EFFECT OF SCREENING ON THERMONUCLEAR FUSION IN STELLAR AND LABORATORY PLASMAS

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ABSTRACT

The fusion-enhancement factor due to screening in the solar plasma is calculated. We use the finite-temperature Green’s function method, and a self-consistent mean field approximation. We reduce this to one-center problems, because in the collision of two fusing ions, the turning point where tunneling may occur lies far inside the screening radius. The numerical results given by this method indicate that screening may be slightly weaker than that obtained in the most recent previous calculations.

Subject headings: elementary particles — nuclear reactions, nucleosynthesis, abundances — plasmas

1. INTRODUCTION

There remains continued interest in the solar neutrino problem, which has not been resolved in terms of the standard solar model and standard particle physics. Neutrinos are generated in thermonuclear reactions, and thermonuclear reaction rates are determined by solar physics (temperature and density), nuclear physics, and atomic shielding. The solar neutrino problem is just one of several examples where there is current interest in thermonuclear reaction rates; others include general stellar structure and laboratory plasmas. We address here the role of atomic shielding, using a finite-temperature Green’s function method. Recent calculations of screening effects in the Sun have been reported by Gruzinov & Bahcall (1998), who also review previous solar screening calculations. Results of those calculations, with which we compare our present work, exhibit a scatter of 10%–30% or more in the effect of screening on fusion rates. As discussed in Gruzinov & Bahcall (1998), all of these previous calculations either are based on Salpeter’s weak screening formula, which is a classical approximation, or else make unphysical approximations in order to go beyond the linear regime. Gruzinov & Bahcall attempted to rectify these limitations by including quantum effects, treating the kinetic energy in perturbation theory. Our model differs from theirs in that we do not rely on perturbation theory.

The physical model we employ is based on self-consistent Hartree plus finite-temperature local density approximation for exchange and correlation, and it assumes thermal equilibrium and adiabaticity in the internuclear coordinates. We solve this model making no further approximations or expansions, except for numerics that are carefully monitored. All previous calculations involve, e.g., expansions in the temperature, density, or quantum corrections. Carraro et al. (1988) also consider dynamic effects. Thus we believe that our approach yields results that are the most accurate to date. These results yield fusion-enhancement factors that are typically a little smaller than those recently reported (Gruzinov & Bahcall 1998).

The rate of thermonuclear fusion in plasmas is governed by barrier penetration. The barrier itself is dominated by the Coulomb repulsion of the fusing nuclei. Because the barrier potential appears in the exponent of the Gamow formula, the result is very sensitive to the effects of screening by electrons and positive ions in the plasma. Screening lowers the barrier and thus enhances the fusion rate; the greater the nuclear charges, the more important it becomes, and thus it plays an important role in the solar neutrino spectrum.

As shown below, the classical turning point radius that enters in the WKB integral for barrier penetration is very small compared with the characteristic screening lengths of interest. Inside this radius, the barrier potential is just the nucleus-nucleus Coulomb repulsion minus a constant due to screening. The constant can be interpreted simply as the difference in free energies of the system between united and separated nuclei. Since both of these are spherically symmetric, one needs only consider one-center problems.

We present here numerical calculations relevant to the solar core. The screening due to electrons in the plasma is calculated quantum mechanically by a novel Green’s function method described in a recent paper (Watrous et al. 1999). The screening due to the ions is treated classically but self-consistently with the electrons. The resultant enhancement factors for several nuclear reactions are presented and compared with earlier results by other authors.

2. FUSION RATE

We work in atomic units, $\hbar = m_e = k_b = 1$; the unit of atomic temperature is $3.159 \times 10^5$ K. As shown by Salpeter (1954; here we follow Clayton 1968, p. 359), the fusion reaction rate between species 1 and 2 is given by

$$r_{1,2} = N_1 N_2 \int_0^{\infty} \psi(E)\nu(E)\sigma(E)dE,$$  \hspace{1cm} (1)

where $N_1$ and $N_2$ are the number densities of the colliding nuclides, $\psi(E)$ is the Maxwellian probability that the center-of-mass energy at large separation is $E$, and the cross section $\sigma$ is written as a product of a penetrability factor $P$ and a nuclear factor $\sigma_{\text{nuc}}$.

$$\sigma(E) = P(E)\sigma_{\text{nuc}}(E).$$ \hspace{1cm} (2)

In the WKB approximation, the s-wave penetration is given by

$$P_0(E) = \left(\frac{E\mu}{E}\right)^{1/2} \times \exp \left[ -2\sqrt{2}\mu \int_{R_0}^{R} \left[ Z_1 Z_2/r + U_{\text{sc}}(r) - E\right]^{1/2}dr \right],$$ \hspace{1cm} (3)
with \( E_B \) the height of the barrier, \( \mu \) the reduced mass, and 
\[ U_{sc}(r) < 0 \] the screening potential; \( R \) is the “touching” 
radius (the top of the barrier), and \( R_0 \) is the classical turning 
radius. The integrand in equation (1) peaks at some characteristic 
energy \( E_0 \). For the solar interior, the corresponding 
classical turning radius \( R_0 \approx z_1 Z_2/\mu E_0 \), is \( \sim 0.005 \) AU, 
compared with a screening radius of \( \sim 0.5 \) AU. For this 
reason, the screening potential can be taken as a constant 
\( U_0 = U_{sc}(r = 0) = 0 \) within the turning radius, acting as an 
effective shift in the energy:

\[
\begin{align*}
    r_{1,2} &= N_1 N_2 \int_0^\infty \psi(E) \sigma(E)(E - U_0) dE \\
    r_{1,2} &\propto \int_0^\infty E^{1/2} e^{-E/T} \sigma(E)(E - U_0) dE \\
    &= \int_{-U_0}^\infty (E' + U_0)^{1/2} e^{-(E' + U_0)/T} \sigma(E') dE'.
\end{align*}
\]

Then, neglecting \( U_0 \) in the limit of integration, 
\[
r_{1,2} \approx e^{-U_0/T} N_1 N_2 \int_0^\infty \psi(E) \sigma(E) dE.
\]

Screening thus enhances the reaction rate by the factor 
\[
f = e^{-U_0/T},
\]

where \( U_0 \) is given by equation (10) below. Since \( U_0 < 0 \), 
\( f > 1 \), corresponding to enhancement.

3. FREE ENERGY AND THE ONE-CENTER PROBLEM

The screening potential is just the change, brought about 
by the approaching ions, in the Helmholtz free energy 
\[
F = U_{\text{internal}} - TS,
\]

as a function of nuclear separation. Because of the smallness 
of the turning radius, it is sufficient to consider the one-
center problems and identify 
\[
U_0 = F(Z_1 + Z_2) - F(Z_1) - F(Z_2).
\]

What we mean here by one-center problems are the calcula-
tions of \( F \) when either charges \( Z_1, Z_2 \), or both lie at the 
center of the plasma. In § 4 we calculate \( F(Z) \) explicitly for 
an independent particle model approximation, akin to the 
temperature dependent Hartree-Fock method. However, the 
free energy has a simple and completely general (for the 
problem at hand) interpretation which does not depend on 
the mean field approximation. It is, by definition, the work 
required at a given temperature to introduce the nuclear 
charge into the plasma. The nucleus interacts with the 
plasma only electrostatically, so \( dF = \phi(Z, r = 0) dZ' \), and 
thus the work required to assemble the charge \( Z \) at, say, 
\( r = 0 \) is

\[
F(Z) = \int_0^Z \phi(Z', r = 0) dZ',
\]

where \( \phi(Z', r) \) is the electrostatic potential generated in the 
plasma due to a nuclear charge \( Z' \),

\[
\phi(Z', r = 0) = 4\pi \int_0^\infty r'dr' \left[ \sum_T \rho_T(r', T) - \rho_T(r', T) \right].
\]

Here \( \rho_T(r, T) \) and \( \rho_T(r, T) \) denote the finite-temperature 
number density (recall \( e = 1 \)) of the electrons and various 
background ions charge densities, respectively.

The one-center screening problem is solved by the 
methods described by Watrous et al. (1999) for the electrons 
with a Kohn-Sham formalism, using the finite-temperature 
local density approximation (Mermin 1965) for exchange 
and correlation. Screening due to ions is included as well as 
that due to electrons. The ions are treated classically 
according to the Debye-Huckel method. Thus the electric 
potential generated by electrons and ions becomes

\[
\Phi(r) = \frac{Z}{r} + \int d^3r' \sum T \rho_T(r', T) - \rho_T(r', T) .
\]

The second term is the function denoted by \( \phi(Z, r) \) above. 
Each ion density is given by

\[
\rho_T(r, T) = \rho_T(\infty) e^{-Z_1 \phi(r)/T}.
\]

Since \( \Phi(r) \) is positive, ions are pushed outward and electrons 
are drawn toward the nucleus. For notational simplicity in 
the following, the temperature dependence of the densities 
will be understood and not specified explicitly.

4. ALTERNATIVE MEAN FIELD DERIVATION OF THE 
FREE ENERGY

We now demonstrate the equivalence of the \( F \) defined by 
equations (9) and (11) in the finite-temperature Hartree-Fock 
approximation, which is similar to the finite-temperature 
local density approximation actually used in our numerical 
calculations. In a transparent, short notation, we describe 
the system by a second-quantized Hamiltonian \( H \) containing 
the kinetic energy operators \( t_i \) of the particles present in the 
plasma, their two-body interactions \( v_{ij} \), and the additional 
one-body operators \( w_i = -Z/r_i \) or \( +Z/r_i \) representing the 
contributions of the additional nuclear charge \( Z \) at the center. The temperature \( T \) enters 
the formalism via the usual Boltzmann factor exp \(-\beta H\), 
where \( \beta = 1/T \). Actually, because the average electronic 
density and background positive charge density are fixed 
parameters of the problem, \( H \) must be replaced by the 
usual constrained Hamiltonian. This will read, in a short 
notation, \( H = -\mu N \). Here \( \mu \) is a several-component 
chemical potential because of the several components in 
the plasma (i.e., electrons and various background ions). 
Accordingly the particle number operator \( N \) must be 
understood as a several-component operator. For simplicity, 
however, the following equations deal with the 
electrons only. This is because the positive ions in 
the background may consist of bosons as well as fermions, 
and we want to spare the reader the cumbersome symmetriza-
tion or antisymmetrization formulae for such backgrounds. 
In any case, the present paper describes the background 
density classically, and this density is not high enough to 
demand exchange terms.

The independent particle Ansatz approximates the eigen-
states of \( H = -\mu N \) by antisymmetrized products of single 
particle states (orbitals) \( |\omega\rangle \), with an approximate spectrum 
made of sums of independent particle levels \( \eta_i \). The \( \infty \) set 
of orbitals \( |\omega\rangle \) and eigenvalues \( \eta_i \) defines a one-body 
operator \( H_0 - \mu N \), presumed optimal from the point 
of view of a variational principle: i.e., stationarity of the grand 
potential or free energy \( F \).

In second quantization, the many-body density matrix 
used as a trial density operator (noted in the following by 
quantities carrying a subscript \( t \)) is

\[
D_t = \exp \left[ -\beta (H_0 - \mu N) \right] = \exp \left( -\beta \sum_i \eta_i c_i^t c_i \right),
\]

sections.
where $c_i^*$ and $c_i$ are the usual fermionic creation and annihilation operators for orbital $|i\rangle$. For electrons the normalization denominator $Z_i$ is

$$Z_i = \prod_i [1 + \exp (-\beta \eta_i)],$$

so the trial density becomes

$$D_t = \prod_i \frac{\exp (-\beta \eta_i c_i^* c_i)}{1 + \exp (-\beta \eta_i)}.$$ (17)

The true density matrix $D = \text{exp} \left[ -\beta (\mathcal{H} - \mu \mathcal{N}) \right]/\text{Tr} \exp \left[ -\beta (\mathcal{H} - \mu \mathcal{N}) \right]$, minimizes the true grand potential, $\Omega = \text{Tr} D (\mathcal{H} - \mu \mathcal{N} + \beta^{-1} \ln D)$. However, with an independent particle approximation, one must be content with minimizing

$$F = \text{Tr} D_t (\mathcal{H} - \mu \mathcal{N} + \beta^{-1} \ln D_t).$$

(18)

It is easy to show that

$$\text{Tr} D_t c_i^* c_i c_j^* c_j = f_i f_j, \quad \text{if} \quad i \neq j,$$

where the Fermi occupation numbers are $f_i \equiv \text{Tr} D_t c_i^* c_i = 1/[1 + \exp (-\beta \eta_i)].$ Furthermore

$$\text{Tr} D_t \{-\beta \eta_i c_i^* c_i - \ln [1 + \exp (-\beta \eta_i)] \} = f_i \ln f_i + (1 - f_i) \ln (1 - f_i).$$

(20)

Finally, because $\mathcal{H} = (\mathcal{F} + \mathcal{W}) + \mathcal{V} = \text{the sum} \text{of} \text{a} \text{one-body} \text{operator} \mathcal{F} + \mathcal{W} \equiv \sum_i t_i + \sum_i w_i$ and a two-body operator $\mathcal{V} \equiv \sum_{i>j} v_{ij}$, we obtain

$$F = \sum_i f_i \langle i | (t + w - \mu') | i \rangle + \frac{1}{2} \sum_{i,j} f_i f_j \langle i j | \tilde{v} | i j \rangle$$

$$+ \beta^{-1} \sum_i [f_i \ln f_i + (1 - f_i) \ln (1 - f_i)].$$

(21)

Here the tilde $\tilde{v}$ means that the matrix element $\langle ij | \tilde{v} | ij \rangle$ is antisymmetrized. The functional derivative of $F$ with respect to $\langle i |$ is then

$$\delta F/\delta \langle i | = f_i \left( t + w - \mu' + \sum_j f_j \langle j | \tilde{v} | ij \rangle \right),$$

(22)

where one recognizes the action of a mean field potential, including both direct and exchange terms

$$\mathcal{V} | i \rangle \equiv \sum_j f_j \langle j | \tilde{v} | ij \rangle.$$ (23)

Stationarity of $F$ with respect to $|i\rangle$ then gives the “finite-temperature Hartree-Fock” equations,

$$\langle t + w - \mu' + \eta | i \rangle = \eta | i \rangle, \quad \forall i,$$

(24)

where one recognizes that $\eta_i$ is the Lagrange multiplier for the normalization of the orbital.

In the same way, the derivative of $F$ with respect to $\eta_i$, or as well $f_i$, yields

$$\frac{\partial F}{\partial f_i} = \eta_i + \beta^{-1} \ln \left[ f_i/(1 - f_i) \right],$$

(25)

which vanishes [see eq. (20)]. It can thus be concluded that

$$F = -\beta^{-1} \ln Z_t - \text{Tr} D_t \mathcal{V},$$

(26)

(which differs from $-\beta^{-1} \ln Z_t$) is stationary with respect to variations of $D_t$. Therefore, since $\mathcal{V}$ is proportional to the additional charge $Z$ at the center, the derivative of $F$ with respect to $Z$ must be given by

$$\frac{\partial F}{\partial Z} = 4\pi \int r^2 dr' \left[ \rho_v(r') - \rho_d(r') \right],$$

(28)

which is the differential form of equations (11–12). Here $\rho_v(r')$ and $\rho_d(r')$ are diagonal matrix elements $\langle r'| D_t | r' \rangle$ in the electron and positive background sectors, respectively. It will be noticed that equation (28) gives the background density as well as the electronic density, while the preceding equations, equations (15)–(27), accounted for the electrons only. In view of the simplicity of the result due to the electrons, this reinstatement of the background contribution is trivial. Notice also that for the one-center problem, $D_t$ is rotationally invariant, hence no vector label $r'$ is needed.

The result, equation (28), is simply a reformulation of equations (11)–(12). The method of Matsubara poles used by Watrous et al. (1999) via the finite-temperature, one-body Green’s function, is perfectly suited to this local calculation of the density and avoids an explicit solution of equation (24). Indeed, as discussed in detail by Watrous et al. (1999), a local density such as $\rho_v(r)$ can be directly derived from diagonal matrix elements $\langle r'| (\eta - t - w - \mu' - \mathcal{W})^{-1} | r' \rangle$ of the one-body Green’s function. Such matrix elements are integrated on a suitable contour in the $\eta$-complex plane. Once $\delta F/\delta Z$ is known for all values of $Z$ smaller than $Z_t + Z_s$, trivial integrals provide the screening $U_0$ according to equation (10).

5. NUMERICAL RESULTS FOR THE SOLAR CORE

Shielding calculations have been performed for $Z = 1, 2, 4, 6, 8$ at a density and temperature relevant to energy and neutrino production in the Sun. From these calculations the enhancement factors are calculated and compared with the results of other researchers. Ricci et al. (1995) have shown that enhancement factors for the relevant fusion reactions are insensitive to the location within the solar
core. We use here the set of parameters similar to those employed by Bahcall & Pinsonneault (1995), corresponding to \( R/R_\odot = 0.06 \). In atomic units, they are \( T = 47, n_e = 7.63, X = 0.432, Y = 0.568 \). The results are displayed in Table 1 for \( \phi(Z, r = 0) \) and \( \Delta \rho_e(Z, r = 0) = \rho_e(Z, r = 0) - n_e \). These quantities for other \( Z \)-values can be obtained by interpolation. \( \phi(Z, r = 0) \) was fitted to a fourth-order polynomial,

\[
\phi(Z, r = 0) \approx - \sum_{n=1}^{4} c_n Z^n .
\]

The integral of this quantity then yields the free energy,

\[
F(Z) \approx - \sum_{n=1}^{4} c_n Z^{n+1}/(n+1) ,
\]

with \( c_1 = 2.0275, c_2 = -0.03661, c_3 = 0.00594, c_4 = -0.000103 \). Note that \( \phi(Z, r = 0) \) is nearly linear in \( Z \).

Table 2 gives the fusion-enhancement factors for several reactions of interest in the solar neutrino problem. The deviation from unity is a result of shielding. Note that the various calculations exhibit a scatter of 10%–30% and more in the deviation from unity. Although our factors are rather close to the recent calculations of Gruzinov & Bahcall (1998), they are usually somewhat lower.

### Table 2

| Reaction | This Work | WES | Mit | GDGC | CSK | GB |
|----------|-----------|-----|-----|------|-----|----|
| \( p + p \) | 1.043 | 1.049 | 1.045 | 1.049 | 1.038 | 1.053 |
| \( \text{He} + \text{He} \) | 1.181 | 1.213 | 1.176 | 1.115 | 1.158 | 1.224 |
| \( \text{Be} + p \) | 1.183 | 1.213 | 1.171 | 1.112 | 1.169 | 1.166 |
| \( \text{N} + p \) | 1.356 | 1.402 | 1.293 | 1.191 | 1.324 | 1.393 |

**Note:**—WES is Salpeter’s weak screening approximation (Salpeter 1954); Mit is Mitler’s Thomas-Fermi-like model (Mitler 1977); GDGC is from Graboske et al. 1973; CSK is the dynamic screening model of Carraro et al. 1988; GB is from Gruzinov & Bahcall 1998.

### 6. SUMMARY AND CONCLUSIONS

The finite-temperature Green’s function method of Watrous et al. (1999) has been applied to the problem of screening of the nucleus-nucleus interaction in the solar plasma. The method is based on a self-consistent, finite-temperature Kohn-Sham formalism with the local density approximation for exchange and correlation. Atomic bound states are included on an equal footing with continuum states. Fusion-enhancement factors (over pure Coulomb) are calculated for various relevant nuclear reactions at mean conditions (temperature and density) of the solar core. Comparisons with several other calculations are presented.

The method appears to have no restriction with respect to temperature or density for stars in “noncatastrophic,” thermal equilibrium states. When implementing calculations for other systems, one may need to extend the range of parameters for the local exchange-correlation term, which is quite small for our solar system.

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