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SCREENING IN THERMONUCLEAR REACTION RATES IN THE SUN

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ABSTRACT

We evaluate the effect of electrostatic screening by ions and electrons on low-Z thermonuclear reactions in the Sun. We use a mean field formalism and calculate the electron density of the screening cloud using the appropriate density matrix equation of quantum statistical mechanics. Because of well-understood physical effects that are included for the first time in our treatment, the calculated enhancement of reaction rates does not agree with the frequently used interpolation formulae. Our result does agree, within small uncertainties, with Salpeter's weak screening formula. If weak screening is used instead of the commonly employed screening prescription of Graboske et al., the predicted ^{8}B neutrino flux is increased by 7% and the predicted chlorine rate is increased by 0.4 SNU.

Subject headings: nuclear reactions, nucleosynthesis, abundances — Sun: abundances — Sun: interior

1. INTRODUCTION

In recent years, an increasing amount of attention has been devoted to calculating more accurately the effects on the rates of solar fusion reactions of electrostatic screening in the solar plasma (Carraro, Schäfer, & Koonin 1988; Johnston et al. 1992; Bahcall & Pinsonneault 1992; Shoppa et al. 1993; Dzitko et al. 1995; Ricci, Degl'Innocenti, & Fiorentini 1995; Gruzinov & Bahcall 1997; Brown & Sawyer 1997; Brüggen & Gough 1997). All of these discussions take as their starting point the classical analysis by Salpeter (1954). The primary reason for making more precise calculations is that nuclear fusion reactions produce the solar neutrino fluxes.[1] The neutrino fluxes are being observed with a number of large new detectors that are expected to yield flux measurements of high accuracy (of the order of a few percent or better, see Bahcall et al. 1995, and, for more details, Totsuka 1996; McDonald 1994; Arpesella et al. 1992).

In this paper, we calculate for the first time the electron density in the vicinity of the fusing nuclei using the partial differential equation for the density matrix that is derived in quantum statistical mechanics. In previous treatments of screening that attempted to go beyond the linear regime, the electron density near the nucleus was either taken to be—without quantitative justification—the unperturbed value $n_e(\infty)$ (Mitler 1977; Dzitko et al. 1995) or left as a free parameter (Ricci et al. 1995) or the electrons were assumed to be completely degenerate (Graboske et al. 1973). We calculate screening corrections in a mean field approximation; we numerically solve the nonlinear Poisson-Boltzmann equation for a mixture of electrons and ions. The electron density distribution calculated from the density matrix equation is included self-consistently and iteratively in the mean field equation.

Our results represent both an improvement on and a simplification of the description of nuclear fusion used in many solar evolution codes.

For simple physical reasons, our results differ from the interpolation formulae that are currently used to describe reaction rates in the Sun (Salpeter & Van Horn 1969; Graboske et al. 1973) and the numerical calculations of Dzitko et al. (1995).

Interpolation formulae describe a transition between Salpeter's weak screening, which is due to both electrons and ions, and strong screening, for which only ions are effective. At the high densities relevant for strong screening, electrons are fully degenerate. The solar core, however, is only weakly degenerate, and the effects of degeneracy are already included into the Debye radius R_D (which is increased 2% by electron degeneracy, cf. eq. [4] of the present paper or eq. [25] of Salpeter 1954). Therefore, the interpolation formulae in use underestimate the electron contribution to screening and give reaction rates lower than ours.

The numerical procedures of Dzitko et al. (1995) and Mitler (1977) predict reaction rates that are too slow for heavy ions because they assumed that the electron charge density near a screened nucleus is the unperturbed value, $en_e(\infty)$. This assumption seriously underestimates the charge density near heavy ions. For example, it is known that a screened beryllium nucleus under solar interior conditions has charge density near the nucleus $\approx -3.85en_e(\infty)$ (Gruzinov & Bahcall 1997; Brown & Sawyer 1997; all quantum mechanical calculations give similar results, see Bahcall 1962 and Iben, Kalata, & Schwartz 1967).

This paper is organized as follows. In § 2 we review the basic concepts, and in § 3 we relate the electrostatic energy to the screening enhancement using the free energy. We describe the calculations in § 4 and summarize the numerical results in § 5. In § 6 we summarize our main results and present the conclusions regarding solar neutrino fluxes. The Appendix evaluates a quantum correction to the kinetic energy of thermal electrons in the electrostatic field of a screened nucleus.

2. ENHANCEMENT OF FUSION RATES

The solar core plasma is dense enough that it noticeably enhances fusion rates as compared to the rates in a rarefied plasma of the same temperature. As explained by Salpeter (1954), the rate of a fusion of two nuclei of charges Z_1 and Z_2 is increased by a factor

$$f = \exp \Lambda , \tag{1}$$

where

$$\Lambda = Z_1 Z_2 \frac{e^2}{TR_D} . \tag{2}$$

[1] See http://www.sns.ias.edu/ jnb.

Here R_D is the Debye radius,

$$\frac{1}{R_D^2} = 4\pi\beta n e^2 \zeta^2 , \tag{3}$$

with

$$\zeta = \left[\Sigma_i X_i \frac{Z_i^2}{A_i} + \left(\frac{f'}{f}\right) \Sigma_i X_i \frac{Z_i}{A_i} \right]^{1/2} . \tag{4}$$

Here $\beta = 1/T$; n is the baryon density; X_i, Z_i, and A_i are, respectively, the mass fraction, the nuclear charge, and the atomic weight of ions of type i. The quantity $f'/f \simeq 0.92$ accounts for electron degeneracy. Equation (4) is the same as equation (25) of Salpeter (1954). In what follows, we will make use of a simplified expression for ζ,

$$\zeta_{\rm simple} \cong [(1 - Y/2) f'/f + 1]^{1/2} , \tag{5}$$

in which the plasma is assumed to consist only of hydrogen and helium (Y is the helium abundance by mass). The approximation of considering only a hydrogen and helium plasma rather than the full solar composition (cf. Grevesse & Noels 1993) causes an error of less than 0.5% in computing solar fusion rates. This error is completely unimportant for our purpose of estimating the ratio of the total screening to the weak screening value given by equations (1)–(4).

The enhancement of fusion rates due to screening depends only very weakly upon location in the solar interior (cf. Ricci et al. 1995) because the primary effect of screening is proportional to ρ/T^3 (cf. eqs. [1]–[4]), which is approximately constant in the solar interior (cf. eq. [41] of Bahcall et al. 1982). The plasma parameters at a characteristic radius in the solar interior, $R/R_\odot = 0.06$, are (Bahcall & Pinsonneault 1995) $R_D = 0.46$ and $T = 47$ in atomic units ($m_e = \hbar = e = 1$). In units that are more common in astronomical discussions, the temperature T_6 in millions of degrees is $T_6 = 0.32T = 15$, and the Debye radius in centimeters is $R_D = 0.46 \times 5.3 \times 10^{-9} = 2 \times 10^{-9}$ cm.

Consider an important example: $Z_1 Z_2 = 4$ for the solar fusion reactions ^{3}He(^{4}He, γ)^{7}Be and ^{7}Be(p, γ)^{8}B. Equation (2) yields $\Lambda = 0.19$. According to equation (1), the calculated rates of these fusion reactions are then 21% faster than they would be if screening were neglected.

Equation (1) is only valid to first order in Λ. Nonlinearities in the electrostatic screening interactions might naively be expected to produce corrections $\sim\Lambda^2$, i.e., of order 4% for a $Z_1 Z_2 = 4$ reaction. In the following sections, we calculate corrections to the Salpeter weak screening formula, equation (1), and find that the numerical corrections are always significantly smaller than Λ^2.

3. ENHANCEMENT FACTORS AND FREE ENERGY

Salpeter's formula (eqs. [1], [2]) can be derived as follows. The screened potential near the nucleus Z_1 in the Debye-Hückel approximation is

$$\frac{Z_1}{r} e^{-r/R_D} \approx \frac{Z_1}{r} - \frac{Z_1}{R_D} . \tag{6}$$

The potential shift Z_1/R_D increases the probability that the charge Z_2 comes close to Z_1 by the Boltzmann factor e^Λ, $\Lambda = \beta Z_1 Z_2/R_D$.

Unfortunately, this clear derivation cannot be used if we go beyond the Debye-Hückel approximation and include nonlinear screening effects. Given a numerically calculated potential around the charge Z_1, $\phi_1(r)$, we cannot assume that the enhancement factor is equal to e^Λ with $\Lambda = \beta Z_2 \times [Z_1/r - \phi_1(r)]|_{r=0}$. This is already obvious from the asymmetry of this expression under the 1-2 permutation; ϕ_1 is not just proportional to Z_1 for nonlinear screening.

In the more general case considered here, the enhancement of fusion rates due to screening can be calculated in terms of an expression involving the free energy of a screened charge Z, $F(Z)$. In terms of free energy, the enhancement factor is simply (DeWitt, Graboske, & Cooper 1973) e^Λ with

$$\Lambda = -\beta F(Z_1 + Z_2) + \beta F(Z_1) + \beta F(Z_2) , \tag{7}$$

which is a manifestly symmetrical expression. Equation (7) expresses the thermodynamic relation that at constant temperature (which is relevant when considering solar fusion reactions) $\delta F = -\delta W$, where δW is the work done by the plasma on the fusing ions. The extra work performed by the plasma due to screening is positive, pushing the fusing ions closer together. For a given relative kinetic energy when the ions fuse, the initial kinetic energy is lower by δW than in the absence of screening. Therefore, the probability of the fusing configuration is increased, i.e., the reaction rates are faster, by a factor $\exp(\beta\,\delta W) = \exp(-\beta\,\delta F) = \exp(\Lambda)$.

The free energy can be calculated in terms of electrostatic energy using the thermodynamic formula

$$\beta F = \int_0^\beta d\beta' U . \tag{8}$$

The lower limit in the integral in equation (8) is chosen so that at high temperature (small β) F goes to zero as $\beta^{1/2}$, as implied by Debye theory (see discussion below). The total electrostatic energy including the self-energy is

$$U_{\rm tot} = \tfrac{1}{2} \int d^3 r \phi(r) \rho(r) . \tag{9}$$

The self-energy of the charges cancels out in performing the difference indicated by equation (7). The fusing nuclei are well separated whenever screening is relevant; their combined self-energies are the same in the fusing state as the sum of the self-energies in the initial (infinitely separated) state. Most of the acceleration of the fusing nuclei occurs at distances larger than $0.1R_D$, which is 4 orders of magnitude larger than nuclear radii. Therefore, the relevant self-energy for the calculation of enhancement factors due to screening does not include the self-energies and is

$$U = \frac{Z}{2} \delta\phi(0) + \frac{1}{2} \int d^3 r \phi(r) \delta\rho(r) , \tag{10}$$

where $\delta\phi = \phi - Z/r$ and $\delta\rho = \rho - Z\,\delta(r)$.

In the Debye-Hückel approximation these expressions reproduce Salpeter's formula (Brüggen & Gough 1997). In the Debye-Hückel approximation, $\phi = (Z/r)e^{-r/R_D}$, $4\pi\,\delta\rho = -\phi/R_D^2$, $\delta\phi(0) = -Z/R_D$, and equation (10) gives $U = -\frac{3}{4}Z^2/R_D$. Since $R_D \sim \beta^{-1/2}$, equation (8) gives $\beta F = -\frac{1}{2}\beta Z^2/R_D$. Then equation (7) gives equation (2).

4. CALCULATIONS

In the mean field approximation, electrostatic screening of a charge Z is described by the Poisson-Boltzmann equa-

tion

$$\nabla^2\phi = 4\pi n\left[\left(1-\frac{Y}{2}\right)e^{\beta\phi} - (1-Y)e^{-\beta\phi} - \frac{Y}{2}\,e^{-2\beta\phi}\right], \tag{11}$$

where the terms on the right-hand side represent, respectively, screening by electrons, protons, and alphas. The boundary condition is $\phi \to Z/r$ for $r \to 0$. In the nonlinear regime, one cannot solve the Poisson-Boltzmann equation as written. Classical electrons recombine, which corresponds formally to the divergence of the classical Boltzmann factor $e^{\beta\phi}$ near the nucleus. This problem does not arise in previous solutions of the Poisson-Boltzmann equation, which were carried out in the linear regime corresponding to weak screening.

Quantum statistical mechanics must be used for calculating terms beyond the weak screening approximation. Fortunately, electron degeneracy makes only a small correction, less than 2% in the Debye radius, see equation (4), and therefore less than 1% for all cases in the reaction rates. Hence, a distinguishable particles approximation can be employed.[2] We use a numerical code that solves the density matrix equation for the density of electrons near the nucleus. The code, which was developed following the discussion of Feynman (1990), is described in Gruzinov & Bahcall (1997).

The average electron density can be calculated by solving the density matrix equation (e.g., Feynman 1990)

$$\partial_\beta \rho = [\tfrac{1}{2}\nabla^2 + \phi(r)]\rho\ , \tag{12}$$

with the initial condition

$$\rho(r,\ \beta = 0) = \delta^{(3)}(r)\ . \tag{13}$$

Since equation (12) appropriately describes the quantum statistical mechanical effects, the solution for the density matrix converges everywhere despite the divergence of the classical potential at $r = 0$. Another great advantage of the density matrix formulation is that the character of the states in the plasma does not have to be specified, and therefore difficult questions concerning the existence or nonexistence of bound states are finessed. The enhancement of the electron density to be used in the Poisson-Boltzmann equation instead of the Boltzmann factor $e^{\beta\phi}$ is the solution of equation (12) for the nuclear charge of Z divided by the solution for $Z = 0$. The solution for the $Z = 0$ case can be obtained analytically and is $\rho_0(\beta) = (2\pi\beta)^{-3/2}$.

As described in Gruzinov & Bahcall (1997), the diffusion with multiplication problem, equation (12), can be solved easily by direct three-dimensional numerical simulations for solar conditions because the inverse temperature β is small (~ 0.02) and the diffusive trajectory stays close to the origin. The mesh size and the regularization procedure were the same as in our previous work.

[2] Brown & Sawyer (1997) calculated electron densities using both Fermi-Dirac and Maxwell-Boltzmann statistics. Degeneracy effects on the value of the central electron density were of order 10% for $Z = 6$. We shall show in the course of this paper that changing the central electron density by almost an order of magnitude does not significantly change the rate of nuclear fusion reactions. Therefore, the small fractional change in the central electron density due to using different statistics is not important for our purposes.

Numerically, we start with an initial guess that $\phi(r) = (Z/r)e^{-r/R_D}$ everywhere and then calculate the electron density using equation (12) for all $r < 0.4$. The particular value of $r = 0.4$ ($\sim R_D$) is not important. For all $r \gtrsim 0.2$, our density matrix code simply reproduces the Boltzmann distribution factor $n(r) = n(\infty)e^{\beta\phi}$. We use the calculated electron density at $r < 0.4$ to solve equation (11) numerically for all r. We then obtain a new potential $\phi(r)$. We use this potential to calculate the electron density at $r < 0.4$ using equation (12) and repeat the procedure. The procedure converges quickly, after one to three iterations.

The electrostatic energy was calculated from equation (10). The calculation was repeated at higher temperatures for the purpose of estimating the free energy using equation (8).

Quantum statistical mechanics implies the existence of an effect that we believe has not been previously considered in the context of fusion reaction rates. The kinetic energy of electrons in the electrostatic field of the nucleus is no longer $(3/2)T$ per electron. Indeed, the kinetic energy of electrons is increased. In the low-temperature limit this effect is the familiar zero-point oscillations. In the high-temperature limit the effect is more subtle, but it can be calculated analytically. In the Appendix we calculate the quantum statistical mechanics corrections to the electron kinetic energy and the resulting correction to the free energy.

5. NUMERICAL RESULTS

Table 1 gives the numerical results for: (1) corrections to the Debye-Hückel electrostatic energy, (2) corrections to the free energy due to the changed electrostatic energy, (3) corrections to the kinetic energy of electrons, (4) corrections to the free energy due to the changed kinetic energy of electrons, and (5) the total correction to free energy.

Figure 1 explains the sources of different corrections to the Debye-Hückel approximation of screening.

1. At large distances (small ϕ), the plasma response is suppressed due to helium ions. To see this, expand equation (11) up to the second order in ϕ: $\nabla^2\phi = \phi(1 - w\beta\phi)/R_D^2$, where $w = 3Y/(8 - 2Y)$.

2. At small distances, the plasma response is suppressed due to the fuzziness of quantum electrons, which is expressed by the density matrix equation (12).

3. At intermediate radii, the plasma response can be enhanced just because $e^{\beta\phi} > \beta\phi$.

TABLE 1

ELECTROSTATIC, KINETIC, AND FREE ENERGY CORRECTIONS (%)

	Z					
PARAMETER	1	2	4	5	7	8
$\beta\,\delta U$	0.34	1.6	6.4	9.2	11.2	7.6
$\beta\,\delta F_U$	0.1	0.6	2.7	3.9	5.7	5.2
$\beta\,\delta K$	0.22	0.57	1.9	3.2	8.1	12.6
$\beta\,\delta F_K$	0.1	0.3	0.8	1.3	2.9	4.4
$\beta\,\delta F$	0.2	0.9	3.5	5.2	8.6	9.6

NOTES.—The symbols represent nuclear charge Z corrections to (1) the electrostatic energy normalized to temperature $\beta\,\delta U$, (2) the free energy due to increased electrostatic energy $\beta\,\delta F_U$, (3) the kinetic energy of electrons $\beta\,\delta K$, (4) the free energy due to increased kinetic energy $\beta\,\delta F_K$, and (5) the total free energy $\beta\,\delta F$. The plasma parameters are taken from the solar model of Bahcall & Pinsonneault 1995 at the representative point $R/R_\odot = 0.06$.

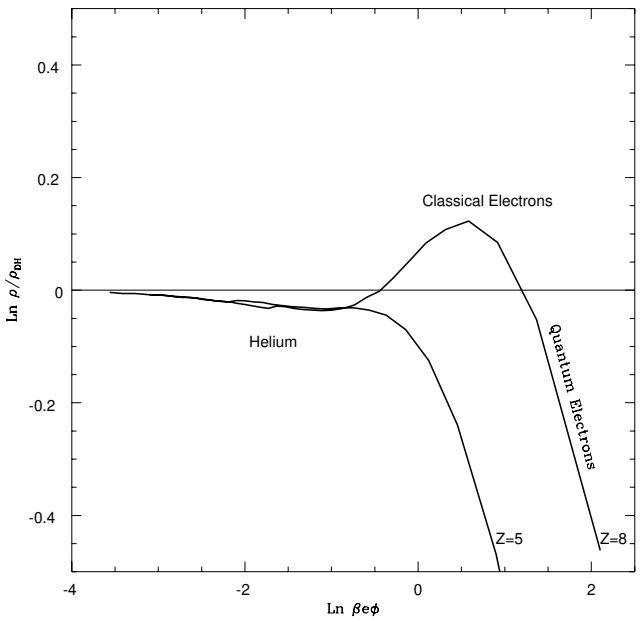

FIG. 1.—Screening of two test charges. The induced charge density ρ normalized to the Debye-Hückel charge density, $\rho_{DH} = \phi/(4\pi R_D^2)$, is shown as a function the electrostatic potential ϕ. For small ϕ (large distances from the screened nucleus), ρ is given by the classical Boltzmann formula (see the right-hand side of eq. [11]). In this region, ρ is smaller than ρ_{DH} due to the presence of helium ions. At large ϕ (close to the screened nucleus), ρ is much smaller than ρ_{DH} due to the quantum fuzziness embodied in the density matrix equation (eq. [12]). At intermediate distances, ρ can be larger than ρ_{DH} (because $\exp \phi > \phi$). For $Z = 8$ the plasma response is larger than linear at intermediate distances. For $Z = 5$ the plasma response is always smaller than linear.

The second column of Table 2 shows the corrections, $-\delta\Lambda$, to reaction rates calculated in this paper (GB) relative to Salpeter's weak screening rates. For example, the correction to the rate of the ^{7}Be(p, γ)^{8}B reaction is $\delta\Lambda = -\beta\,\delta F(5) + \beta\,\delta F(4) + \beta\,\delta F(1) = -5.2\% + 3.5\% + 0.2\% = -1.5\%$. This means that the reaction is only 1.5% slower in the Sun than predicted by the Salpeter formula. Table 2 also compares our corrections with those predicted by Graboske et al. (1973, hereafter GDGC), by Salpeter & Van Horn (1969), and by Dzitko et al. (1995).

Our corrections are typically an order of magnitude smaller than the corrections calculated by GDGC (cf. cols. [2] and [3] of Table 2). The intermediate screening prescription of GDGC (their Table 4, p. 465) uses the intermediate screening formula from DeWitt et al. (1973, p. 455; their eq. [70]); the DeWitt et al. (1973) formula was obtained as an illustration assuming completely degenerate electrons, which is inappropriate for the solar interior. The GDGC intermediate screening prescription underestimates the enhancement of fusion reactions by a factor $\exp(\delta\Lambda_{GDGC} - \delta\Lambda_{GB})$, which varies from about 7% for the important ^{3}He(^{4}He, γ)^{7}Be and ^{7}Be(p, γ)^{8}B reactions to about 16% for the ^{14}N(p, γ)^{15}O reaction (cf. Table 2 of Ricci et al. 1995).

TABLE 2

REACTION RATE CORRECTIONS (%)

Reaction (1)	GB (2)	GDGC (3)	SVH (4)	DTDL (5)
$p + p$	0.5	0.0	0.5	0.2
^{3}He + ^{4}He.....	1.7	8.2	2.4	1.8
$p + {}^7$Be	1.5	8.5	2.6	2.3
$p + {}^{14}$N.....	0.8	15.2	6.3	6.3

NOTES.—Corrections to weakly screened reaction rates. Nuclear fusion reactions in the Sun are enhanced by a factor $\exp(\Lambda + \delta\Lambda)$, where Λ is given by Salpeter's expression, which is eq. (2). The table shows the corrections, $-\delta\Lambda$, calculated in this paper (GB), by Graboske et al. 1973 (GDGC), by Salpeter & Van Horn 1969 (SVH), and by Dzitko et al. 1995 (DTDL). The corrections refer to a representative point $R/R_\odot = 0.06$.

The discrepancies between our results and those of Dzitko et al. (1995) only become large when relatively heavy nuclei are involved. In this case, the electron density in the vicinity of the fusing nuclei is much larger than the value, $n_e(\infty)$, assumed by Dzitko et al. (1995).

For heavier nuclei like nitrogen, the large classical enhancement of electron density near the nucleus competes with the smearing effect due to quantum fuzziness, resulting in a net correction that is smaller than for the lighter nuclei (see Fig. 1).

6. SUMMARY AND CONCLUSION

We use the density matrix equation to determine from quantum statistical mechanics the electron density in the near vicinity of the fusing nuclei. Our treatment is the first to describe properly the electron density in screening calculations that are appropriate for solar interior conditions. Previously, the lack of understanding of what to use for the electron density near the fusing nuclei has been the principal cause for uncertainty in estimating nonlinear corrections to screening calculations (see, e.g., Ricci et al. 1995 and references therein).

The nonlinear corrections that we calculate to the Salpeter weak screening formulae, equations (1)–(4), are, for solar conditions, $\sim$1% for all the important nuclear fusion reactions. The principal uncertainty in our calculations is caused by thermal fluctuations, which are not included in the present treatment. For the analogous case of electron capture, thermal fluctuations affect the average rate by $\leq$1% (Gruzinov & Bahcall 1997). Since the nonlinear effects calculated in the present paper are small and of the same order as the effects of fluctuations that occur in the electron capture problem, we recommend using the Salpeter weak screening formula for solar fusion rates.

What difference do the present results make for the solar neutrino problem? This question is answered by Table 3 of Bahcall & Pinsonneault (1992). Keeping all other input data constant, the weak screening approximation gives, relative to the Graboske et al. (1973) prescription, a 0.4 SNU larger result in the chlorine (Homestake) experiment, a 2 SNU increase in the gallium experiments, and a 7% larger ^{8}B neutrino flux (measured in the Super Kamiokande, Kamiokande, and Sudbury Neutrino Observatory experiments). The Graboske et al. (1973) prescription was used previously by Bahcall and Pinsonneault and in many other stellar evolution codes (cf. Ricci et al. 1995).

An error in the screening enhancement is equivalent to an error in the low-energy cross section factor. Therefore, one can use the well-known power-law dependences of the neutrino fluxes on cross section factors (Bahcall 1989) to estimate the uncertainties introduced by inaccuracies in the screening calculations. A 1% uncertainty in the screening calculation causes a $\sim$1% uncertainty in the predicted ^{8}B

neutrino flux and a smaller uncertainty for other fluxes in the pp chain. For the crucial ^{8}B neutrino flux, the uncertainty in the measurement of the low-energy cross section factor for the ^{7}Be$(p, \gamma)^8$B reaction causes a much larger uncertainty, more than 10% (see Bahcall & Pinsonneault 1995).

The nonlinear effects in ion and electron screening that are evaluated in this paper cause differences in the solar model neutrino fluxes that are small compared to the order-of-unity differences between the rates measured in solar neutrino experiments and the fluxes predicted by standard models (assuming nothing happens to the neutrinos after they are created).

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APPENDIX

QUANTUM CORRECTIONS TO THE (3/2)T KINETIC ENERGY PER PARTICLE RULE

In classical statistical mechanics, the kinetic energy of particles, interacting or noninteracting, in an external potential or in free space, is (3/2)T per particle. In quantum statistical mechanics, the kinetic energy at a given temperature depends on the external potential. This is obvious in the low-temperature limit: the kinetic energy of the ground state is positive if the external potential is not constant (the zero-point oscillations).

Thermal electrons in an electrostatic field of a nucleus have kinetic energy larger than (3/2)T. The effect depends on Z and reduces the reaction rates (as compared to Salpeter's weak screening rates). The correction to kinetic energy can be calculated if the diagonal of the density matrix (e.g., Feynman 1990) $\rho(r, \beta) \equiv \rho(r, r, \beta)$ is known,

$$\delta K = n_e (2\pi\beta)^{3/2} \int d^3 r [-\partial_\beta \rho - (\tfrac{3}{2}\beta^{-1} + V)\rho] , \tag{A1}$$

that is, the correction to the kinetic energy is the total energy minus the unperturbed kinetic energy (3/2)T minus the potential energy V. In classical statistical mechanics

$$\rho = (2\pi\beta)^{-3/2} e^{-\beta V} , \tag{A2}$$

and equation (A1) gives $\delta K = 0$.

We calculated the density matrix of electrons analytically and used equation (A1) to calculate the kinetic energy correction for $V = -(Z/r)e^{-r/R_D}$ assuming $\beta \ll 1$, $Z \sim$ few, $R_D > \beta^{1/2}$. These conditions are satisfied in the solar interior where $\beta \approx 0.02$ and $R_D \approx 0.5$. Two different approaches were used at distances from the nucleus greater than the de Broglie wavelength $\beta^{1/2}$ and at distances smaller than the Debye radius R_D. These two approaches are explained below.

A1. $r \gg \beta^{1/2}$: HIGH-TEMPERATURE EXPANSION

Thermal electrons have "a characteristic size" $\sim\beta^{1/2}$. If the potential energy does not change by much over this distance (which in our case is true for $r > \beta^{1/2}$), the density matrix is approximately given by equation (A2) with small corrections. The corrections are due to the fact that a fuzzy thermal electron samples potential not only at a given point but in the $\beta^{1/2}$ vicinity of the given point.

Let (x, y, z) be a small deviation of coordinates from $(r, 0, 0)$. Potential energy is, up to the second order,

$$\delta V = V' x + \frac{1}{2} V'' x^2 + \frac{1}{2}\frac{V'}{r} y^2 + \frac{1}{2}\frac{V'}{r} z^2 , \tag{A3}$$

where primes denote the r derivatives, and we assume that V is spherically symmetrical. The path integral giving the density matrix (e.g., Feynman 1990, Chap. 3) is Gaussian and can be calculated. In fact, the answer can be constructed without the actual calculation from the known density matrix of the linear harmonic oscillator (e.g., Feynman 1990, Chap. 2). It reads

$$\rho = (2\pi\beta)^{-3/2} e^{-\beta V}\left[1 + \frac{1}{24}\beta^3 V'^2 - \frac{1}{12}\beta^2\left(V'' + \frac{2}{r}V'\right)\right] . \tag{A4}$$

The kinetic energy correction is given by equation (A1)

$$\delta K = n_e \int 4\pi r^2 dr e^{-\beta V}\left[-\frac{1}{8}\beta^2 V'^2 + \frac{1}{6}\beta\left(V'' + \frac{2}{r}V'\right)\right] . \tag{A5}$$

In our case equation (A4) is valid only at $r \gtrsim \beta^{1/2}$, but if potential energy V were smooth at all r, we could have integrated the last term by parts

$$\delta K = \tfrac{1}{24} n_e \beta^2 \int 4\pi r^2 dr e^{-\beta V} V'^2 , \tag{A6}$$

showing that kinetic energy correction is positive in the high-temperature limit. In our calculation we used equation (A4) at $r > r_0$, and results from the next section were used at $r < r_0$. The final answer does not depend on the choice of r_0 as long as $R_D \gtrsim r_0 \gtrsim \beta^{1/2}$.

A2. $r \ll R_D$: HYDROGENIC DENSITY MATRIX

At distances from the screened nucleus $r \ll R_D$, the potential energy is

$$V = -\frac{Z}{r}\exp\left(-\frac{r}{R_D}\right) \approx -\frac{Z}{r} + \frac{Z}{R_D}\,. \tag{A7}$$

The only effect of the constant correction Z/R_D is to lower electron density by the Boltzmann factor $e^{-\beta Z/R_D}$. The density matrix in the Coulomb potential can be obtained from hydrogenic eigenstates.

The kinetic energy correction is

$$\delta K = n_e e^{-\beta Z/R_D}(2\pi\beta)^{3/2}\int d^3r[-\partial_\beta \rho - (\tfrac{3}{2}\beta^{-1} + V)\rho]\,. \tag{A8}$$

The diagonal of the density matrix is

$$\rho(r, \beta) = \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\left[\sum_{n=1}^{\infty}|R_{nl}(r)|^2 e^{\beta/2n^2} + \int_0^\infty \frac{dk}{2\pi}|R_{kl}(r)|^2 e^{-\beta k^2/2}\right]. \tag{A9}$$

Here the bound states of hydrogen are (e.g., Landau & Lifshitz 1977)

$$R_{nl}(r) = \frac{2}{n^{l+2}(2l+1)!}\left[\frac{(n+l)!}{(n-l-1)!}\right]^{1/2}(2r)^l e^{-r/n}F\left(-n+l+1, 2l+2, \frac{2r}{n}\right), \tag{A10}$$

where F is the confluent hypergeometric function. The continuum states are

$$R_{kl}(r) = 2ke^{\pi/2k}\left|\Gamma\left(l+1-\frac{i}{k}\right)\right|(2kr)^l e^{-ikr}F\left(\frac{i}{k}+l+1, 2l+2, 2ikr\right), \tag{A11}$$

and for $Z \neq 1$ we scale $r \to Zr$, $\beta \to Z^2\beta$.

We used these formulae to calculate the kinetic energy shift at small r. Results of this subsection match the high-temperature results if $\beta^{1/2} < r < R_D$. We repeated the calculation at smaller β to obtain the free energy shift due to the quantum correction to kinetic energy of electrons,

$$\beta\,\delta F = \int_0^\beta d\beta'\,\delta K(\beta')\,. \tag{A12}$$

Results are shown in Table 1.

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