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 $^7Be$ ion and other plasma ions and smeared-out electrons. Our results are in agreement with previous calculations that are based on a different physical picture, a picture which 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 a 1% accuracy, the effects of screening can be described at high temperatures by a Salpeter-like factor of $\exp(-Z e^2/kT R_D)$, which can be derived from the density matrix equation. The total theoretical uncertainty in the electron capture rate is about ±2%.

Subject headings: nuclear reactions
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 underway to study in more detail the rare high-energy neutrinos from $^8\text{B}$ beta-decay (Takita 1993; McDonald 1994; Icarus Collaboration 1995) and the lower energy neutrinos from the relatively common $^7\text{Be}$ electron capture in the sun (Arpesella 1992). The solar rate of electron capture on the ambient $^7\text{Be}$ ions is almost a thousand times faster than the rate of proton-capture (which produces $^8\text{B}$ neutrinos). Therefore, the predicted flux of $^8\text{B}$ neutrinos that is studied in the Kamiokande, Superkamiokande, SNO, and ICARUS experiments is inversely proportional to the electron capture rate on $^7\text{Be}$.

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, Kolbe, Koonin, & Langanke 1992) to calculate accurately the rate at which $^7\text{Be}$ 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).

In the present treatment, we evaluate directly the total electron capture rate on $^7\text{Be}$ ions by integrating numerically the density matrix equation for a thermal electron in the field of a $^7\text{Be}$ nucleus in 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 account of 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 (cf. discussion of the Stark effect in §3 of the paper)

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 provide in §6 a heuristic argument 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 $^7Be$ 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)

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

For the non-relativistic solar plasma, $k = v/Z$ is the wavenumber, and the 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 $^7Be$ 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 due to electrons in continuum states is $w_c = 3.18$.

### 2.1. Bound States plus Continuum States

Iben, Kalata, & Schwartz (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

$$w_b = \pi^{1/2}(2\beta)^{3/2} \sum n^{-3} \exp(\beta Z^2/2n^2),$$  \hspace{1cm} (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, Kalata, & Schwartz (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, $\chi$, and the probability densities, $\psi^2$, at the nucleus for a screened Coulomb potential with $Z$ taking on values from 1 to 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 due to screening,

$$F_{IKS} = \psi^2 e^{\beta \chi}/\psi_0^2 e^{\beta \chi_0},$$  \hspace{1cm} (3)

where the subscript 0 indicates unscreened values. Thus, we see from Table 1 that bound state screening reduces the total capture rate by a factor

$$R = (w_c + F_{IKS}w_{b1})/(w_c + w_b) = 0.85,$$  \hspace{1cm} (4)
or by 15%.

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

$$F_{BM} = \langle \psi^2 \rangle / \langle \psi_0^2 \rangle.$$ (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 $\beta$ and $R_D$.

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

$$w_{IKSBM} = F_{BM} w_c + F_{IKS} w_{bl},$$ (6)

where we make the excellent approximation that screened excited bound states give a negligible contribution. For $Z = 4$, Eq. (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 Eq. (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

$$\phi = \frac{Z}{r} e^{-r/R_D} \approx \frac{Z}{r} - \frac{Z}{R_D}.$$ (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 Eq. (6), and the simple Salpeter-like formula, Eq. (8). The agreement between the two results is about 1% for $Z$ less than 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 which represents the solar plasma by a screened nucleus and a sea of non-interacting 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 due to 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.

Asymmetric fluctuations might plausibly 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 $^7\text{Be}$ nucleus) experiences an electric field, $\mathcal{E}$, 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 $\psi^2$. The first effect increases the
capture rate since the ionization potential increases. In second order of the perturbation theory (eg. Landau & Lifshitz 1977)

\[ \chi = \frac{Z^2}{2} + \frac{9E^2}{4Z^4}. \]  

(9)

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

\[ \psi = 2 - \frac{81E^2}{8Z^6}, \]  

(10)

which reduces the capture rate. The two effects together alter the ground state electron density by a factor, \( F_E \), where

\[ F_E = \frac{\psi^2}{4} e^{\delta \chi} \approx 1 - \left( \frac{81}{8} - \frac{9\beta Z^2}{4} \right) \frac{E^2}{Z^6} \approx 1 - 0.0023E^2, \]  

(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 due to the Stark effect, we need to know the size of the fluctuating field, \( E^2 \). For an illustrative model calculation, one can use the well-known Holtsmark probability distribution for the electric field. This distribution is exact for unscreened non-interacting ions (low densities). The Holtsmark probability distribution is

\[ P_H(x) = \frac{2x}{\pi} \int_0^\infty dy \sin(xy)y \exp(-y^{3/2}). \]  

(12)

Here \( x \) is the normalized electric field, \( x = E/E_H \), and the characteristic electric field is

\[ E_H = 2.6n^{2/3} \approx 11. \]  

(13)

We do not consider very large electric fields, \( x \gg 1 \), since in this domain the assumption of non-interacting ions is obviously incorrect. We therefore take \( P(x) = 0 \) for large \( x \) where the factor (11) becomes negative. We find, upon averaging Eq. (11), \( F = 0.21 \) - a strong effect.
Both second order perturbation theory and the Holstmark 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 Schroedinger 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 number - the density of thermal electrons at the nucleus. The average density can be calculated by solving the density matrix equation (e.g. Feynman 1990)

\[ \partial_\tau \rho = \left\{ \frac{1}{2} \nabla^2 + \frac{Z}{r} e^{-r/R_D} + V(r) \right\} \rho, \]

\[ \rho(r, \tau = 0) = \delta^{(3)}(r). \]

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 Eq. (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

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

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

The diffusion with multiplication problem, Eq. (14), can be solved easily by direct three-dimensional numerical simulations for solar conditions, because the inverse temperature $\beta$ is small ($\sim 0.02$), and the diffusive trajectory stays close to the origin. We simulated Eq. (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

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

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 Eq. (16) is $(2\pi\beta)^{-3/2}$. We used the code to compute the numerator of Eq. (16) for $R_D = \infty$, and for $R_D = 0.45$, 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 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 I) and Boltzmann distributed ions (case II).

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

$$U = Z \sum \frac{1}{r_j} e^{-r_j/R_D} + \sum \frac{1}{r_{jk}} e^{-r_{jk}/R'_D}. \tag{18}$$

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

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

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 Eq. (16).

The probability distribution for potentials is different in the two models. In case I, the nucleus can experience arbitrarily high electric fields, while in case II, 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 seen from the
Table, 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 $\mathcal{E}$ are described by the fluctuating potential $V = \mathcal{E}x$ in Eq. (14). As a result, both the un-normalized density at the nucleus $\rho_Z$, and the density normalization $\rho_0$ are shifted by the fluctuating field. The Coulomb attraction keeps the diffusing thermal electron (as described by the density matrix equation (14)) in the vicinity of the nucleus, and we may suppose that the shift in $\rho_Z$ is smaller than the shift in $\rho_0$. The density matrix equation for $\rho_0$ is simple, and one can calculate the shift in $\rho_0$ using the perturbation expansion of the density matrix (e.g. Feynman 1990). In second order perturbation theory, we find

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

For the characteristic microfield ($\mathcal{E} \sim \mathcal{E}_H \approx 11$) and the inverse temperature ($\beta = 0.0215$), Eq. (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, Eq. (13), for $E$, 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, $a_0 \sim R_D$, Eq. (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

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

7. Summary and Discussion

The rate of electron capture by $^7Be$ 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 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 $^7Be$ using the density matrix formalism (cf. 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 due to the small number (about 3) of ions in a Debye sphere surrounding a $^7Be$ 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 $^7\text{Be}$ electron capture rate in the Sun (see, e.g., Iben, Kalata, & Schwartz 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 $R/R_\odot = 0.0, 0.06, \text{ and } 0.15$.

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 $^7\text{Be}$ 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. we conclude that the total fractional uncertainty, $\delta R/R$, is small and that

$$\delta R/R < 0.02.$$  \hspace{1cm} (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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Table 1. Mean Field Theories

|        | 1     | 2     | 3     | 4     | 5     | 6     |
|--------|-------|-------|-------|-------|-------|-------|
| $\chi/\chi_0$ | -     | .0034 | .12   | .25   | .35   | .43   |
| $\psi^2/\psi_0^2$ | -     | .098  | .52   | .70   | .80   | .85   |
| $F_{IKS}$ | .0    | .09   | .48   | .62   | .67   | .68   |
| $F_{BM}$  | .965  | .985  | .98   | .978  | .979  | .991  |
| $w_{IKS\overline{BM}}$ | 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 ($\chi$) and electron density ($\psi^2$), bound state reduction factor ($F_{IKS}$), continuum reduction factor ($F_{BM}$), density enhancement ($w$). Results are given for an inverse temperature $\beta = 0.0215$ and a Debye radius $R_D = 0.45$. 
Table 2. Monte Carlo Results

|       | $N_{MC}$ | 1     | 2     | 5     | 10    | 20    | 50    | 100   |
|-------|----------|-------|-------|-------|-------|-------|-------|-------|
| I, $\rho_Z$ | 4.84   | 4.91  | 4.93  | 4.90  | 4.99  | 4.84  | 4.73  |
| I, $\rho_0$  | 1.26   | 1.27  | 1.28  | 1.27  | 1.29  | 1.26  | 1.23  |
| I, $w$       | 3.84   | 3.87  | 3.85  | 3.86  | 3.87  | 3.84  | 3.85  |
| I, %         | -0.3   | +0.5  | 0.0   | +0.3  | +0.5  | -0.3  | 0.0   |
| II, $\rho_Z$ | 5.40   | 5.46  | 5.43  | 5.52  | 5.60  | 5.57  | 5.53  |
| II, $\rho_0$ | 1.37   | 1.40  | 1.39  | 1.40  | 1.44  | 1.42  | 1.41  |
| II, $w$      | 3.90   | 3.86  | 3.87  | 3.90  | 3.85  | 3.88  | 3.88  |
| II, %        | +1.3   | +0.3  | +0.5  | +1.3  | 0.0   | +0.8  | +0.8  |

Note. — The number of Monte Carlo realizations, $N_{MC}$, is given in the first row for case I. For case II, the number of realizations is $10 \times N_{MC}$. The table also lists the average density, $\rho_Z$, the normalization $\rho_0$, and the density enhancement $w$. The last row for each case is the % deviation from the mean field result of 3.85.