1 e$ gives a charge density

$$\rho_0 = -\frac{3}{4} \frac{Z_1 e}{\pi a^3} . \qquad (4)$$

In order to assess the validity of that density we can consider the hydrogen-like atom $Z_1 e$ which will also be used in this section . The charge density at the center of the cloud of such an atom (when the electron is in its ground state) is

$\rho_0^{\text{g.s.}} = -e \left(Z_1/a_0 \right)^3 /\pi$. It is obvious that for $Z_1 = Z_2 = 1$ we obtain $\rho_0 \simeq - \left(e/a_0^3 \right)$ and $\rho_0^{\text{g.s.}} = - \left(e/a_0^3 \right) /\pi$, that is the simplified model in question overestimates the central density by a factor of π.

Consequently it is obvious that if low-energy nuclear reactions are to be treated by means of a mean-field potential a more sophisticated treatment is necessary.

As a first step we consider a more plausible charge distribution:

$$\rho (r) = \rho_0 \left(1 - \frac{r^2}{a^2} \right) , \qquad (5)$$

which takes into account the depletion of charge with respect to distance from the center. The radius a is the screening radius given by eq. (3) and the charge density ρ_0 at the center of the cloud can be found by means of the normalization condition:

$$\int_0^a \rho (r) \, 4\pi r^4 \mathrm{d}r = -Z_1 e . \qquad (6)$$

This integral yields a central value of

$$\rho_0 = -\frac{15}{8} \frac{Z_1 e}{\pi a^3} . \qquad (7)$$

Note that for a collision $Z_1 = Z_2 = 1$ we have a central charge density $\rho_0 = 7.68 \left(e/a_0^3 \right) /\pi$ which gives an even larger core density than the constant density assumption. An alternative approach would be to consider the value ρ_0 equal to the corresponding hydrogen-like one and then calculate the screening radius using eq. (6). The latter treatment gives a screening radius

$$a = \left(\frac{15}{8 Z_1^2 \pi} \right)^{1/3} a_0 , \qquad (8)$$

which is independent of the charge of the projectile. For hydrogen isotopes eq. (8) gives a radius of $a = 0.842 a_0$.

We can calculate the electrostatic energy by solving the equation of Poisson for the above charge distribution with the appropriate boundary conditions, so that

$$\Phi (r) = -\frac{15}{12} \frac{Z_1 e}{a} \left[\frac{3}{2} - \left(\frac{r}{a} \right)^2 + \frac{3}{10} \left(\frac{r}{a} \right)^4 \right] . \qquad (9)$$

Whenever a bare nucleus $Z_2 e$ impinges on the target nuclei surrounded by the electron cloud of eq. (5) the total interaction potential in the atom-nucleus reaction channel is

$$V (r) = \frac{Z_1 Z_2 e^2}{r} - \frac{15}{12} \frac{Z_1 Z_2 e^2}{a} \left[\frac{3}{2} - \left(\frac{r}{a} \right)^2 + \frac{3}{10} \left(\frac{r}{a} \right)^4 \right] . \qquad (10)$$

Although the above potential energy is more plausible than the constant charge density one, a more reliable charge distribution should be considered which could account for various other atomic effects as well as for the atom-atom reaction channel.

Let us consider a hydrogen-like atom with atomic number Z_1. When the wave function of the electron is given

by $\Psi_{nl}(r, \theta)$ then the charge density around the point-like nucleus is

$$\rho(r, \theta) = -e |\Psi_{nl}(r, \theta)|^2 \qquad (11)$$

by which it is obvious that both the previous screening model and that of ref. [7] are imperfect. If we solve the equation of Poisson for hydrogen atoms (or hydrogen-like ions) whose electron is in its ground ($1s$) state we obtain

$$\Phi_{00}(r) = -\frac{e}{r} + \frac{e}{r}\left(1 + \frac{r}{2r_0}\right)\exp(-r/r_0), \qquad (12)$$

where the screening radius is

$$r_0 = \frac{a_0}{2Z_1}. \qquad (13)$$

If a positive projectile $Z_2 e$ interacts with the above screened nucleus then the total potential energy is

$$V_{00}(r) = \frac{Z_1 Z_2 e^2}{r} - \frac{Z_2 e^2}{r} + \frac{Z_2 e^2}{r}\left(1 + \frac{r}{2r_0}\right)\exp\left(-\frac{r}{r_0}\right). \qquad (14)$$

On the other hand, if we assume that the electron is in an excited state ($2s$) then the potential energy is found to be

$$V_{10}(r) = \frac{Z_1 Z_2 e^2}{r} - \frac{Z_2 e^2}{r} + \frac{Z_2 e^2}{r} \cdot$$
$$\cdot \left(1 + \frac{3}{8}\frac{r}{r_0} + \frac{r^2}{16 r_0^2} + \frac{r^3}{64 r_0^3}\right)\exp\left(-\frac{r}{2r_0}\right). \qquad (15)$$

It should be emphasized that in the derivation of the above potentials we have assumed an unperturbed wave function of the target nuclei, throughout the tunnelling process. In fact at astrophysical energies the electron cloud responds rapidly and by the time tunneling begins the nuclei are so close that the wave function is actually that of a hydrogen-like atom with charge $Z_1^* = (Z_1 + Z_2)$ and a screening radius $r_0^* = a_0/2Z_1^*$

3 Nuclear reactions at astrophysical energies

At astrophysical energies reactions between light nuclei take place via s-interactions, thus enabling us to investigate them by means of the WKB.

If we assume that a bare nucleus $Z_2 e$ collides at very low energy E with a screened nucleus whose electron is in its ground state then the tunneling probability according to the WKB method is

$$P(E) = \exp\left[-\frac{2\sqrt{2\mu}}{\hbar}\int_R^{r_c(E)}\sqrt{V_{00}(r) - E}\,\mathrm{d}r\right]. \qquad (16)$$

We can assume that the lower limit of the WKB integral is given in terms of the mass number A of the reacting nuclei: $R = 1.4\left(A_1^{1/3} + A_2^{1/3}\right)$. For most practical purposes this lower bound is set equal to zero as all the nuclear effects of the fusion reaction are included in the cross-section factor.

The classical turning point can be obtained by equating the relative collision energy E with the potential energy of the interaction. The collision energy is set equal to the Gamow peak of the corresponding reaction in the plasma so that

$$V_{00}(r_c) = 1.220 \cdot \left(Z_1^2 Z_2^2 A T_6^2\right)^{1/3} \text{ keV}, \qquad (17)$$

where A the reduced mass number and T_6 the temperature in million degrees kelvin. For a wide range of light nuclei we have performed extensive numerical solutions for eq. (17) as well as numerical integrations of eq. (16). At astrophysical energies, just as is the case with the Debye-Hückel model in plasma conditions [14], the results indicate that throughout the potential barrier the potential energy $V_{00}(r)$ of eq. (14) can be safely replaced by the much simpler formula:

$$V_{00}(r) \simeq \frac{Z_1 Z_2 e^2}{r} - \frac{Z_1^* Z_2 e^2}{a_0}. \qquad (18)$$

Therefore the WKB penetration factor can be written as

$$P(E) = \exp\left[-\frac{2\sqrt{2\mu}}{\hbar}\right.$$
$$\left.\times \int_R^{r_c(E)}\sqrt{\frac{Z_1 Z_2 e^2}{r} - \frac{Z_1^* Z_2 e^2}{a_0} - E}\,\mathrm{d}r\right]. \qquad (19)$$

The equation for the classical turning point is modified accordingly:

$$\frac{Z_1 Z_2 e^2}{r_c} = 1.220 \cdot \left(Z_1^2 Z_2^2 A T_6^2\right)^{1/3} \text{ keV}, \qquad (20)$$

where we have ignored the screening shift given by

$$U_e = \frac{Z_1^* Z_2 e^2}{a_0}. \qquad (21)$$

It is now obvious that the relative energy of the reaction has been increased by U_e. In that case the penetration factor can be easily found to be [10]:

$$f_{1s}(E) \simeq \exp\left[\pi n(E)\frac{U_e}{E}\right], \qquad (22)$$

where the subscripts indicate the excitation state of the target atom. If we follow the same methodology for the $2s$ state we obtain

$$f_{2s}(E) \simeq \exp\left[\pi n(E)\frac{U_e}{4E}\right]. \qquad (23)$$

The much simpler potential model of eq. (10) gives a screening factor:

$$f_0(E) \simeq \exp\left[\pi n(E)\frac{\widetilde{U_e}}{E}\right] \qquad (24)$$

with an energy shift of

$$\widetilde{U_e} = \frac{15}{8}\frac{Z_1 Z_2 e^2}{a}, \qquad (25)$$

where a is given either by eq. (3) or eq. (8).

4 Magnetically catalyzed screening

By now it is obvious that any shift $U_e \ll E$ of the interaction potential energy $V(r)$

$$V(r) = \frac{Z_1 Z_2 e^2}{r} - U_e \qquad (26)$$

accelerates the fusion cross-section of hydrogen isotopes by a factor $f_{1s}(E)$ given by eq. (22). That observation will prove very useful in the study of the effects of a superstrong magnetic field on laboratory hydrogen fusion reactions which follows.

As a matter of fact under such extreme conditions the electron-screening cloud is deformed in the sense that it becomes compressed perpendicular and parallel to the magnetic field so that the screening potential energy for the strongly magnetized hydrogen atom is [15]

$$U_e(\rho, z; \alpha) = \frac{e^2}{\widehat{\rho}} \frac{1}{\sqrt{2\pi}} \int_0^\infty \frac{\exp\left[-\frac{1}{2}\left(\frac{\overline{\rho}^2}{1+u} + \frac{\overline{z}^2}{\alpha^2+u}\right)\right]}{(1+u)\sqrt{\alpha^2+u}} \mathrm{d}u,$$
$$(27)$$

where ρ, z are the coordinates in a cylindrical frame of reference whose origin coincides with the point-like nucleus of the hydrogen atom.

The natural length unit in the above formula is of course the cyclotron radius so that $\overline{\rho} = \rho/\widehat{\rho}$, $\overline{z} = z/\widehat{\rho}$, and α is a parameter which depends on the magnetic field and is determined by the variational method. The above formula was shown to be reliable for very strong fields whereas it becomes inaccurate below the threshold of the intense magnetic field regime given by

$$B_{\mathrm{IMF}} = 4.7 \times 10^9 \,\mathrm{G}. \qquad (28)$$

In ref. [15] potential (27) was applied at zero relative energies in order to obtain the mean-life times of hydrogen isotopes in neutron star surfaces. However, a more recent work [16] used that potential in a problem where the relative energies were of the order of keV showing that for energies $E > 0.5$ keV and fields of the order of $B_{12} = 0.047$ (B_{12} being the field measured in 10^{12}G) the classical turning point is so deep inside the cloud that the screening shift can be considered constant and equal to the value of the potential at the center of the cloud given in ref. [15]:

$$U_e(0,0;\alpha) = \frac{e^2}{\widehat{\rho}} \frac{2}{\sqrt{2\pi}} \frac{\ln\left(\alpha + \sqrt{\alpha^2-1}\right)}{\sqrt{\alpha^2-1}}. \qquad (29)$$

In the present work that approximation has been tested for various other fields and energies. The results show that for fields as high as $B_{12} = 4.7$ and interaction energies $E > 0.5$ keV the screening effect is independent of the angle at which the projectile enters the electron cloud and can be considered equal to eq. (29).

Therefore if the target hydrogen nuclei are in such a magnetic field the reaction is going to be accelerated
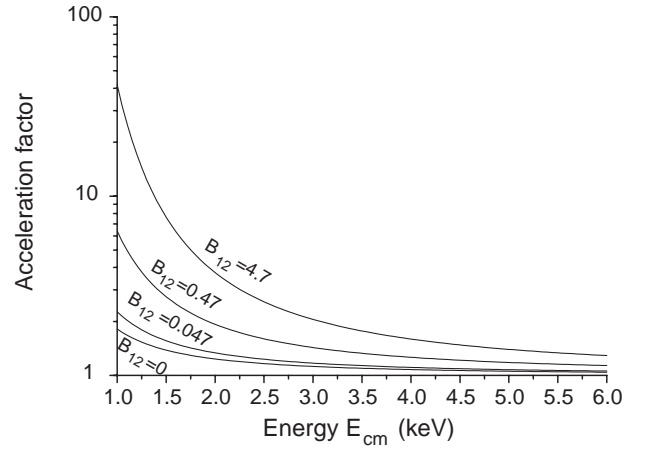
Fig. 1. The screening (acceleration) factor f_{1s} with respect to the relative interaction energy of two fusing protons for various superstrong magnetic fields (in units of 10^{12}G).
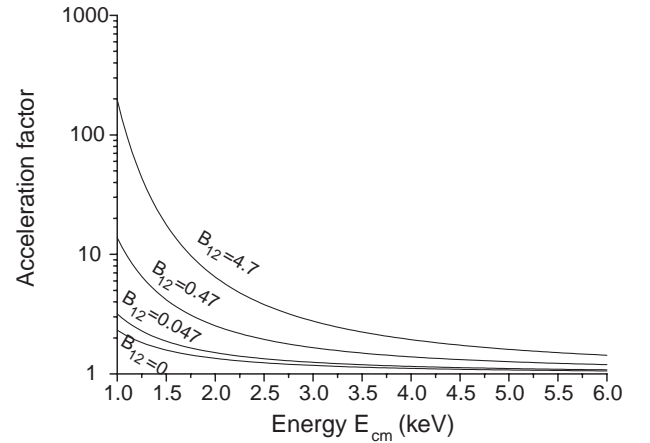
Fig. 2. The screening (acceleration) factor f_{1s} with respect to the relative interaction energy of two fusing deuterons for various superstrong magnetic fields (in units of 10^{12}G).

by a factor

$$f_{1s}(E) \simeq \exp\left[\pi n(E) \frac{U_e(0,0;\alpha)}{E}\right]. \qquad (30)$$

Figures 1 and 2 depict the acceleration of the pp and dd reactions, respectively, for various magnetic fields and interaction energies. Especially for the pp reaction it is obvious that even in such a strong field the cross-section is still significantly small. Namely, as the corresponding zero energy astrophysical factor is $S_{\mathrm{pp}}(0) \simeq 4 \times 10^{-22}$ keV-b, the screening effect in a superstrong field $B_{12} = 4.7$ can only increase $S_{\mathrm{pp}}(0)$ by roughly one order of magnitude compared to the unmagnetized case. If we take into account that the most powerful magnet currently available does not exceed 10^6 G, it is obvious that any hope of magnetically catalizing the pp reaction in the laboratory (in the near future) is futile.

The dd reaction, on the other hand, can be significantly affected by such a magnetic field as it is already much faster than the pp one. At very low energies the in-

crease can be as high as two orders of magnitude compared to the unmagnetized case.

5 The astrophysical factor of dd nuclear reactions.

Despite the fact that the reactions $H^2(d,p)H^3$, $H^2(d,n)He^3$ have been investigated since the early days of accelerators [17–19], the effect of screening on the associated astrophysical $S(E)$, which will eventually be used in theoretical calculations, is still under investigation. In the discussion that follows we will show that our model is compatible with the experimental data of that reaction.

The appropriate treatment of a low-energy experiment should take into account screening effects in order to calculate the respective values of $S(E)$. As a matter of fact once a screening model and the associated screening energy U_e are adopted, the corrected bare-nucleus astrophysical factor of the experiment is actually given by

$$S_b(E) = E\sigma(E)\exp(2\pi n)\exp\left(-\pi n\frac{U_e}{E}\right). \qquad (31)$$

Then eq. (2) is fitted to the data corrected through eq. (31) in order to obtain the zero-energy coefficient $S(0)$.

Any effort to extrapolate from higher-energy data or fit all the uncorrected data with formula (2) is bound to induce errors.

There are three different ways to analyze low-energy fusion data [3] which must of course be consistent with each other. We will apply those methods on the available data [20] for dd reactions ($E > 2$ keV) and compare them with the analytic model proposed in the present paper. First we note that for energies $E > 20$ keV any screening correction is meaningless since the exponential term of eq. (31) is very close to unity at such high energies. Therefore we can obtain the asymptotic behavior of the astrophysical factor by using the available high-precision experimental data [21] for higher energies which yielded

$$S_b(E) = 55.49\,(0.46) + 0.094\,(0.0054)\,E. \qquad (32)$$

We can now reasonably assume that this should be a fair approximation of the bare-nucleus astrophysical factor provided its use consistently describes the low-energy experimental data. In fact the screened value of $S(E)$ will now be given by

$$S(E) = (55.49 + 0.094E)\exp\left(\pi n\frac{U_e^{as}}{E}\right), \qquad (33)$$

where the screening energy U_e^{as} is determined by fitting eq. (33) to the uncorrected data of ref. [20], so that $U_e^{as} = 0.019\,(0.003)$ keV with $\chi^2 = 0.028$.

The second method which will corroborate the validity of the proposed models entails fitting all four parameters $S(0)$, $S'(0)$, $S''(0)$, U_e simultaneously to the uncorrected experimental data. Thus we obtain a screening energy of $U_e^{all} = 0.017\,(0.003)$ keV and a bare nucleus astrophysical factor:
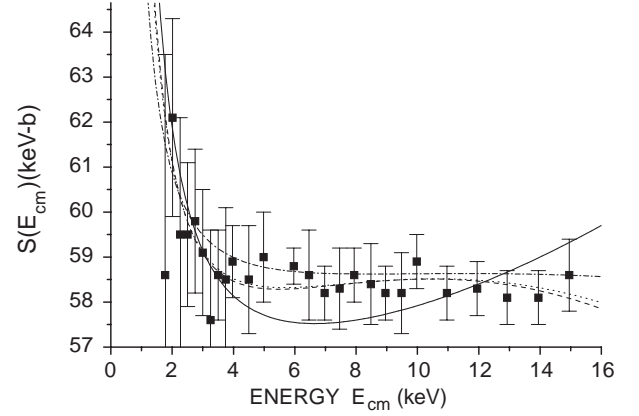
Fig. 3. The $H^2(d,p)H^3$ astrophysical factor $S(E)$ measured in keV-b with respect to the center-of-mass interaction energy E_{cm} (keV). The data (squares) are taken from ref. [20]. The solid curve represents eq. (33), which makes use of the asymptotic form given in ref. [21]. The dashed curve represents eq. (34) where all four parameters $S(0)$, $S'(0)$, $S''(0)$, U_e are fitted simultaneously. The dotted curve is obtained by adopting as a screening energy the value given by eq. (25), while the dash-dotted curve stands for the astrophysical factor obtained by using eq. (21).

$$S_b(E) = 54.54\,(1.39) + 0.608\,(0.265)\,E - 0.026\,(0.026) \qquad (34)$$

with $\chi^2 = 0.011$. Obviously, the two previous approaches give results which are compatible with each other as expected. Figure 3 shows that both the previous fits provide a satisfactory description of the screening effect.

The third method is a straightforward application of the theoretical models derived in the present paper. However, in order to apply those models on the experimental data we have to take into account that the data refer to a molecular target while our models refer to atomic ones. Hence, we have to allow for the energy which will be carried away by the spectator nuclei plus the reduction due to the molecular binding energy. Although this assumption has been argued against [11], the actual energy reduction for a deuteron molecular target has been calculated [23] by a Coulomb explosion process to be of the order of 44 eV. Therefore modifying our models for a molecular deuteron target we derive a screening energy $U_e = 0.010$ keV (eq. (21)) and $\widetilde{U_e} = 0.016$ keV (eq. (25)) which are in reasonably good agreement with the experimentally obtained values. We can now fit the formula

$$S(E) = \left[S(0) + S'(0)E + 0.5S''(0)E^2\right]\exp\left(\pi n\frac{U_e}{E}\right) \qquad (35)$$

by using the screening shift of our models. The results are as follows:

$$U_e = 0.010,$$

$$S_b(E) = 57.3\,(0.41) + 0.160\,(0.125)\,E - 0.0056\,(0.002)E^2 \qquad (36)$$

with $\chi^2 = 0.013$ and

$$\widetilde{U_e} = 0.016,$$

$$S_b(E) = 54.93\,(0.38) + 0.537\,(0.1149)\,E - 0.0225\,(0.007)E^2 \qquad (37)$$

with $\chi^2 = 0.011$.

Although our models are fairly compatible with the experiment there is an inevitable degree of uncertainty in the associated astrophysical factors due to the actual amount of energy that is carried away by the spectator nuclei of the molecular target. In any case the models proposed here turn out to provide a simple and effective way of describing fusion reactions between hydrogen-like atoms.

6 Conclusions

This work proposes a simple and efficient model for the study of the screening enhancing effect on low-energy nuclear fusion reactions. In that model, the fusing atoms are considered hydrogen-like atoms whose electron probability density is used in Poisson's equation in order to derive the corresponding screened Coulomb potential energy. This way atomic excitations and deformations of the reaction participants can be taken into account. The derived mean-field potentials are then treated semiclassically, by means of the WKB, in order to derive the screening enhancement factor which is shown to be compatible with the experimentally obtained one for the $\mathrm{H}^2\,(\mathrm{d},\mathrm{p})\,\mathrm{H}^3$ reaction, although some ambiguity remains regarding the molecular nature of the deuteron target. Moreover, by means of the proposed model the effect of a superstrong magnetic field on laboratory hydrogen fusion reactions is investigated for the first time showing that despite the remarkable increase in the cross-section of the dd reaction, the pp reaction is still too slow to justify experimentation.

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