Atomic effects in astrophysical nuclear reactions

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Abstract

Two models are presented for the description of the electron screening effects that appear in laboratory nuclear reactions at astrophysical energies. The two-electron screening energy of the first model agrees very well with the recent LUNA experimental result for the break-up reaction $^3\text{He}(^3\text{He},2p)^4\text{He}$, which so far defies all available theoretical models. Moreover, multi-electron effects that enhance laboratory reactions of the CNO cycle and other advanced nuclear burning stages, are also studied by means of the Thomas-Fermi model, deriving analytical formulae that establish a lower and upper limit for the associated screening energy. The results of the second model, which show a very satisfactory compatibility with the adiabatic approximation ones, are expected to be particularly useful in future experiments for a more accurate determination of the CNO astrophysical factors.

PACS number(s): 25.10.+s, 25.55.-e, 25.45.-z, 26.65.+t

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I. INTRODUCTION

The screening enhancement effect in laboratory nuclear reactions at astrophysical energies has attracted a lot of attention recently, especially after the recent accomplishments of the LUNA collaboration at Gran Sasso [1]. The very low energies attained for the break-up reaction $^3\text{He} \, (^3\text{He}, 2p)^4\text{He}$, which is extremely important to the solar neutrino production [2], revealed the real magnitude of the problem, as the screening energy obtained in that experiment still exceeds all available theoretical predictions. Other low energy experiments of the proton-proton chain [3,9] (past, current or planned) still need a theoretical model that could account for the observed enhancement.

On the other hand the astrophysical factors for the reactions of the CNO chain have been obtained by performing measurements well above the Gamow peaks ([10] and references therein) and extrapolating to lower energies without correcting for screening, thus committing a notable error in certain cases as it will become apparent in this work.

Various theoretical models have been proposed so far, some of which are in conflict with each other (e.g. accepting [7], or rejecting [11] the influence of the spectator nuclei) while others [12] were applied at a time when experimental measurements [4] were too sparse and inaccurate, thus their actual validity has been obscured.

There have even been suggestions [13,14] that this discrepancy between theoretical and experimental results is due to an overestimation of the energy losses in the experiment, which cause that apparent enhancement of the cross section. The most recent relevant experiment [1] reports no such energy-loss deficit which means that all energy losses have been taken into account, and yet the observed screening energy is still higher than the adiabatic limit.

Nevertheless, the prevalent belief nowadays is that a model is needed which could give a screening energy higher than the adiabatic limit. Although the adiabatic limit [15,16] is generally accepted, in a recent paper [17] a simple and efficient model was proposed for the study of the screening effect on low-energy nuclear fusion reactions which exceeded that limit. In that model, the fusing atoms were considered hydrogen-like atoms whose electron probability density was used in Poisson’s equation in order to derive the corresponding screened Coulomb potential energy. That way atomic excitations and deformations of the reaction participants could also be taken into account. The derived mean-field potentials were then treated semiclassically, by means of the WKB, in order to derive the screening enhancement factor which was also shown to be compatible with the experiment. In that work the screened Coulomb potentials were given without details of their derivation. However, a detailed derivation is necessary here before two-electron configurations are studied such as the $^2H \, (^2H, n)^3\text{He}$ reaction with a neutral projectile or the break-up reaction $^3\text{He} \, (^3\text{He}, 2p)^4\text{He}$. This need arises from the fact that the conventional use of a screened Coulomb potential is that of a Yukawa one. Nevertheless, the Yukawa one is only an approximation (truncation) of the complete screened potential arising from the solution of Poisson’s equation, as it will soon become apparent. Disregarding a priori higher order terms can possibly induce errors, especially when the experiment takes place at astrophysical energies of a few keV.

The layout of the paper is as follows: In Sec. II the screened Coulomb potentials for
hydrogen-like atoms are derived in a detailed fashion, which turns out to be very useful in Sec. III, where those potentials are modified in order to account for two-electron effects in nuclear reactions at astrophysical energies. Notably, in Sec. III, the screening energy for the $^3$He ($^3$He, 2p) $^4$He reaction which so far remains inexplicably high is reproduced to a very good approximation. Sec IV deals with multi-electron effects by means of the Thomas-Fermi model, which enables us to derive analytical formulas for the screening enhancement factors for reactions encountered in advanced nuclear burning stages of stellar evolution. A final concluding section summarizes the novelties and the results of the present work.

II. ONE-ELECTRON SCREENING EFFECTS

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

$$\rho_{nl} (r, \theta) = -e |\Psi_{nl} (r, \theta)|^2$$  (1)

Assuming spherically symmetric wavefunctions for simplicity we can solve the equation of Poisson for the above charge density in order to derive a screened Coulomb potential $\Phi (r)$ around the nucleus. Note that this potential will take into account the repulsive effects of the point-like nucleus, by imposing the appropriate boundary conditions:

$$\Phi (\infty) = 0 , \quad \Phi (0) = \frac{Z_1 e}{r}$$  (2)

The second boundary condition indicates that if a positive projectile ($Z_2 e$) is in contact with the nucleus ($Z_1 e$) at the center of the electron cloud then there is no negative charge between them to reduce the Coulomb barrier.

Let us define the screening form factor of the screened Coulomb as a function $f (r)$ so that:

$$\Phi (r) = \frac{Z_1 e}{r} f (r)$$  (3)

If we insert Eq. (3) and Eq. (1) into the equation of Poisson we obtain

$$\frac{d^2 f_{nl} (r)}{dr^2} = \frac{4\pi}{Z_1} r |\Psi_{nl} (r)|^2$$  (4)

which is to be solved with the boundary conditions

$$f_{nl} (\infty) = finite , \quad f_{nl} (0) = 1$$  (5)

Equation (4) with the corresponding boundary conditions constitutes a generator of screened Coulomb potentials which correspond to a particular excitation and ionization of the atomic target. According to the quantum state of the hydrogen-like atom we can use Eq. (4) in order to obtain the corresponding screened Coulomb potentials.
Actually in the above treatment there is an implicit assumption of independence between the nuclear and electronic degrees of freedom. This assumption can be expressed in a quantitative form by the formula:

$$V_{sc} (r) = V_c (r) + \Phi_e (r)$$  \hspace{1cm} (6)

The above formula states that the screened Coulomb potential is actually the sum of the bare nucleus Coulomb potential $V_c (r)$ plus the electrostatic potential energy of the electron cloud. Therefore one can calculate $\Phi_e (r)$ and then add it to the bare nucleus potential which simplifies the calculations especially when multi-electron atoms are considered. We now proceed to give an alternative approach according to the above assumption, which will be particularly useful in our study of two-electron effects.

Let us assume a hydrogen-like atom $Z_1$ in its ground state, whose electron charge distribution of Eq. (1) can be written:

$$\rho (r) = \rho (0) \exp (-r/r_0)$$  \hspace{1cm} (7)

where $r_0 = a_0 / (2Z_1)$.

The charge density at the center of the electron cloud is:

$$\rho (0) = -\frac{e}{\pi} \left( \frac{Z_1}{a_0} \right)^3$$  \hspace{1cm} (8)

while the electrostatic potential of the distribution is given by the solution of Poisson’s equation:

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d\Phi_e (r)}{dr} \right) = -4\pi \rho (0) \exp (-r/r_0)$$  \hspace{1cm} (9)

Upon integration we obtain:

$$\Phi_e (r) = C_1 + \frac{C_2}{r} - 4\pi \rho (0) r_0^2 \exp \left(-\frac{r}{r_0}\right) \left(1 + 2\frac{r_0}{r}\right)$$  \hspace{1cm} (10)

The electrostatic potential $\Phi_e (r)$ must go to zero at infinity which gives $C_1 = 0$. At very large distances $r \gg r_0$, due to the spherical symmetry of the distribution, any projectile impinging on that cloud will actually "see" a Coulomb potential of the form:

$$\Phi_e (r \gg r_0) = -\frac{e}{r}$$  \hspace{1cm} (11)

so that $C_2 = -e$. Inserting the values of the parameters $r_0$ and $\rho (0)$ into the above equation we obtain the formula used without details of its derivation in Ref. [17]:

$$\Phi_e (r) = \frac{e}{r} + \frac{e}{r} \left(1 + \frac{r}{2r_0}\right) \exp (-r/r_0)$$  \hspace{1cm} (12)

If a positive projectile $Z_2 e$ impinges onto the above hydrogen-like atom the total interaction potential energy $V (r)$ between the two nuclei will be due to the above electrostatic potential, that is $Z_2 e \Phi_e$, plus the repulsive potential of the nucleus $Z_1 e$:
\[ V_{sc}(r) = \frac{Z_1 Z_2 e^2}{r} - \frac{Z_2 e^2}{r} + \frac{Z_2 e^2}{r} \left( 1 + \frac{r}{2 r_0^*} \right) \exp \left( -\frac{r}{r_0^*} \right) \]  
(13)

where

\[ r_0^* = \frac{a_0}{2 (Z_1 + Z_2)} \]  
(14)

The reason for replacing \( r_0 \) with \( r_0^* \) is that, at astrophysical energies, the electrons move at higher velocities than the nuclei themselves. For example in laboratory \( d - D \) reactions the relative nuclear velocity equals the typical electron velocity \( v_e = \alpha c \) for \( E = 25 \text{keV} \). Although the above assumption is particularly valid at such low energy collisions between hydrogen nuclei, when reactions between heavier nuclei are considered (see next section), an inevitable small error is involved at intermediate energies (e.g. in the vicinity of the Gamow peak). As it will soon become clear the WKB treatment of the penetration factor disregards all effects beyond the classical turning point. Therefore, inside the tunneling region, the wavefunction of the electron actually corresponds to a combined nuclear molecule \((Z_1 + Z_2)\) instead of the initial \( Z_1 \) atom. Of course this is an approximation and, in our model, the intermediate stages of the wavefunction deformations are assumed to play a minor role.

When the electron of the target atom/ion is in an excited state, we can obtain in the same way the corresponding potential energy used in Ref. [17].

III. TWO-ELECTRON SCREENING EFFECTS

Let us now assume that a hydrogen-like atom \( Z_2 e \) impinges on a resting target nucleus \( Z_1 e \). Let us further assume that the target atom has two electrons orbiting the nucleus. In a Hartree-Fock approximation the total potential energy of the interaction will be:

\[ V_{sc}(r) = V_c(r) + V_{n_2e_1}(r) + V_{n_2e_2}(r) + V_{n_1e}(r) + V_{e_1e_2} + V_{e_1e} + V_{e_2e} \]  
(15)

that is the sum of: a) the Coulomb potential energy \( V_c(r) \) between the two bare nuclei plus b) the interaction between the projectile \((n_2)\) and the electrons \((e_1, e_2)\) of the target nucleus, plus c) the interaction between the target nucleus \((n_1)\) and the electron of the projectile \((e)\), plus d) the interaction between the electrons of the target \( V_{e_1e_2} \) and of course, the interaction \((e_1e, e_2e)\) between the electron of the projectile and those of the target. In the above equation only the terms associated with the nuclei will be considered functions of the relative internuclear distance, while the electron-electron interactions will be treated as perturbations which will actually raise the Coulomb barrier between the two reacting nuclei. We consider the following channels:

a) The nucleus-nucleus channel

That interaction has been thoroughly studied in most text books [10] and needs no further elaboration.

b) The atom-atom channel for hydrogen like atoms.

In most experiments, the projectile has been considered fully stripped of its electrons which is the case at relatively high energies. However, when the projectile is in a neutral state, or at least not fully ionized, its electron cloud has to be taken into account [7].
For such an interaction the total potential energy can be written:

\[ V_{sc} (r) = V_c (r) + V_{n2e1} (r) + V_{n1e} (r) + V_{e1e} \]  

(16)

When the two electron clouds interact, their mutual ground state wavefunction must be antisymmetric, since the electrons are identical fermions. The spatial wavefunction is necessarily symmetric therefore antisymmetry is arranged by considering an antisymmetric spin singlet state. Since we still work with hydrogen-like atoms, the electron-electron spatial wavefunction is

\[ \Psi_{e1e} (\vec{r}_1, \vec{r}_2) = \Psi_{00} (\vec{r}_1) \Psi_{00} (\vec{r}_2) \]  

(17)

where \( \Psi_{00} (\vec{r}) \) is actually the usual ground state wavefunction of hydrogen-like atoms.

The electrostatic potential energy of the two electrons is:

\[ V_{e1e} = \int \int \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \left| \Psi_{00} (\vec{r}_1) \right|^2 \left| \Psi_{00} (\vec{r}_2) \right|^2 d^3r_1 d^3r_2 \]  

(18)

where \( \vec{r}_{1,2} \) are the positions of the two electrons. As it will soon become apparent the effective interaction between the two participants of the reaction begins upon reaching the classical turning point. At astrophysical energies the classical turning point is hundreds of times smaller than the atomic radius, therefore we can safely assume that throughout the Coulomb barrier the two colliding nuclei constitute a combined nuclear molecule. Under that assumption the above integral can be calculated \[19\] so that for \( Z_1 = Z_2 = Z \) we obtain:

\[ V_{ee} = \frac{5 Ze^2}{8 a_0} \]  

(19)

That positive energy will be transferred to the relative nuclear motion, increasing the height of the Coulomb barrier.

The equal charge assumption combined with the fact that during tunneling the reacting nuclei practically coincide with respect to the electron cloud dimensions yields: \( V_{n2e1} (r) \simeq V_{n1e} (r) \)

On the other hand each of the two electrons is actually subject to the repulsive effect of a screened nucleus due to the presence of the other electron. For the combined nuclear molecule, we have \( Z_t = Z_1 + Z_2 \), while the usual variational procedure yields an effective atomic number for each electron \( Z^{**} = Z_t - 5/16 \).

Therefore for the low energy reaction of two hydrogenlike atoms in their ground state, with equal atomic numbers \( Z \), the interaction potential energy is:

\[ V_{sc} (r) = \frac{Z^2e^2}{r} - 2 \left[ \frac{Ze^2}{r} + \frac{Ze^2}{r} \left( 1 + \frac{r}{2r_0^{**}} \right) \exp \left(-r/r_0^{**}\right) \right] + \frac{5 Z^{**}e^2}{8 a_0} \]  

(20)

where

\[ r_0^{**} = \frac{a_0}{2Z^{**}} \]  

(21)
In the same way we can calculate the potential energy when one (or both) atoms are in an excited state.

c) The nucleus-atom channel.

For the hydrogen-like atom target an extensive study has already been given [17]. However, for a two electron target atom further elaboration is needed. In that case the potential energy is:

\[ V(r) = V_c(r) + V_{n_2 e_1}(r) + V_{n_2 e_2}(r) + V_{e_1 e_2} \]  \hspace{1cm} (22)

If we compare Eq. (14) with Eq. (22) we see that the two potentials must be approximately the same. Therefore the potential energy (21) can account for the nucleus-atom channel with a two-electron target atom, as well.

The penetration factor \( P(E) \) multiplied by the astrophysical factor \( S(E) \) in the \( s \)-wave cross section formula

\[ \sigma(E) = \frac{S(E)}{E} P(E) \]  \hspace{1cm} (23)

is given by the WKB method:

\[ P(E) = \exp \left[ -\frac{2\sqrt{2\mu}}{\hbar} \int_{R}^{r_c(E)} \sqrt{V_{sc}(r) - E} \, dr \right] \]  \hspace{1cm} (24)

where the classical turning point is given by

\[ V_{sc}(r_c) = E \]  \hspace{1cm} (25)

At astrophysical energies the potential energy is found to be shifted by a constant screening energy \( U_e \) which is added to the relative energy of the collision.

For the nucleus-nucleus channel the calculation is trivial leading to \( P(E) = \exp(-2\pi n) \) where \( n \) is the Sommerfeld parameter and \( U_e = 0 \).

For the nucleus-hydrogen-like atom channel the screening energy has already been calculated [17]

\[ U_e = -(Z_1 + Z_2) \frac{Z_2 e^2}{a_0} \]  \hspace{1cm} (26)

For two hydrogen-like atoms with equal charges \((Ze)\) we have performed numerical integrations of Eq. (24) and numerical solutions of Eq. (25). At astrophysical energies where screening becomes important the screened coulomb potential can be safely replaced by the quantity

\[ V_{sc}(r) = \frac{Z^2 e^2}{r} + U_e \]  \hspace{1cm} (27)

where:

\[ U_e = -2Z (2Z - 5/16) \frac{e^2}{a_0} + \frac{5}{8} (2Z - 5/16) \frac{e^2}{a_0} \]  \hspace{1cm} (28)
which is also the screening energy for the collision of a bare nucleus ($Ze$) with a two-electron target atom.

For the astrophysical reaction $^3He(^3He,2p)^4He$ we have $Z_1 = Z_2 = Z = 2$ and the corresponding screening energy obtained through the above model is $U_e = -338\text{ eV}$. Our result is very close to the experimental result of the LUNA collaboration $U_{ee}^{ex} = -294 \pm 47\text{ eV}$. The small difference could be plausibly attributed to energy losses and experimental errors had it not been for another, as yet unidentified, uncertainty source for the screening energies and the associated astrophysical factors, which causes a small increase in the uncertainty for the solar neutrino fluxes. In fact the LUNA experimental results were first fitted using three different approaches: a) fixing the screening energy at the value given by the adiabatic limit, b) allowing all three parameters $(S(0), S'(0), S''(0))$ of the astrophysical factor and the screening energy $U_e$ to vary simultaneously, c) using higher energy data to fix the parameters of the astrophysical factor while varying the screening energy. The two model independent methods (b,c) gave considerably different screening energies in that work, that is $U_e^{(b)} = -323 \pm 51\text{ eV}$ and $U_e^{(c)} = -432 \pm 29$ respectively. In their final article only the (b) method was used yielding the above mentioned value of $U_{ee}^{ex} = 294 \pm 47\text{ eV}$. It is obvious that if the (c) method had been used the screening energy would have been higher, and the adiabatic limit would have been considerably exceeded again. The two methods (b,c) gave respectively the following zero energy astrophysical factors: $S^{(b)}(0) = 5.30 \pm 0.08$ and $S^{(c)}(0) = 5.1 \pm 0.1$, that is a 3.9% difference. Regarding the solar neutrino problem that percentage admittedly leads to a negligible neutrino flux uncertainty for the $pp$ and $hep$ neutrinos (0.1%). However the uncertainty for the $^8B$ and $^7Be$ ones can be as high as 1.5% , which should not be disregarded. Although the author agrees that method (b) seems more plausible than the (c) one, a better justification is needed for the choice of the fitting method when such low energy experiments are considered as it obviously constitutes a source of uncertainty.

IV. MULTI-ELECTRON SCREENING EFFECTS

In the framework of the Thomas-Fermi (TF) model the screened Coulomb potential for a neutral multi-electron atom $Z_1$ is \cite{18}:

$$V_{sc}^{TF}(r) = \frac{Z_e}{r} \phi(r)$$

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The dimensionless function $\phi(r)$ can be obtained by the solution of the universal differential equation

$$
\frac{d^2\phi(x)}{dx^2} = \frac{\phi^{3/2}(x)}{\sqrt{x}}
$$

where $x = r/a$ and the screening radius is $a = 0.8853Z_1^{-1/3}a_0$.

In our approach, instead of solving numerically the differential equation, we will make use of an analytic approximation of the function $\phi(r)$ given by Tietz [21]. Namely:

$$
\phi(x) = \frac{1}{(1 + bx)^2}
$$

with $b = 0.536$.

At first we will consider the interaction of very light nuclei with a heavy multi-electron atom so that we can disregard the perturbation induced by the impinging particle to the average electron density of the target atom, which is the sudden limit (SL) approximation.

If we expand the TF screened potential using Tietz’s approximation we obtain the screened potential energy of the interaction:

$$
V_{TF}^{sc} = \frac{Z_1Z_2e^2}{r} - 2\frac{bZ_1Z_2e^2}{a} + 3\frac{Z_1Z_2b^2e}{a^2}r + O(r^2)
$$

The third term of the above potential, as well as terms $O(r^2)$, are negligible with respect to the constant screening energy shift given by the second term. For example for relative energies of 20 keV the tunneling region for a $p + ^{14}N$ reaction begins at a classical turning point of $r_c = 500 fm$. At such a distance the second term is 440 eV while the third is only 7 eV. Therefore, inside the barrier, where $r < r_c$, terms proportional to the scaled distance $r/a$ practically vanish.

Inserting the above screened Coulomb potential (32) with Tietz’s approximation into the WKB integral of Eq. (24) and working in the same way as with the potentials of the previous section we obtain the screening energy for the collision of a light bare nucleus ($Z_2e$) with a neutral multi-electron atom ($Z_1e$):

$$
U_{TF}^{SL} = -1.21\frac{Z_1^{4/3}Z_2e^2}{a_0}
$$

Let us now suppose that the impinging nucleus (not necessarily a light one) has been neutralized so that it can also be considered a TF atom. We can obtain the maximum screening energy transferred to the relative nuclear motion by using the formula for the total energy of a TF atom. In fact there are three contributions to the total energy of the atom: The kinetic energy of the electrons, the potential energy of their interaction with the nucleus and the potential energy of their mutual interaction. For a neutral TF atom with charge $Z_1e$ the total energy is given by [20]:

$$
E_{TF}^{tot} = -\frac{Z_1^2e^2}{a}\left(\frac{2}{5}\mu - \frac{J}{10}\right)
$$
where $\mu = -\phi'(0)$ and

$$J = \int_0^\infty \left( \frac{d\phi}{dx} \right)^2 dx \quad (35)$$

Numerically,

$$E_{TF}^{\text{tot}} = -20.93 \frac{Z_1^{7/3}}{eV} \quad (36)$$

It is therefore plausible to assume that for an adiabatic limit (AL) interaction of two neutral TF atoms the screening energy $U_{TF}^{\text{AL}}$ will be the difference between the total energy of the combined molecule and that of the two separate atoms:

$$U_{TF}^{\text{AL}} = -20.93 \left[ (Z_1 + Z_2)^{7/3} - Z_1^{7/3} - Z_2^{7/3} \right] \text{eV} \quad (37)$$

We can compare the results of Eqs. (33) and (37) with the ones obtained in Ref. [16]. For a reaction $p + \frac{1}{3} X$ between a bare proton $p$ and neutral atom $\frac{1}{2}X$ we obtain:

**Table I.** The screening energies for various proton-induced astrophysical reactions as obtained through the sudden $(U_{e}^{\text{SL}})$ and the adiabatic $(U_{e}^{\text{AL}})$ limit of Ref. [16] versus the screening energies obtained through the present TF sudden $(U_{TF}^{\text{SL}})$ and adiabatic $(U_{TF}^{\text{AL}})$ limit.

| Reaction        | $U_{e}^{\text{SL}}$ (eV) | $U_{e}^{\text{AL}}$ (eV) | $U_{TF}^{\text{SL}}$ (eV) | $U_{TF}^{\text{AL}}$ (eV) |
|-----------------|--------------------------|--------------------------|--------------------------|--------------------------|
| $p + \frac{7}{3} L$ | 186                      | 259                      | 281                      | 592                      |
| $p + \frac{11}{5} B$ | 347                      | 426                      | 462                      | 717                      |
| $p + \frac{12}{6} C$ | 441                      | 441                      | 441                      | 527                      |
| $p + \frac{14}{7} N$ | 544                      | 570                      | 570                      | 847                      |
| $p + \frac{18}{8} O$ | 653                      | 653                      | 653                      | 653                      |

We observe that Eq. (33) practically reproduces the sudden limit $U_{e}^{\text{SL}}$ of Ref. [16], while Eq. (37) gives a higher adiabatic limit than the one $(U_{e}^{\text{AL}})$ given in Ref. [16]. Despite the fact that for the reaction $^3\text{He} (^3\text{He}, 2p)^4\text{He}$ the electrons involved are too few to justify use of the above formulas it will give a sense of the validity of the present models if we apply our formulas on that reaction as well. In fact Eq. (33) gives $U_{TF}^{\text{SL}} = 166 \text{eV}$ while Eq. (37) gives $U_{TF}^{\text{AL}} = 426 \text{eV}$, which are admittedly reasonable bounds.

Regarding the acceleration effects produced by the above screening energies on the non-resonant wings of astrophysical nuclear reactions, we can apply the usual enhancement factor [22]

$$f_{TF}^{(\text{SL,AL})}(E) = \exp \left( \pi n \frac{U_{TF}^{(\text{SL,AL})}}{E} \right) \quad (38)$$

where $n$ is the Sommerfeld parameter and $E$ is the center-of-mass energy. We obtain for the sudden and the adiabatic limit respectively:
\[ f_{TF}^{SL}(E) \simeq \exp \left( \frac{Z_1^{7/3} Z_2^2 A^{1/2}}{2E_{(keV)}^{3/2}} \right) \]  
\[ \text{and} \]
\[ f_{TF}^{AL}(E) \simeq \exp \left[ \frac{Z_1 Z_2 \left( (Z_1 + Z_2)^{7/3} - Z_1^{7/3} \right) A^{1/2}}{3E_{(keV)}^{3/2}} \right] \]

where \( A = A_1 A_2 (A_1 + A_2)^{-1} \) is the reduced mass number.

The above formula will be particularly useful in laboratory experiments where such nuclear reactions are involved as those of the CNO cycle and the ones encountered in the final stages of stellar evolution (e.g. supernova nucleosynthesis). In such reactions, it is often impossible to measure a nonresonant cross section in the laboratory at a sufficiently low energy due to technical difficulties \[10\] (large background of counts, beam instability etc.). Therefore the associated astrophysical factor cannot be accurately extrapolated to zero energies as required for the calculation of the effective astrophysical factor \( S_{eff} \) that appears in the thermonuclear reaction rate formulas (Ref. \[23\] and references therein). However, the recent accomplishments of the LUNA collaboration with the \( ^3\text{He} \left( ^3\text{He}, 2p \right)^4\text{He} \) reaction inspire hope that similar low-energy experiments will soon be conducted for heavier nuclei (multi-electron atoms) as well, in which case the above formula will help correct the low energy cross section measurements.

Let us consider for example the first member of the CNO cycle, namely the radiative direct capture reaction \( ^{12}\text{C} \left( p, \gamma \right)^{13}\text{N} \). The low energy cross section is dominated by an s-wave resonance \( \left( \frac{1}{2}^+ \right) \) at \( E_{cm} = 424 \text{ keV} \), while its Gamow peak at central solar conditions is \( 24.5 \text{ keV} \). The usually employed \( S_{eff} \) for that reaction is the one obtained by an experiment \[24\] which measured cross sections at energies as low as \( E_{cm} = 138 \text{ keV} \) disregarding all screening effects. According to the present models the screening enhancement of the cross section at such an energy would be between 2\% and 3.4\% which is not a negligible correction. It is now obvious that in any future attempt to improve the accuracy of the extrapolation by lowering the energy of the experiment the proposed model of this work will be very useful.

The corrections are even more important for other reaction of the CNO cycle such as the slowest one, which controls the energy generation of that cycle, that is \( ^{14}\text{N} \left( p, \gamma \right)^{15}\text{O} \). Various investigations \[25\] (and references therein) have obtained data for that reaction to center-of-mass energies as low as 93 \text{ keV} without correcting for screening. The error committed at such low energies for that particular reaction can be as high as 9\% (AL). Finally, the corrections can be dramatic if we consider very low resonances such as the 66 \text{ keV} one of the \( ^{17}\text{O} \left( p, a \right)^{14}\text{N} \) reaction, namely of the order of 12\% (AL). Such considerable enhancement could presumably lead even to shifts of the resonance energies themselves, compared to the bare nuclei measurements.

In figures 1 and 2, there is plotted the screening enhancement factor for the most important astrophysical nuclear reactions of the CNO bi-cycle with respect to the center-of-mass energy. Close to the Gamow peaks of those reactions (Fig.1) the predicted enhancement of the nonresonant cross section is already 5\% (at least) while at very low energies (Fig.2)
2 \leq E_{cm} \leq 5\text{keV}, the nonresonant cross section of the screened reaction is expected to be several times larger than that of the bare nucleus one.

Before concluding this section we should emphasize that our results agree well with the ones obtained by the adiabatic assumption \cite{15} according to which the screening energy of the reaction between atoms $A$ and $B$ is given by the formula:

$$U_{e}^{BE} = E_{el}(A + B) - E_{el}(A) - E_{el}(B)$$

(41)

where $E_{el}(A + B)$ is the total binding energy of the electrons in the combined atom $A + B$, and $E_{el}(A)$, $E_{el}(B)$ are the total electronic binding energies of the asymptotically separated atomic reaction partners $A, B$. For example for the $^{12}\text{C}(p, \gamma)^{13}\text{N}$ and the $^{14}\text{N}(p, \gamma)^{15}\text{O}$ reactions respectively, the latter model gives screening energies $U_{e}^{BE} = 444 \text{eV}$ and 546 \text{eV}, which are bracketed by the energies derived through the present models (see table).

V. CONCLUSIONS

Two very efficient models are presented here which reproduce the screening enhancement effects that appear in laboratory nuclear reactions at astrophysical energies. The first model, which describes two-electron effects, relies on the Hartree-Fock approximation and agrees very well with the recent LUNA experimental screening energy for the reaction $^{3}\text{He}(^{3}\text{He}, 2p)^{4}\text{He}$, which so far remains unexplained.

The second model is based on the Thomas-Fermi theory and yields the screening energies for reactions encountered in advanced nuclear burning stages of stellar evolution, where multi-electron effects dominate. To the author’s knowledge, for multi-electron laboratory effects, there have never been any closed formulas such as Eqs. (39) and (40), which can be readily used in order to correct the cross section measurements. Moreover, the latter model compares well with other available theories and its use is expected to be particularly useful in any future attempt to improve the accuracy of the CNO astrophysical factors by lowering the energy of the experiment.

Finally, the fitting method used in the determination of the astrophysical factor is identified here as a source of uncertainty for the solar neutrino fluxes, which needs further elaboration and justification.

VI. APPENDIX

The screened potential model approach needs some elaboration regarding its actual effects. In Refs. \cite{10} and \cite{14} the screening energy for a collision between the atomic target ($Z_{1}e$) and the projectile ($Z_{2}e$) was identified as

$$U_{e} = \frac{Z_{1}Z_{2}e^{2}}{R_{a}}$$

(42)

where the screening radius was set equal to the radius of the innermost electrons of the target ($R_{a} = a_{0}/Z_{1}$) labeling that as the ”worst case”. In that model, the electron cloud is
assumed to be unperturbed, which is the definition for the sudden limit, and there is no special consideration for multi-electron effects, either.

However, in our study of hydrogen-like atomic targets [17] we have shown that the screening radius $R_a$, for the same sudden limit, is actually independent of the atomic number $Z_1$ and equal to the Bohr radius $R_a = a_0$, thus obtaining a smaller screening energy when $Z_1 > 1$ than the one used in Refs. [10] and [15]. Note that if we adopt the "worst case" approach for the reaction $^{12}\text{C}(p, \gamma)^{13}\text{N}$, then Eq. (12) gives the unrealistic screening energy $U_e = 1000 \text{ eV}$ which is beyond the present TF adiabatic limit value, too.

On the contrary, it is easy to show our approximation is valid for most practical purposes. The screening term $U^{(r)}_e$ that we disregarded when treating Eq. (13) via the WKB is actually proportional to the scaled relative internuclear distance $r/a_0$:

$$U^{(r)}_e = -2Z_1^2Z_2^2\frac{e^2}{a_0} \frac{r}{a_0}$$  \hspace{1cm} (43)

For a typical classical turning point $r_c \sim 10^{-2}a_0$ we have, throughout the barrier, $r < 10^{-2}a_0$. Hence, in the sudden limit, the ratio of the term that we considered significant $U_e$ (Eq. (26)) to the insignificant one, given by Eq. (43), is $U_e/U^{(r)}_e > 50Z_1^{-1}$. Obviously for small $Z_1$, which is usually the case in astrophysical reactions, our formulas becomes increasingly accurate.

**ACKNOWLEDGMENTS**

This work was financially supported by the Greek State Grants Foundation (IKY) under contract #135/2000. It was initiated at ECT* during a nuclear physics fellowship. The author would like to thank the director of ECT* Prof. Malfliet for his kind hospitality and support.
FIGURE CAPTIONS

Figure 1. The screening enhancement factor $f_{TF}(E)$ for the most important astrophysical nuclear reactions of the CNO bi-cycle with respect to the center-of-mass energy $E$ in the region of the Gamow peaks ($E_{GP}$) as calculated for central solar conditions. The lower (upper) solid curve represents the enhancement of the $^{13}C(p,\gamma)^{14}N$ reaction ($E_{GP} = 24.5$ keV) as calculated by the above TF sudden (adiabatic) limit. Likewise, the dashed curves stand for the $^{14}N(p,\gamma)^{15}O$ reaction ($E_{GP} = 27.2$ keV), while the dotted ones for the $^{16}O(p,\gamma)^{17}F$ reaction ($E_{GP} = 29.8$ keV). Lower and upper curves always indicate sudden and adiabatic limits respectively.

Figure 2. The screening enhancement factor $f_{TF}(E)$ for the most important astrophysical nuclear reactions of the CNO bi-cycle with respect to the center-of-mass energy in the
region $2 \leq E \leq 5keV$. The enhancement effect is particularly accentuated at such low energies. The notation is the same as in Fig.1.
