Multi-electron SEFs for nuclear reactions involved in advanced stages of stellar evolution

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Abstract

Multi-electron screening effects encountered in laboratory astrophysical reactions are investigated by considering the reactants Thomas-Fermi atoms. By means of that model, previous studies are extended to derive the corresponding screening enhancement factor (SEF), so that it takes into account ionization, thermal, exchange and relativistic effects. The present study, by imposing a very satisfactory constraint on the possible values of the screening energies and the respective SEFs, corrects the current (and the future) experimental values of the astrophysical factors associated with nuclear reactions involved in advanced stages of stellar evolution.

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I. INTRODUCTION

The astrophysical factors for the nuclear reactions of the CNO bi-cycle (solar center, upper main-sequence stars etc.) and of other advanced nuclear burning stages, such as those ignited in classical novae, have been obtained by performing measurements well above the Gamow peak, ( [1] and references therein) and extrapolating to lower energies thus committing a significant error in certain cases. After the accomplishments of the LUNA collaboration [2] in probing deep into the Gamow-peak region of the most important break-up reaction \( He^3(He^3,2p)He^4 \) the nuclear astrophysics community hopes that similar low-energy experiments will follow for astrophysical nuclear reactions involving heavier nuclei. However, the screening effect, which has been studied extensively ( [3,9] and references therein) regarding nuclear reaction of the proton-proton chain, is particularly accentuated when heavier ions are considered due to their multi-electron nature. It is the purpose of this paper to investigate the enhancement of the astrophysical factor that appears (or will appear) when astrophysical energies are attained in nuclear reaction experiments.

In a recent paper [3] the Thomas-Fermi (TF) model was used in order to derive a lower (sudden) limit (SL) and an upper (adiabatic) limit (AL), thus imposing a constraint on the possible values of the screening energies. In the present work we will improve that study by tightening that constraint while studying, at the same time, ionization, relativistic, thermal and exchange effects.

The TF model is one of the most thoroughly studied models of atomic physics (for a detailed study see Ref. [10]). In brief, if \( n(r) \) is the electron number density around the screened nucleus then the self-consistent potential \( \Phi(r) \), which results from the combined field (nucleus plus electrons), is obtained by solving the Poisson equation \( \nabla^2\Phi(r) = -4\pi\rho(r) \) where \( \rho(r) = -en(r) \) is the charge density of the electron cloud. Using quantum statistical arguments [10] we can show that for the TF atom at each point \( r \) the fermi energy \( p_f \) must be

\[
\frac{p_f^2}{2m_e} = e \left[ \Phi(r) - \Phi(r_0) \right]
\]

where \( r_0 \) is the ionic radius which gives the boundary conditions

\[
\Phi(r_0) = \frac{Ze_e}{r_0}, \quad \left( \frac{d\Phi}{dr} \right)_{r_0} = -\frac{\Phi(r_0)}{r_0}
\]

and the degree of ionization is a function of the number of electrons \( (N) \) and protons \( (Z) \), respectively, so that \( q = 1 - N/Z \).

Following some well cited transformations [10] the self-consistent potential can be written:

\[
\Phi(r) = \Phi(r_0) + \frac{Ze_e}{r} \phi
\]

Setting \( r = \alpha x \), the universal function \( \phi(x) \) is given by the dimensionless TF equation:
\[
\frac{d^2 \phi(x)}{dx^2} = \frac{\phi^{3/2}(x)}{\sqrt{x}}
\]

(4)

to be solved with the boundary conditions \(\phi(0) = 1\), \(\phi'(x_0) = -q/x_0\). Note that the scaling parameter \(\alpha\) has its usual value \(\alpha = 0.88534Z^{-1/3}a_H\), with \(a_H\) representing the Bohr radius.

II. IONIZATION, EXCHANGE AND THERMAL EFFECTS

We will exploit the advantages of the TF theory in order to derive the effects of ionization, electron-electron (exchange) interactions and temperature on multi-electron SEFs. The adiabatic limit (AL) SEF of Ref. [3] for neutral atoms seems to be well justified and it is the largest available. However, the sudden limit (SL) SEF of the same work needs improvement as it has been derived using Tietz’s approximation [11] which is actually a rough model that can only approximate the self-consistent potential of neutral atoms at average distances from the nucleus, disregarding all relativistic, thermal and ionization effects. As far as astrophysical reaction are concerned, screening becomes important very close to the nucleus and therefore a more appropriate approximation is needed, which could also account for ionization effects. To solve that problem we resort to Baker’s [12] small \(x\) expansion where the expansion coefficients are themselves functions of the initial slope \(S(q) = \phi'(0)\). The first few terms are given by:

\[
\phi_B(x) = 1 + S(q)x + \frac{4}{3}x^{3/2} + \frac{2}{5}S(q)x^{5/2} + \frac{1}{3}x^3 + \frac{3}{70}S^2(q)x^{7/2} + \frac{2}{15}S(q)x^4 + ...
\]

(5)

There exists a unique value \(S(0) = -1.588\) which gives \(x_0 = \infty\) and \(\phi(x_0) = 0\) corresponding to the neutral TF atom \((q = 0)\). Every other value \(S(q) < S(0)\) gives finite values for \(x_0\) corresponding to positive TF ions \((0 < q < 1)\). By selecting various initial slopes we obtain relations of the form: \(S = S(q)\) and \(x_0 = x_0(q)\) (see Figures 1 and 2).

Hence, the screened Coulomb potential around the target nucleus will now be given by:

\[
\Phi(r) = \frac{Z_1eQ}{\alpha x_0(q)} + \frac{Z_1e}{r} \phi_B \left(\frac{r}{\alpha}\right)
\]

(6)

where from now on \(Z_1\) and \(Z_2\) represent the atomic numbers of the target nucleus and the projectile, respectively.

An alternative approach would be to adopt Moliere’s approximation [13] for the solution of Eq. (6):

\[
\phi_M(x) = \sum_{i=1}^{3} B_i \exp(-\beta_i x)
\]

(7)

with the fitting parameters

\[
B_1 = 0.1, \quad B_2 = 0.55, \quad B_3 = 0.35, \quad \beta_1 = 6.0, \quad \beta_2 = 1.2, \quad \beta_3 = 0.3
\]

(8)
However, Molière’s function is less accurate than Baker’s one since the former underestimates the initial slope. For example, for neutral atoms $\phi'_{M}(0) = -1.365$, while $\phi'_{B}(0) = -1.588$

When positive ions are considered the total binding energy $E_{TF}^{tot} = -20.93 Z^{7/3} eV$ used in Ref. [3] for neutral TF atoms must be modified to account for ionization. In such a case

$$E_{TF}^{tot}(q) = F(q) Z^{7/3} \tag{9}$$

where

$$F(q) = \frac{12}{7} \left( \frac{2}{9 \pi^2} \right)^{1/3} \frac{e^2}{a_H} \left[ S(q) + \frac{q^2}{x_0(q)} \right] \tag{10}$$

We can now derive the screening enhancement factor for astrophysical nuclear reactions. The energy dependent penetration factor $P(E)$ multiplied by the astrophysical factor $S(E)$ in the $s$-wave cross section formula

$$\sigma(E) = \frac{S(E)}{E} P(E) \tag{11}$$

is given by the WKB method:

$$P^{SC}(E) = \exp \left[ -\frac{2\sqrt{2}\mu}{\hbar} \int_{r_n}^{r_c(E)} \sqrt{V_{sc}(r) - E} dr \right] \tag{12}$$

where $(SC)$ stands for screening and the classical turning point $r_c$ is given by

$$V_{sc}(r_c) = E \tag{13}$$

while the nuclear radius $r_n$ is a function of the mass numbers $A_{1,2}$ of the reactants, so that $r_n = 1.4 \left( A_{1}^{1/3} + A_{2}^{1/3} \right) fm$.

At astrophysical energies in the laboratory 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 no-screening (NOS) nucleus-nucleus channel the calculation is easy leading to

$$P^{NOS}(E) = \exp \left[ -2\pi n \left( 1 - \frac{4}{\pi} \left( \frac{r_n}{r_c} \right)^{1/2} + \frac{2}{3\pi} \left( \frac{r_n}{r_c} \right)^{3/2} + ... \right) \right] \tag{14}$$

where $n$ is the Sommerfeld parameter and $U_e = 0$. The general SEF $f(E)$ is defined as

$$f(E) = \frac{P^{SC}(E)}{P^{NOS}(E)} \tag{15}$$

which for weak screening (WES) shifts $U_e << E$ can be written

$$f^{WES}(E) = \exp \left( \pi n \frac{U_e}{E} \right) \tag{16}$$
In fact all measurements in the laboratory should be corrected by means of the above SEF so that the bare-nucleus astrophysical factor is not overestimated. Following the treatment of Ref. [3] which was used for neutral TF atoms, we can derive an approximate analytic formula for the TF screening shifts $U_{TF}^{(SL,AL)}$ and the corresponding SEFs $f_{TF}^{(SL,AL)}(E)$ in the SL and the AL respectively, where the degree of ionization is also taken into account. Combining Eqs. (16), (12), and (6) we obtain the following formulas:

Sudden Limit

$$U_{TF}^{SL}(q) = 4 \left( \frac{2}{9 \pi^2} \right)^{1/3} Z_1^{1/3} Z_2 \left[ S(q) + \frac{q}{x_0(q)} \right] \frac{e^2}{a_H}$$  \hspace{1cm} (17)

$$f_{TF}^{SL}(E) \simeq \exp \left[ -0.482 \frac{Z_1^{7/3} Z_2^2 A^{1/2}}{E_{(keV)}^{3/2}} \left[ S(q) + \frac{q}{x_0(q)} \right] \right]$$  \hspace{1cm} (18)

Adiabatic Limit

$$U_{TF}^{AL} = \left[ F(q_{12}) (Z_1 + Z_2)^{7/3} - F_1(q_1) Z_1^{7/3} - F_2(q_2) Z_2^{7/3} \right]$$  \hspace{1cm} (19)

$$f_{TF}^{AL}(E) \simeq \exp \left[ -15.64 Z_1 Z_2 \frac{F(q_{12}) (Z_1 + Z_2)^{7/3} - F_1(q_1) Z_1^{7/3} - F_2(q_2) Z_2^{7/3}}{E_{(keV)}^{3/2}} A^{1/2} \right]$$  \hspace{1cm} (20)

where the subscripts (1, 2, 12) of $q$ in the adiabatic limit formulas take into account the different degrees of ionization of the reactants and the combined nuclear molecule.

The present sudden limit formulas are more accurate than the ones obtained by means of Tietz’s approximation, therefore improving the constraint on the possible range of screening energies. For example the lower limit for neutral atoms given by Eq. (17) is 40% larger than the corresponding one of Ref. [3], thus greatly narrowing the gap between the sudden and the adiabatic limit SEFs.

Further simplifications are possible by noting that, for small ionization numbers $q$, the second additive term $q^2/x_0(q)$ in Eq. (14) is much smaller than the initial slope $S(q)$ and can therefore be neglected. If we further assume proton induced nuclear fusion reactions where the ionization state before and after the collision is the same then the AL formulas can be written as

$$U_{TF}^{AL} = \frac{12}{7} \left( \frac{2}{9 \pi^2} \right)^{1/3} \left[ (Z_1 + 1)^{7/3} - Z_1^{7/3} \right] \left[ S(q) + \frac{q^2}{x_0(q)} \right] \frac{e^2}{a_H}$$  \hspace{1cm} (21)

$$f_{TF}^{AL}(E) \simeq \exp \left[ -\frac{S(q) + q^2/x_0(q)}{5E_{(keV)}^{3/2}} Z_1 Z_2 \left[ (Z_1 + 1)^{7/3} - Z_1^{7/3} \right] A^{1/2} \right]$$  \hspace{1cm} (22)

Note that if we set $q = 0$ in all the above SL and AL formulas we recover the respective ones for neutral targets [3]. However, the $f_{TF}^{SL}(E)$ SEF given by Eq. (18) must be used...
with caution. It has been derived by truncating Baker’s series but at very low energies and moderately heavy nuclei that approximation begins to break down. Its actual validity will be investigated along with the relativistic effects in Sec.III.

We can assess the quality of the constraint imposed by our model on the possible values of the screening energies and the associated SEFs by studying Fig. 3 and Fig. 4. In the former, the SL and AL screening energy $U_{TF}^{(SL,AL)}$ for the most important astrophysical nuclear reactions of the CNO bi-cycle are plotted with respect to the degree of ionization of the TF positive ionic target. Along the whole profile of the $q$ values the upper (AL) and lower (SL) screening energy limits differ by roughly $100\text{eV}$ (or less) which is a very satisfactory constraint for most practical purposes.

On the other hand in Fig.4 we can observe the SL/AL SEFs for the most important astrophysical nuclear reaction of the CNO bi-cycle, namely $N^{14}(p,\gamma)O^{15}$, with respect to the center-of-mass energy $E$ in the region of the solar Gamow peaks ($E_{GP} = 27.2\text{keV}$) for various degrees of ionization. Naturally, the more ionized the atomic target the smaller the screening energy (see also Fig. 3) and, consequently, the smaller the respective SEF at a particular energy. The quality of the SL/AL constraint on the SEF is very good as has already been indicated by the corresponding screening energy limits (see Fig.3.)

Before we proceed to study relativistic effects, we should consider the influence of thermal and exchange effects. It should be emphasized that we have defined the sudden limit for a cold electron gas ($T = 0$) disregarding all exchange effects which, on the contrary, have been taken into account in the derivation of the total TF binding energy $E_{TF}^{tot}(q)$. Of course, the latter also includes the total potential energy $E_{TF}^{(n,e)}$ between the nucleus and the electrons and the total kinetic energy $K_{TF}^{tot}$ of the bound electrons. Actually, the exchange energy $E_{TF}^{(e,e)}$ is expected to lower the relative collision energy as recently shown in a relevant study $[4]$. For a neutral atom the above components of the total binding energy $E_{TF}^{tot}(q)$ can be written $[18]$:

$$K_{TF}^{tot} = +20.99Z^{7/3}, E_{TF}^{(e,e)} = +7.00Z^{7/3}, E_{TF}^{(n,e)} = -48.99Z^{7/3}$$

where we observe that exchange effects play a less important screening role than the kinetic energy ones.

It is now obvious that the adiabatic limit SEF can be written as

$$f_{TF}^{AL}(E) = f_{K_{TF}^{tot}}^{AL}(E) \times f_{E_{TF}^{(e,e)}}^{AL}(E) \times f_{E_{TF}^{(n,e)}}^{AL}(E)$$

where the first two factors of the right-hand side decrease rather than increase the cross section of the astrophysical fusion reaction.

The above factorization of multi-electron SEFs allows some qualitative investigation of the phenomenon. Obviously, according to the third factor, by increasing the binding energy of the electrons we can enhance the cross section of the reaction. That is for the same number of electrons, the larger the atomic number the larger the cross section at a particular collision energy. However, by increasing the atomic number the kinetic energy of electrons is also increased and according to the first factor that will cause a decrease in the cross section. On the other hand exchange effects also increase with the atomic number.
reducing further the cross section. Note that the dependence of the SEF on the atomic number is more complex than the simple monotonous increase indicated by Eq. (24) and Eq. (23). The TF model, being a statistical one, gives a net dependence of the total energy on the atomic number proportional to $Z^{7/3}$. Unfortunately this conceals all shell effects, which are very important, as each shell carries a different screening capacity. For example, the K-shell electrons are expected to play a much more important role than those lying in the L-shell and so on. In fact the sudden limit SEFs which were derived [3] for the first and second excited states in hydrogen-like atoms, showed that a single electron of the K-shell increases the relative collision energy four times more than a single electron of the L-shell. As the screening energy enters the SEF exponentially (Eq. (16)) that translates into a K-shell SEF being equal to the L-shell SEF raised to the fourth power. Higher shells can be shown to play an even minor role. Notably, the present TF approach for the sudden limit disregards the fast response of the electron cloud due to the combined nuclear molecule [3], thus obtaining an even more conservative value for the SL screening energy.

In order to study the relative importance of shell effects we can consider the screening energy generated by the collision of a bare Carbon nucleus ($Z = 6$) with an atom of the same nuclear charge with only two electrons in its closed K-shell. Disregarding the fast response of the two-electron cloud, so that we are consistent with the present TF model, the Hartree-Fock (HF) screening energy is [3]

$$U_{HF}^{SL} = \left[ -2Z (Z - 5/16) + \frac{5}{8} (Z - 5/16) \right] \frac{e^2}{a_H}$$

with a numerical value of $U_{HF}^{SL} = 1760 \text{ eV}$.

On the other hand the Thomas-Fermi SL model (Eq. (17)) for $q = 0$ gives $U_{TF}^{SL} = 3191 \text{ eV}$. If we also take into account the exchange effects disregarded by Eq. (17) the TF screening energy should be smaller. In any case, according to our models, more than 50% of the six-electron TF screening energy originates from the two K-shell electrons, which emphasizes the importance of shell effects.

The TF formulas derived in this paper show a direct dependence of multi-electron SEFs on the ionization state ($q$) of the reacting atoms. The ionization number $q$ is of course a function of temperature (see for example the Saha equation [16]) so that at very high temperatures the atom is completely ionized (e.g. stellar plasma). Thus, the cold electron gas assumption is no longer valid when the temperature rises. For thermal energies of a few $eV$, corresponding to a few thousand degrees Kelvin, Eq. (4) should be replaced by the Marshak-Bethe equation [19]:

$$\frac{d^2 \phi_{MB}(x, T)}{dx^2} = \frac{\phi_{MB}^{3/2}(x, T)}{x^{1/2}} \left[ 1 + \zeta(T) \frac{x^2}{\phi_{MB}^2(x, T)} \right]$$

where the dimensionless temperature-dependent parameter is $\zeta(T) = 10^{-11} Z_1^{-8/3} T^2$, with $T$ measured in degrees Kelvin. The solution of that equation can be found by a perturbation method [20] and reads:

$$\phi_{MB}(x, T) = \phi_0(x) + \zeta(T) \phi_1(x)$$

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where the unperturbed term $\phi_0(x)$ is the solution of Eq. (11) and the trial function $\phi_1(x)$ is approximated by the truncated series $\phi_1(x) \simeq (4/35)x^{7/2} - (4/63)S(0)x^{9/2} + \ldots$. Consequently, in our study there is now a temperature dependent screening correction $U_e(T)$ to be taken into account. After some algebra that term for small distances can be written

$$U_e(T) = \frac{4}{35} \zeta(T) \frac{Z_1 Z_2 e^2}{\alpha} \left( \frac{r}{\alpha} \right)^{5/2}$$  \hspace{1cm} (28)$$

Actually, in obtaining Eq. (17) we disregarded radially dependent terms arising from Baker’s expansion since even the largest of those neglected terms, given by

$$U^{SL}_{TF}(r) = \frac{4}{3} \frac{Z_1 Z_2 e^2}{\alpha} \left( \frac{r}{\alpha} \right)^{1/2}$$  \hspace{1cm} (29)$$
is much smaller than the constant screening shift throughout the tunnelling region. By comparing Eq. (28) and Eq. (29) it is obvious that for temperatures of several thousand degrees Kelvin (so that $kT << e\Phi(r_0)$) the multi-electron screening enhancement of astrophysical reactions is the same as in a cold electron gas.

III. RELATIVISTIC EFFECTS

We can now proceed to include relativistic corrections to screening energies and the respective SEFs, which are expected to become important when studying the screening effects of lower shell electrons on a heavy atomic nucleus. For example a K-shell electron of an Oxygen atom has a Bohr velocity of $u_e = 0.058c$, which indicates that relativity may further modify the screening effect and therefore warrants further investigation. For simplicity, in the study that follows we will focus on neutral targets, as any degree of ionization will simply diminish the associated relativistic corrections.

The sudden limit can be obtained by using the Dirac-Hartree-Fock-Slater (DHFS) calculations of Salvat et al [21], which provide us with screening functions accounting for relativistic effects. In that work Moliere’s approximation was used and the corresponding $B_i(Z)$, $\beta_i(Z)$ parameters were tabulated for $Z = 1 - 92$. Therefore, when relativistic effects are considered, the SL screening shift can be written as

$$U^{SL}_{DHFS} = -4 \left( \frac{2}{9\pi^2} \right)^{1/3} Z_1^{4/3} Z_2 \left[ \sum_{i=1}^{3} B_i(Z_1) \beta_i(Z_1) \right] \frac{e^2}{a_H}$$  \hspace{1cm} (30)$$

Unfortunately, Eq. (30) is an very rough approximation. Moliere’s approach was previously shown to underestimate the non-relativistic (neutral atom) SL screening energy by 14%. In our study we have used the relativistic and non-relativistic screened Moliere potentials given in Ref. [13] and Ref. [21], respectively. Although they both satisfy the condition that relativistic effects result in more bound systems none of them is reliable close to the nucleus. For example Eq. (30) for the reaction $C^{13}(p, \gamma)N^{14}$ yields $U^{SL}_{DHFS} = 406eV$ which is even lower than the non-relativistic SL screening energy given by Eq. (17). Therefore, the DHFS screening energy turns out to be inappropriate as a lower bound of the relativistic screening energy.
The most accurate way to calculate the screened Coulomb potential would be to use the Vallarta-Rosen relativistic TF equation \[ \frac{d^2 \phi_{rel}(x)}{dx^2} = \frac{\phi_{rel}^{3/2}(x)}{\sqrt{x}} \left[ 1 + \lambda \frac{\phi_{rel}(x)}{x} \right]^{3/2} \] (31)

with \( \lambda = 3 \times 10^{-5} Z_1^{4/3} \). The V-R potential has been approximated with respect to the distance \( x_c = \lambda + S(0) \lambda^2 \), by a two-branch function \[ \phi_{rel}^{out}(x) = \sum_{n=0}^{\infty} \left[ \lambda^n \phi_n(x) \right] - 1.206 \lambda^{3/2} (1 + 0.553 \ln Z) \] (32)

where \( \phi_0(x) \) is the non-relativistic Baker’s expansion given by Eq. (5) and

\[
\phi_1(x) = -6x^{1/2} + 11.733x + 5S(0)x^{3/2} + \ldots
\]

\[
\phi_2(x) = \frac{1}{2}x^{1/2} - \frac{21}{4}S(0)x^{1/2} + \ldots
\]

The only significant terms added to Baker’s expansion through the sum of Eq. (32) are those raised to powers \( n = 0, 1 \). The remaining terms \( (n > 1) \) are negligible throughout the tunneling region as they are multiplied by the very small number \( \lambda^n \) and therefore vanish at distances smaller than the classical turning point (see also previous section and the Appendix in Ref. \[3\]).

For distances shorter than \( x_c \) (but larger than the minimum internuclear distance given by \( x_n = r_n/\alpha \)) the approximation is

\[
\phi_{rel}^{in}(x) = 1 + sx + \frac{3}{2} \lambda^{1/2} [(x_n - x) + x \ln (x/x_n)] + \lambda^{3/2} \left[ \left( \frac{x - x_n}{x_n} \right) - \ln \left( \frac{x}{x_n} \right) \right] + \ldots
\]

where \( s \) is given by

\[
s = S(0) - \lambda^{1/2} \ln Z - 0.1388\lambda^{1/2} + 11.733\lambda + 5.157S(0)\lambda^{3/2} + \ldots
\]

Instead of seeking an approximate analytic formula for the relativistic \( SL \) SEF we have numerically evaluated the quantity given by Eq. (15) for the non-relativistic and relativistic regime. This approach will also provide a measure of the accuracy of the non-relativistic \( SL \) SEF analytic formula given by Eq. (18).

In Fig. 5 we have plotted the sudden limit \( SEF s \) 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 solar Gamow peaks \( (E_{GP}) \) with and without relativistic corrections (middle and lowermost curves, respectively), obtained by integrating numerically the penetration factors appearing in Eq. (13). In the same plot we have also included the non-relativistic SEF (uppermost curves) obtained through the analytic formula given by Eq. (18). We observe that the analytic formula overestimates the \( (CNO) \) \( SEF s \) by roughly 2% at the
Gamow peak energies, with the discrepancy becoming larger at lower energies. In nuclear astrophysics experiments, as far as astrophysical factors are concerned, energies lower than the Gamow peaks are not needed for most practical purposes, unless of course there are suspicions about the existence of resonances. If resonances can be ruled out, or the experimental energies are higher than the Gamow peaks (as expected to happen in future experiments) then the analytic ($SL$) SEF formula of Eq. (18) is a very reliable lower bound of our non-relativistic constraint.

In the same figure, regarding the lowermost and middle curves of each reaction, although it is obvious that the SL relativistic curves are almost indistinguishable from the non-relativistic ones, their divergence is increased when moderately heavy atoms are considered at very small energies. Admittedly, such small effects can be neglected at the currently attained experimental energies (or at the even lower energies expected to be attained in the future). Consequently, in any case, the non-relativistic $SL$ SEF is lower than the relativistic one and therefore can safely play the role of the lower bound of our constraint.

The upper (adiabatic) limit ($AL$) is expected to be more reliable as it has been calculated under well established models. In fact the total (neutral atom) TF energy can be given by:

$$E^{rel}_{TF}(Z) = Z^{7/3} \sum_{n=0}^{\infty} (c_n + k_n \ln Z) Z^{2n/3}$$

(37)

where the coefficients $c_n, k_n$ have been tabulated in Ref. [23]. Following the treatment used in Ref. [5] the relativistic AL screening energy for proton induced reactions will be:

$$U^{AL}_{RTF} = (Z_1 + 1)^{7/3} \sum_{n=0}^{\infty} [c_n + k_n \ln (Z_1 + 1)] (Z_1 + 1)^{2n/3} - Z_1^{7/3} \sum_{n=0}^{\infty} [c_n + k_n \ln (Z_1)] Z_1^{2n/3}$$

(38)

The corresponding relativistic $AL$ SEF can be found using Eq. (16) and the above screening energy. In Fig. 6 we have plotted the adiabatic limit SEFs 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 solar Gamow peaks ($E_{GP}$) with and without relativistic corrections (neutral targets). Upper and lower curves always indicate relativistic and non-relativistic regimes, respectively. As expected the divergence between the relativistic and the non-relativistic curves is an increasing function of the atomic number and a decreasing function of the relative collision energy. The screening energy given by Eq. (38) and the SEFs originating from it (through Eq. (16)) are the highest possible values and constitute the upper bounds of the constraints derived in this paper.

IV. CONCLUSIONS

The astrophysical factors $S(E)$ for nuclear reactions ignited during advanced stages of stellar evolution (solar center, upper main sequence, classical novae etc.) have been obtained by performing measurements in the laboratory well above the Gamow peak, and
extrapolating to lower energies. Any attempt to increase the accuracy of $S(E)$ by lowering the experimental energies introduces a significant error as multi-electron screening effects enhance the cross sections at astrophysical energies, thus yielding an overestimated zero-energy astrophysical factor $S(0)$. The tool for correcting the respective data is the SEF which, in the present work, is derived both analytically and numerically for the most important nuclear reactions of the CNO bi-cycle by means of Thomas-Fermi model. By means of that model lower ($SL$) and upper ($AL$) limits are derived for the possible values of the screening energies and the respective SEFs imposing a very reliable constraint on the corrections which are necessary before fitting the bare-nucleus astrophysical factor polynomial to the experimental data.

Moreover, we have also investigated the effects of the degree of ionization ($q$) of the reacting atoms deriving analytically the functional dependence of SEF on it. As expected, the SEF is a decreasing function of $q$, which is again well constrained by lower and upper limits. Other effects studied here, are exchange, relativistic and thermal ones. The actual contribution of exchange effects is analysed while relativistic and thermal effects are shown to be negligible for most practical purposes. Finally the importance of shell effects, an aspect the TF model cannot take into account, is underlined by showing that the lower shell are mostly responsible for the screening effect while higher ones play a minor role even in multi-electron atomic systems.

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FIGURE CAPTIONS

Figure 1. The initial slope $S(q) = \phi'(0)$ of the TF function $\phi(x)$ plotted with respect to the degree of ionization $q = 1 - N/Z$ of the TF positive ion.

Figure 2. The ionic radius $x_0(q)$ of the TF positive ion plotted with respect to the degree of ionization $q = 1 - N/Z$.

Figure 3. The SL and AL screening energy $U^{SL,AL}_{TF}$ for the most important astrophysical nuclear reactions of the CNO bi-cycle plotted with respect to the degree of ionization $q = 1 - N/Z$ of the TF positive ion. The upper (lower) solid curve represents the enhancement of the $^{13}C(p, \gamma)^{14}N$ reaction as calculated by the TF sudden (adiabatic) limit. Likewise, the dashed curves stand for the $^{14}N(p, \gamma)^{15}O$ reaction, while the dotted ones for the $^{16}O(p, \gamma)^{17}F$ reaction. Upper and lower curves always indicate sudden and adiabatic limits respectively.

Figure 4.
The SEFs for the most important astrophysical nuclear reactions of the CNO bi-cycle $\text{N}^{14} (p, \gamma) \text{O}^{15}$ reaction with respect to the center-of-mass energy $E$ in the region of the solar Gamow peaks ($E_{GP} = 27.2 \text{ keV}$) for various degrees of ionization $q = 1 - N/Z$. The lower (upper) solid curve represents the enhancement of the reaction as calculated by the TF sudden (adiabatic) limit for neutral atoms (Eqs. (18) and 20). Likewise, the dashed curves stand for a degree of ionization $q = 0.3$, while the dotted ones for $q = 0.8$. Lower and upper curves always indicate sudden and adiabatic limits, respectively.

Figure 5.

The sudden-limit SEFs 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 solar Gamow peaks ($E_{GP}$) with and without relativistic corrections (neutral targets). The solid curves represent the enhancement of the $\text{C}^{13} (p, \gamma) \text{N}^{14}$ reaction ($E_{GP} = 24.5 \text{ keV}$) with the lowermost and middle curves standing for the non-relativistic and relativistic SEFs, respectively, obtained by integrating numerically the penetration factors appearing in Eq. (15). The uppermost solid curve represents the non-relativistic SEF obtained through the analytic formula given by Eq. (15). Likewise, the dashed curves stand for the $\text{N}^{14} (p, \gamma) \text{O}^{15}$ reaction ($E_{GP} = 27.2 \text{ keV}$), while the dotted ones for the $\text{O}^{16} (p, \gamma) \text{F}^{17}$ reaction ($E_{GP} = 29.8 \text{ keV}$), with their lowermost, middle and uppermost curves having the same meaning as in the $\text{C}^{13} (p, \gamma) \text{N}^{14}$ reaction.

Figure 6.

The adiabatic limit SEFs 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 solar Gamow peaks ($E_{GP}$) with and without relativistic corrections (neutral targets). The upper (lower) solid curve represents the relativistic (non-relativistic) enhancement of the $\text{C}^{13} (p, \gamma) \text{N}^{14}$ reaction as calculated by the TF model. Likewise, the dashed curves stand for the $\text{N}^{14} (p, \gamma) \text{O}^{15}$ reaction, while the dotted ones for the $\text{O}^{16} (p, \gamma) \text{F}^{17}$ reaction. Upper and lower curves always indicate relativistic and non-relativistic regimes, respectively.
Atomic TF radius: $x_0(q)$

Degree of Ionization: $q = 1 - N/Z$
Screening Energy $U_{TF}^{(SL,AL)}$ (eV) vs. Degree of Ionization: $q=1-N/Z$
