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THE ^{7}Be ELECTRON CAPTURE RATE IN THE SUN

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ABSTRACT

For solar conditions, we numerically integrate the density matrix equation for a thermal electron in the field of a ^{7}Be ion and other plasma ions and smeared-out electrons. With this technique, we can calculate the capture rate without either assuming the existence of bound states or requiring fluctuations to be spherical. Our results are in agreement with previous calculations that are based on a different physical picture, a picture that postulates the existence of distinct continuum and bound-state orbits for electrons. The density matrix calculation of the electron capture rate is independent of the nature of electron states in the solar plasma. To within 1% accuracy, the effects of screening can be described at high temperatures by a Salpeter-like factor of exp $(-Ze^2/kTR_D)$, which can be derived from the density matrix equation. We show that nonspherical fluctuations change the reaction rate by less than 1%. The total theoretical uncertainty in the electron capture rate is about $\pm 2\%$.

Subject heading: nuclear reactions, nucleosynthesis, abundances

1. INTRODUCTION

Observations of solar neutrinos by four different experiments (Davis 1994; Hirata et al. 1991; Anselmann et al. 1995; Abdurashitov et al. 1994) have revealed important information about the interior of the Sun and also about neutrino properties (Bahcall 1996). Further experiments are under way to study in more detail the rare high-energy neutrinos from ^{8}B beta decay (Takita 1993; McDonald 1994; Icarus Collaboration 1995) and the lower energy neutrinos from the relatively common ^{7}Be electron capture in the Sun (Arpesella et al. 1992). The solar rate of electron capture on the ambient ^{7}Be ions is almost 1000 times faster than the rate of proton capture (which produces ^{8}B neutrinos). Therefore, the predicted flux of ^{8}B neutrinos studied in the Kamiokande, Superkamiokande, SNO, and ICARUS experiments is inversely proportional to the electron capture rate on ^{7}Be.

Over the past 35 years, a number of different studies have been undertaken (Bahcall 1962; Iben, Kalata, & Schwartz 1967; Bahcall & Moeller 1969; Watson & Salpeter 1973; Johnson et al. 1992) to calculate accurately the rate at which ^{7}Be ions in the solar plasma capture electrons from continuum and bound states. Successive improvements have been introduced into the calculations, but in all cases the changes have been rather small.

All previous calculations have been based upon a simplified model of the solar plasma in which the different quantum configurations were idealized into separate bound and continuum states. Bound electron captures were imagined to occur from isolated atoms in which the plasma was represented by a mean field (Iben et al. 1967).

We perform here the first calculations that do not assume the existence of bound states with Saha probabilities in the solar plasma and that allow for nonspherical fluctuations. We evaluate directly the total electron capture rate on ^{7}Be ions by integrating numerically the density matrix equation for a thermal electron in the field of a ^{7}Be nucleus in a plasma environment. We use Monte Carlo simulations to represent the relatively large fluctuations that result from the small number of ions within a Debye sphere. Our technique avoids the necessity for defining separate bound states within the solar plasma and allows us to take into account the departures from spherical symmetry that result from the fluctuations in the number of ions near the ^{7}Be nucleus. We thus finesse complicated questions concerning the properties and meaning of electron "bound states" in a dense plasma in which electrons have appreciable probabilities to be at different ion sites (see the discussion of the Stark effect in § 3 of the paper). Our most surprising result is that nonspherical fluctuations affect the capture rate by less than 1%, even though, as Watson & Salpeter (1973) first stressed, the average number of ions in the Debye sphere is small.

In § 2 we summarize previous results obtained with the mean field approximation. We then give in § 3 an approximate analytic calculation that suggests that the effects of fluctuating electric fields caused by ions near the ^{7}Be nucleus might change significantly the capture rate for bound electrons. We summarize the density matrix formulation in § 4 and present the results of our Monte Carlo simulations in § 5. We show that the density matrix formulation leads naturally to a description of the plasma corrections to the electron capture reaction rate by a Salpeter-like formula. We provide in § 6 a heuristic argument showing why, as found in numerical simulations, the effects of fluctuations on a total electron capture rate are small. We summarize our results in § 7.

2. MEAN FIELD SCREENING

The rate of electron capture is proportional to the density of electrons at the ^{7}Be nucleus. In the solar plasma, there are continuum (positive energy) and bound (negative energy) electrons. If the plasma density is sufficiently low, the density of continuum electrons at the nucleus is greater than the mean plasma density by a well-known Coulomb correction factor (Bahcall 1962)

$$w_c = \langle |\psi_k(0)|^2 \rangle = \left\langle \frac{2\pi/k}{1 - e^{-2\pi/k}} \right\rangle . \quad (1)$$

For the nonrelativistic solar plasma, $k = v/Z$ is the wavenumber, and the angular brackets indicate the average over thermal distribution of electron velocities v. Atomic units ($\hbar = e = m_e = 1$) are used here and throughout the paper. The ^{7}Be electron capture is maximal at $R/R_\odot = 0.06$

(Bahcall 1989), where the inverse temperature is $\beta = 0.0215$ (Bahcall & Pinsonneault 1995). For this typical solar environment, the density enhancement at the nucleus because of electrons in continuum states is $w_c = 3.18$.

2.1. *Bound States plus Continuum States*

Iben et al. (1967) pointed out that under solar conditions bound electrons give a substantial contribution to the density at the nucleus. The bound-state enhancement factor is given by

$$w_b = \pi^{1/2}(2\beta Z^2)^{3/2} \sum n^{-3} \exp(\beta Z^2/2n^2) , \quad (2)$$

and equals $w_b = 1.20 + 0.21 = 1.41$, where $w_{b1} = 1.20$ is the ground-state contribution. The total density enhancement factor is 4.59.

Iben et al. (1967) realized that Debye-Hückel screening would reduce electron densities at the nucleus for bound electrons and evaluated this reduction for isolated atoms. We first present the results of the Iben et al. model.

Table 1 gives the calculated ground-state ionization potentials, χ, and the probability densities, ψ^2, at the nucleus for a screened Coulomb potential with Z taking on values 1–6 and Debye radius $R_D = 0.45$, which is the solar value at $R/R_\odot = 0.06$. For $Z = 1$, Debye-Hückel screening destroys all the bound states. Following Iben et al., we define the rate reduction factors, F_{IKS}, by which the bound-state capture rate is reduced because of screening,

$$F_{IKS} = \psi^2 e^{\beta\chi}/\psi_0^2 e^{\beta\chi_0} , \quad (3)$$

where the subscript zero indicates unscreened values. Thus, we see from Table 1 that bound-state screening reduces the total capture rate by a factor of

$$R = (w_c + F_{IKS} w_{b1})/(w_c + w_b) = 0.85 , \quad (4)$$

or by 15%. Screening effects on continuum electrons were studied by Bahcall & Moeller (1969), who integrated the Schrödinger equation numerically for continuum electrons. For ^7Be under solar conditions, screening corrections are small but larger than our calculational accuracy. Let the screening corrections for continuum electrons be represented by

$$F_{BM} = \langle\psi^2\rangle/\langle\psi_0^2\rangle . \quad (5)$$

Table 1 gives values of F_{IKS} and F_{BM} for different nuclear charges Z; solar values at $R/R_\odot = 0.06$ were used for β and R_D.

TABLE 1

MEAN FIELD THEORIES

	Z					
PARAMETER	1	2	3	4	5	6
χ/χ_0	...	0.0034	0.12	0.25	0.35	0.43
ψ^2/ψ_0^2	...	0.098	0.52	0.70	0.80	0.85
F_{IKS}	0.0	0.09	0.48	0.62	0.67	0.68
F_{BM}	0.965	0.985	0.98	0.978	0.979	0.991
w_{IKSBM}	1.38	1.94	2.73	3.85	5.50	7.91
w_S	1.38	1.92	2.70	3.81	5.41	7.73

NOTE.—The symbols represent nuclear charge (Z), screened ground-state ionization potential (χ), electron density (ψ^2), bound-state reduction factor (F_{IKS}), continuum reduction factor (F_{BM}), and density enhancement (w). Results are given for an inverse temperature $\beta = 0.0215$ and a Debye radius $R_D = 0.45$.

The total electron capture rate should be calculated using a density enhancement factor

$$w_{IKSBM} = F_{BM} w_c + F_{IKS} w_{b1} , \quad (6)$$

where we make the excellent approximation that screened excited bound states give a negligible contribution. For $Z = 4$, equation (6) gives $w = 0.978 \times 3.18 + 0.62 \times 1.20 = 3.85$, which is 16% smaller than the unscreened value of 4.59.

2.2. *Salpeter Formula*

The numerical results summarized by equation (6) are well approximated by a simple analytical expression analogous to the formula derived by Salpeter (1954) for weak screening of thermonuclear reactions. The derivation is simple. Consider a screened potential in the vicinity of the origin, $r = 0$. The first-order expansion of the potential gives

$$\phi = \frac{Z}{r} e^{-r/R_D} \approx \frac{Z}{r} - \frac{Z}{R_D} . \quad (7)$$

Thus the potential near the nucleus is a Coulomb potential plus an approximately constant correction. In statistical equilibrium, the constant change in the potential reduces the electron density at the nucleus by a Boltzmann factor, $F_S = \exp(-\beta Z/R_D)$, and the density enhancement factor is given by

$$w_S = F_S(w_c + w_b) . \quad (8)$$

Table 1 compares, in the last two rows, our numerical values obtained from the detailed quantum-mechanical calculations summarized by equation (6), and the simple Salpeter-like formula, equation (8). The agreement between the two results is about 1% for $Z < 6$.

3. FLUCTUATIONS AND THE NAIVE STARK EFFECT

The density enhancement obtained previously by solving the Schrödinger equation (eq. [6]), or by the statistical equilibrium argument (eq. [8]), is based on a model that represents the solar plasma by a screened nucleus and a sea of noninteracting electrons. At $R/R_\odot = 0.06$, the effective plasma density is $n = (8\pi\beta R_D^2)^{-1} = 9.1$, and there are, on average, only 3.5 ions in a Debye sphere (we use a hydrogen plasma model). Watson & Salpeter (1973) suggested that the small number of ions in the Debye sphere implies that thermal fluctuations in the screening might be of importance. They calculated corrections because of a fluctuating number of ions close to the nucleus. Spherical symmetry was assumed in their calculations; that is, plasma ions were represented by spherical shells centered at the nucleus. Watson & Salpeter found a 7% decrease in the bound-state capture rate, which implies a 2% decrease in a total capture rate.

It is plausible that asymmetric fluctuations might have an even stronger effect on the bound-state capture rate. We give a crude argument that shows that the effects of fluctuations must be evaluated carefully. In the first approximation, asymmetry implies that an ion (e.g., a ^7Be nucleus) experiences an electric field, $\mathscr{E}$, produced by the other plasma ions and smeared-out plasma electrons. The electric field changes the ground-state energy $-\chi$ (the Stark effect) and the probability density at the nucleus, ψ^2. The first effect increases the capture rate, since the ionization potential increases. In the second-order perturbation theory (e.g., Landau & Lifshitz 1977)

$$\chi = \frac{Z^2}{2} + \frac{9\mathscr{E}^2}{4Z^4} . \quad (9)$$

On the other hand, the value of the wave function at the nucleus decreases,

$$\psi = 2 - \frac{81\mathscr{E}^2}{8Z^6} , \quad (10)$$

which reduces the capture rate. The two effects together alter the ground-state electron density by a factor, $F_{\mathscr{E}}$, where

$$F_{\mathscr{E}} = \frac{\psi^2}{4} e^{\beta\delta\chi} \approx 1 - \left(\frac{81}{8} - \frac{9\beta Z^2}{4}\right)\frac{\mathscr{E}^2}{Z^6} \approx 1 - 0.0023\mathscr{E}^2 , \quad (11)$$

for $Z = 4$ and $\beta = 0.0215$. Thus, the fluctuating electric field suppresses the bound-state capture rate.

To estimate quantitatively the reduction factor resulting from the Stark effect, we need to know the size of the fluctuating field, $\mathscr{E}^2$. For an illustrative model calculation, one can use the well-known Holtsmark probability distribution for the electric field. This distribution is exact for unscreened noninteracting ions (low densities). The Holtsmark probability distribution is

$$P_{\rm H}(x) = \frac{2x}{\pi} \int_0^\infty dy \sin(xy) y \exp(-y^{3/2}) . \quad (12)$$

Here x is the normalized electric field, $x = \mathscr{E}/\mathscr{E}_{\rm H}$, and the characteristic electric field is

$$\mathscr{E}_{\rm H} = 2.6 n^{2/3} \approx 11 . \quad (13)$$

We do not consider very large electric fields, $x \gg 1$, since in this domain the assumption of noninteracting ions is obviously incorrect. We therefore take $P(x) = 0$ for large x where the factor (eq. [11]) becomes negative. We find, upon averaging equation (11), $F = 0.21$, a strong effect.

Both the second-order perturbation theory and the Holtsmark distribution were used in the calculation outside of their domains of applicability. Also, the effects of the fluctuating fields on the continuum capture rate were not considered. We do see from these simplified arguments that fluctuation effects on the electron capture rate have to be carefully investigated.

4. DENSITY MATRIX FORMULATION

To compute the mean density of electrons at a nucleus, one could solve the Schrödinger equation many times for a large, representative set of distributions of ions and smeared electrons. Given the numerical results for a set of configurations, the density at the nucleus would be computed as the average of the individual densities over the Boltzmann weighted-ion configurations. This is a difficult but, fortunately, unnecessary task. We do not even have to know all the quantum states for a given ion configuration, which is a hard problem by itself.

For a given ion configuration, we are interested in just one quantity: the density of thermal electrons at the nucleus. The average density can be calculated by solving the density matrix equation (e.g., Feynman 1990, chap. 2)

$$\partial_\tau \rho = \left[\frac{1}{2}\nabla^2 + \frac{Z}{r} e^{-r/R_{\rm D}} + V(r)\right]\rho , \quad (14)$$

$$\rho(r, \tau = 0) = \delta^{(3)}(r) . \quad (15)$$

Here V is the fluctuating potential created by neighboring ions and smeared electrons. In the density matrix formulation, bound and continuum electrons are treated equally. One solves equation (14) for a number of different realizations of V and computes the average $\langle \rho_Z(r = 0, \tau = \beta)\rangle$. The density enhancement factor, w, is then given by the ratio

$$w = \frac{\langle \rho_Z(0, \beta)\rangle}{\rho_0(\beta)} , \quad (16)$$

where $\rho_0(\beta)$ is the normalization factor computed by averaging the solution of equation (14) with $Z = 0$ [for $V = 0$, one finds $\rho_0(\beta) = (2\pi\beta)^{-3/2}$].

Equation (14) makes it clear why the effects of screening should be accurately described by a Salpeter-like factor $\exp(-\beta Z/R_{\rm D})$ if the temperature is high enough and the effects of the fluctuating potential are unimportant. At small β, the diffusing particle described by equation (14) stays close to the origin. At small distances, the expansion of the screened potential, equation (7), is valid. According to equation (14), a constant potential U causes the density to be multiplied by a factor $\exp(U\tau)$.

The diffusion with multiplication problem, equation (14), 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. We simulated equation (14) using a 30^3 mesh in a cube with a side 0.6. This gives a spatial resolution $\Delta = 0.02$, which should suffice because the Bohr radius for $Z = 4$ is 0.25. The Coulomb potential was regularized by the prescription

$$1/r \rightarrow (r^2 + \Delta^2/7.7)^{-1/2} \quad (17)$$

in all of our calculations.

To test our code we calculated the mean field theoretical results of § 2 using our solutions of the density matrix equation. In the absence of the fluctuation potential, the denominator in equation (16) is $(2\pi\beta)^{-3/2}$. We used the code to compute the numerator of equation (16) for $R_{\rm D} = \infty$, and for $R_{\rm D} = 0.45$, for Z from 1 to 6. In all cases, our code reproduced the mean field results with an accuracy better than 1%; expression (6) was used to determine a theoretical mean field value in the screened case.

5. MONTE CARLO SIMULATIONS OF FLUCTUATING FIELDS

We studied by Monte Carlo techniques the effects of fluctuations, V, on the density enhancement factor, w, for $Z = 4$, $\beta = 0.0215$, and the ion density $n = 9.1$. Since the probability functional for the field V is unknown, we simulated two extreme cases: randomly distributed ions (case 1) and Boltzmann distributed ions (case 2).

For case 1, screened ions with mean density 9.1 were randomly distributed within a cube of unit length around the ^{7}Be nucleus of charge $Z = 4$. For case 2, both the surrounding ions and the central nucleus were screened only by electrons ($R_{\rm D} \rightarrow R'_{\rm D} = 2^{1/2} R_{\rm D}$) but the ion configurations were weighted by $e^{-\beta U}$, where

$$U = Z \sum \frac{1}{r_j} \exp\left(-\frac{r_j}{R'_D}\right) + \sum \frac{1}{r_{jk}} \exp\left(-\frac{r_{jk}}{R'_D}\right) . \quad (18)$$

Here r_j are positions of ions, which were assumed to be confined to a sphere of radius $R = 1$ around the nucleus; r_{jk} are the inter-ion distances. The Boltzmann weights take account of the ion part of the screening. In fact, plasma ions that are at distances greater than R also contribute to the screening of the nucleus. Their contribution to the potential at the nucleus is

$$\delta\phi = \frac{Z}{2R_D} e^{-R/R_D} . \quad (19)$$

We take this additional potential into account by subtracting a small Salpeter-like correction, $\delta w = w\beta\,\delta\phi = 0.04$, from the density enhancement given by equation (16).

The probability distribution for potentials is different in the two models. In case 1, the nucleus can experience arbitrarily high electric fields, while in case 2, the stronger fields do not contribute because they have smaller Boltzmann weights.

Numerical results are shown in Table 2 for different values, N_{MC}, of Monte Carlo realizations of ion configurations. The percent deviations shown are fractional differences with respect to the mean field theoretical result of 3.85. As can be seen from Table 2, the average effects are smaller than 1%. We repeated the calculation for different parameters (solar center and the outer edge of the reaction, $R/R_{\odot} = 0.15$) and got similar results; fluctuation effects change the reaction rate by less than 1%.

6. HEURISTIC ESTIMATE OF FLUCTUATION EFFECTS

Our numerical simulations show that fluctuations have little effect on the electron capture rate. However, the second-order perturbative calculations in § 3 predict a strong effect for the bound-state captures. Moreover, Watson & Salpeter (1973) suggested that the effects of fluctuations might be significant if the average number of ions in the Debye sphere, N, is small. In the solar case, N is of the order of a few, and strong effects might be expected.

How can we understand the fact that the total capture rate is insensitive to fluctuating electric microfields? In the density matrix formulation (§ 4), electric microfields $\mathscr{E}$ are described by the fluctuating potential $V = \mathscr{E}x$ in equation (14). As a result, both the unnormalized density at the nucleus ρ_Z, and the density normalization ρ_0 are shifted by the fluctuating field. The Coulomb attraction keeps the diffusing thermal electron (as described by the density matrix equation, eq. [14]) in the vicinity of the nucleus, and we may suppose that the shift in ρ_Z is smaller than the shift in ρ_0. The density matrix equation for ρ_0 is simple, and one can calculate the shift in ρ_0 using the perturbation expansion of the density matrix (e.g., Feynman 1990). In second-order perturbation theory, we find

$$\frac{\delta\rho_0}{\rho_0} = \frac{\beta^3 \mathscr{E}^2}{24} . \quad (20)$$

For the characteristic microfield ($\mathscr{E} \sim \mathscr{E}_H \approx 11$) and the inverse temperature ($\beta = 0.0215$), equation (20) gives $\delta\rho_0/\rho_0 = 5 \times 10^{-5}$, which is indeed a small effect.

Taking the estimate (20) as an upper bound for the fluctuation effects, and substituting the Holtsmark field, equation (13), for $\mathscr{E}$, one has (restoring dimensions)

$$\frac{\delta w}{w} < C \frac{a_0}{R_D} N^{-5/3} . \quad (21)$$

Here C is a dimensionless number and a_0 is the Bohr radius. Since, $a_0 \sim R_D$, equation (21) should give large effects when N is sufficiently small. The reason for the calculated small effect of fluctuations is the size of the dimensionless number C, which is

$$C = \frac{(2.6)^2}{24} \left(\frac{3}{4\pi}\right) 6^{-3} = 2 \times 10^{-4} . \quad (22)$$

7. SUMMARY AND DISCUSSION

The rate of electron capture by ^{7}Be ions in the solar plasma has traditionally been computed as the sum of two different processes: capture from continuum orbits plus capture from bound orbits. But the high density of electrons

TABLE 2
MONTE CARLO RESULTS

PARAMETER	N_{MC}: 1	2	5	10	20	50	100
Case 1							
ρ_Z	4.84	4.91	4.93	4.90	4.99	4.84	4.73
ρ_0	1.26	1.27	1.28	1.27	1.29	1.26	1.23
w	3.84	3.87	3.85	3.86	3.87	3.84	3.85
Percent derivation......	−0.3	+0.5	0.0	+0.3	+0.5	−0.3	0.0
Case 2							
ρ_Z	5.40	5.46	5.43	5.52	5.60	5.57	5.53
ρ_0	1.37	1.40	1.39	1.40	1.44	1.42	1.41
w	3.90	3.86	3.87	3.90	3.85	3.88	3.88
Percent derivation......	+1.3	+0.3	+0.5	+1.3	0.0	+0.8	+0.8

NOTE.—The number of Monte Carlo realizations, N_{MC}, for case 1 is given in the headings for the last seven columns. For case 2, the number of realizations is $10 \times N_{MC}$. The table also lists the average density, ρ_Z, the normalization, ρ_0, and the density enhancement, w. The last row for each case is the percent deviation from the mean field result of 3.85.

and ions in the solar interior makes this separation of quantum states a delicate issue; bound states are continually being formed and dissolved as the result of plasma interactions. We illustrate one aspect of this complexity in § 3, where we discuss the Stark effect caused by the fluctuating electric microfield.

In this paper, we have calculated the total rate of electron capture by ^{7}Be using the density matrix formalism (see eq. [14] and Feynman 1990) without reference to the individual (bound or continuum) quantum states. Our numerical code successfully reproduced the results of the previously used mean field theory to an accuracy of better than 1% (§ 4 and the last two rows of Table 1).

One of the most troublesome aspects of the previous mean field calculation is the possible effect of fluctuations caused by the small number (about three) of ions in a Debye sphere surrounding a ^{7}Be ion. The density matrix formulation permits us to evaluate (in § 5) the effects of fluctuations assuming different (extreme) models for the spatial distribution of the ions. In both cases, the effect of fluctuations in the distribution of ions is less than 1% (see Table 2).

The overall result of our calculations is to confirm to high accuracy the standard calculations for the ^{7}Be electron capture rate in the Sun (see, e.g., Iben et al. 1967; Bahcall & Moeller 1969; Bahcall 1989). The results of numerical simulations (see Table 2) show that the standard formula (Bahcall 1989) is accurate to better than 1%. We obtained similar results for $R/R_\odot = 0.0, 0.06$, and 0.15.

How accurate is the present theoretical capture rate, R? The excellent agreement between the numerical results obtained using different physical pictures (a specific model for bound and continuum states and the density matrix formulation) suggests that the theoretical capture rate is relatively accurate. The largest recognized uncertainty arises from the possible inadequacies of the Debye screening theory. Johnson et al. (1992) have performed a careful self-consistent quantum mechanical calculation of the possible effects on the ^{7}Be electron capture rate of departures from the Debye screening. They conclude that Debye screening describes the electron capture rates to within 2%. Combining the results of Table 2 and of Johnson et al. (1992), we conclude that the total fractional uncertainty $\delta R/R$ is small, and that

$$\delta R/R < 0.02 \,. \tag{23}$$

Simple physical arguments suggest that the effects of electron screening on the total capture rate can be expressed by a Salpeter factor (see discussion in the text following eq. [7] and eq. [16]). The simplicity of these physical arguments provides supporting evidence that the calculated electron capture rate is robust.

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