SYSTEMATIC QUANTUM CORRECTIONS TO SCREENING IN THERMONUCLEAR FUSION

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ABSTRACT

We develop a series expansion of the plasma screening length away from the classical limit in powers of $\hbar^2$. It is shown that the leading-order quantum correction decreases the fusion rate by approximately 2%. We also calculate the next higher order quantum correction, which turns out to be approximately an order of magnitude smaller.

Subject heading: nuclear reactions, nucleosynthesis, abundances

1. INTRODUCTION

Salpeter (1954) wrote a seminal paper more than half a century ago concerning screening effects on thermonuclear reaction rates. He made the basic point that screening effects are small at the center of the Sun.

There has been renewed interest more recently in using the Sun as a source of neutrinos to test the standard model of unification of electroweak forces. The measured neutrino flux deviates from predictions of the standard model by a factor of 2 (Bahcall & Bethe 1990). The measurement uncertainty is ~1% (Bahcall & Bethe 1990; Gruzinov & Bahcall 1998). Therefore, it would be meaningful to quantify the theoretical estimate with equal precision. The structure and dynamics of the Sun are complex (Thoul et al. 1994). Various phenomena need to be identified and estimated correctly. The screening of Coulomb repulsion between nuclei at extremely short distances is one of them. Many calculations of screening have been made since Salpeter’s original paper, attempting to refine the degree of screening (Brown & Sawyer 1997; Brown et al. 2006; Fiorentini et al. 2004), dynamic effects (Carraro et al. 1988), and quantum fluctuations (Gruzinov & Bahcall 1998; Gervino et al. 2005; Bahcall et al. 2002). Here we focus on quantum corrections to screening. The most sophisticated calculation of this effect is that of Gruzinov & Bahcall (1998). In that paper, the electronic density matrix was evaluated accurately using Feynman’s formulation in terms of a Schroedinger equation, with the inverse temperature playing the role of imaginary time. Fermion statistics were ignored due to the high solar temperature. They sustained Salpeter’s original conclusion that quantum corrections are minor. These calculations are essentially right, but cannot estimate in a systematic fashion the next higher order quantum correction. We eliminate that deficiency in this paper.

This paper was written for the sake of completeness, since the Super-Kamiokande experiment has been successful in obtaining evidence for neutrino mass (see Oyama 2006 for recent results). The results of this paper may yet prove useful for more precise quantitative interpretation of stellar experimental data (Pinsonneault & Delahaye 2006). In fact, our approach will be useful for studying the quantum enhancement of fusion rates in highly dense stellar interiors (Itoh et al. 1990; Ogata 1997).

2. NONRELATIVISTIC QUANTUM CORRECTIONS

We treat ions in a thermonuclear plasma as classical objects, while applying a quantum treatment to electrons. The resulting partition function is evaluated as a deviation from the classical limit for electrons. A series expansion is developed in powers of a dimensionless ratio involving $\hbar^2$.

Let us begin with the classical Poisson-Boltzmann equation for a single species of ions and electrons:

$$-\nabla^2 \phi = 4\pi \rho,$$

$$\rho = \rho_+ + \rho_-,$$

$$\rho_+ = eNZ \exp \left(-Ze\phi/k_B T\right),$$

$$\rho_- = -eN \exp \left(e\phi/k_B T\right),$$

where $e$ is the magnitude of the electronic charge, $k_B$ is Boltzmann’s constant, $n$ is the average number density, $Z$ is the atomic number, and $T$ is the temperature of the system. We work in the linear regime, which is expected to apply in the solar interior (Brown et al. 2006), by retaining only terms to first order in $\phi$.

$$\nabla^2 \phi \approx \left[4\pi n(Z^n + Zn)e^2\right]/k_B T \phi \equiv \Lambda_0^{-2} \phi,$$

$$\Lambda_0 = \sqrt{\frac{k_B T}{4\pi ne^2(Z^2 + Z)}},$$

where $\Lambda_0$ is the classical screening length.

The quantum mechanical version of this approximate Poisson-Boltzmann equation for a single species of ions and electrons can be written analogously to equation (1):

$$-\nabla^2 \phi = 4\pi \rho,$$

$$\rho = \rho_+ + \rho_-,$$

$$\rho_+ = eN Z \left(1 - \frac{Ze\phi}{k_B T}\right),$$

$$\rho_- = -e|\psi(\{r\})|^2,$$

where $\psi$ is the many-body quantum wave function for electrons, $\{r\}$ refers collectively to the electrons in the system, and $\phi$ is the electrostatic potential.

We now invoke the following scaled variables, in order to ease subsequent calculations:

$$\tilde{\phi} = \frac{e\phi}{k_B T},$$

$$\tilde{\psi} = \Lambda^{3/2} \psi,$$

$$\Lambda = \sqrt{\frac{k_B T}{4\pi Z^n ne^2}},$$

$$r' = \frac{r}{\Lambda},$$

$$\Gamma = \frac{e^2}{\Lambda k_B T}.$$
Note that the first equation of equations (4) shows that we are using $k_B T$ as the energy scale. The electrostatic potential is then given by
\[ \nabla^2 \phi = \phi + 4\pi \Gamma |\psi|^2 - Z^{-1}. \] (5)

This equation can be obtained from a Lagrangian density:
\[ \mathcal{L}_0 = -\frac{1}{2} |\nabla \phi|^2 - v(\phi, \psi), \]
\[ v(\phi, \psi) = \frac{1}{2} \phi^2 + 4\pi \phi \Gamma |\psi|^2 - Z^{-1} \phi. \] (6)

The corresponding Hamiltonian density can be easily derived:
\[ \mathcal{H}_0 = \frac{1}{2} |\nabla \phi|^2 + v(\phi, \psi). \] (7)

We now introduce second-quantized notation to deal with the statistics of electrons,
\[ v(\phi, \psi) \rightarrow v(\phi, \psi_+), \]
\[ = \frac{1}{2} \phi^2 - Z^{-1} \phi \]
\[ + 4\pi \phi \Gamma (\psi_+^\dagger \psi_+ + \psi_-^\dagger \psi_-), \] (8)

where $\psi_\pm$ are Grassmann variables and the subscripts refer to the spin of the electrons. The coexistence of Grassmann variables and scalars in equation (8) is not problematic, since we use this discussion solely to define a partition function for the entire system. And thereafter we integrate over the electron degrees of freedom, so that only a functional involving the scalar potential survives.

The total Hamiltonian $\mathcal{H}$ for the system, including the quantum mechanical part for the electrons, is
\[ \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_Q, \]
\[ \mathcal{H}_Q = \Delta_Q \left( |\nabla \psi_+|^2 + |\nabla \psi_-|^2 \right). \] (9)

The quantum correction has been encapsulated in the following dimensionless parameter:
\[ \Delta_Q = \frac{\hbar^2 \Lambda^{-2}}{2mk_B T}, \] (10)

where $m$ is the mass of the electron. Since solar temperatures are $\sim O(1 \text{ keV})$, and the rest energy of the electron is 0.55 MeV, it follows that the nonrelativistic approximation employed in equation (9) is valid.

The partition function can be written in scaled variables as
\[ Z = \int D\phi D^2 \tilde{\psi}_\pm \exp \left[ -\int d^3x' (\mathcal{H}_0 + \mathcal{H}_Q) \right], \] (11)

where it is understood that $k_B T = 1$ in the units we are using. Note that the total number of electrons associated with each ion of charge $Ze$ is $Z$ and is obtained via $\langle \psi_+^\dagger \psi_+ + \psi_-^\dagger \psi_- \rangle = Z n$ (where the angular brackets indicate an expectation value). We indicate below how one can impose this constraint on the system using a Lagrange multiplier. In condensed matter physics, this is done via the electronic chemical potential. In our problem, it turns out to be more convenient to institute this constraint via a functional involving just the electrostatic potential.

Note that the parameter $\Gamma$ is analogous to the usual plasma parameter. It is much less than 1 for solar conditions. For solar conditions, viz., a density of 100 g cm$^{-3}$, $T = 15 \times 10^6$ K, and $Z = 2$, it turns out that $\Lambda_0 \approx 0.281$ Å and $\Gamma \approx 0.04$. The value of $\Delta_Q$ turns out to be approximately 0.032. This is already an indication that quantum corrections will be small. In making these estimates, we have assumed a helium plasma with thermodynamic properties similar to those at the center of the Sun (Gruzinov & Bahcall 1998).

The quadratic nature of the energy functional in equation (11) allows us to perform a functional integration over the Grassmann variables associated with the electronic degrees of freedom (Ramond 1981), allowing us to obtain
\[ Z \sim \int D\tilde{\phi} \exp \left[ -\int d^3x' \left( \frac{1}{2} |\nabla \tilde{\phi}|^2 \right. \right. \]
\[ + \frac{1}{2} \tilde{\phi}^2 - Z^{-1} \tilde{\phi} \left. \right) \right] \det(\mathcal{F}), \]
\[ \det(\mathcal{F}) = \exp \left( \text{Tr} \ln \mathcal{F} \right), \]
\[ \mathcal{F} = -\Delta_Q \nabla^2 + 4\pi \Gamma \tilde{\phi}, \] (12)

where $\text{Tr}$ is the trace of the operator appearing to the right of the symbol.

Having integrated over the electronic degrees of freedom, we are left with an effective energy density in terms of the electrostatic potential alone. We choose to impose charge neutrality, which was discussed just below equation (11), via a Lagrange multiplier by making the following addition ($\Delta \mathcal{H}$) to the energy density:
\[ \Delta \mathcal{H} = 4\pi \nu \tilde{\phi}. \] (13)

Here $\nu$ can be interpreted physically as a uniform charge density, which will be adjusted to ensure the overall charge neutrality.

We need to evaluate the determinant of the operator obtained in the process of performing the quadratic functional integral over fermionic variables. This is conveniently performed in Fourier space:
\[ \text{Tr} \ln \mathcal{F} \equiv \int \frac{d^3k}{(2\pi)^3} \ln \left[ 4\pi \Gamma \tilde{\phi}(k) + \Delta_Q k^2 \right], \] (14)

where $\tilde{\phi}(k)$ is the Fourier transform of $\tilde{\phi}$.

Now the estimates below equation (11) indicate that $4\pi \Gamma \gg \Delta_Q$ near the center of the Sun, so we propose a series expansion in powers of $\Delta_Q$:
\[ \ln \left[ 4\pi \Gamma \tilde{\phi}(k) + \Delta_Q k^2 \right] \approx \ln \left[ 4\pi \Gamma \tilde{\phi}(k) \right] \]
\[ + \frac{\Delta_Q k^2}{4\pi \Gamma \tilde{\phi}(k)} - \left( \frac{\Delta_Q k^2}{4\pi \Gamma \tilde{\phi}(k)} \right)^2 + \ldots \] (15)

Furthermore, we conform to the linear screening limit, which is expected to apply in the solar interior (Brown et al. 2006). By this we mean that we seek an expansion of the determinant obtained above to the quadratic order of the scalar potential; higher order terms can be accounted for using diagrammatic techniques. We have the freedom to choose the value of the potential around which to perform the expansion. We choose this value to be $\phi_0$, such that in the limit $\hbar \to 0$, we recover the standard expression...
for the screening length obtained from the linearized Poisson-Boltzmann equation. The power series to quadratic order yields

\[
\ln[4\pi\Gamma \hat{\phi}(k) + \Delta_\phi k^2] \approx \ln(4\pi\Gamma) + \left\{ \ln(\phi_0) + \frac{\hat{\phi}(k) - \phi_0}{\phi_0} - \frac{[\hat{\phi}(k) - \phi_0]^2}{2\phi_0^2} \right\} + \frac{\Delta_\phi k^2}{4\pi\phi_0} \left\{ 1 - \frac{\hat{\phi}(k) - \phi_0}{\phi_0} + \frac{[\hat{\phi}(k) - \phi_0]^2}{\phi_0^2} \right\}. \tag{16}
\]

The constant terms are unimportant, as they can be absorbed into the normalization constant. To be consistent, the rest of the effective energy density must also be expanded around \(\phi_0\). The net result would yield, in addition to a quadratic term, a term linear in \(\hat{\phi}\). The coefficient of this linear term is an effective background charge density, which must be zero in our neutral system. The coefficient can be set to zero by appropriately adjusting \(\nu\), the Lagrange multiplier, defined in equation (13).

With the proper charge neutrality constraint imposed, the screening length expression can be matched with the linearized classical Poisson-Boltzmann equation (2) when \(h \to 0\), by setting \(\phi_0 = Z^{1/2}\). Then the energy density can be written to leading order in \(\Delta_\phi\) in Fourier space as:

\[
\mathcal{H} \approx \frac{1}{2} k^2 \left( 1 + \frac{2\Delta_\phi}{Z^{3/2}\Gamma} \right) \hat{\phi}(k)^2 + \frac{1}{2} \left( 1 + \frac{1}{Z} \right) \hat{\phi}(k)^2. \tag{17}
\]

The corresponding Lagrangian density in real space is

\[
\mathcal{L} = -\frac{1}{2} \left( 1 + \frac{2\Delta_\phi}{Z^{3/2}\Gamma} \right) \nabla \Phi(r)^2 - \frac{1}{2} \left( 1 + \frac{1}{Z} \right) \Phi(r)^2. \tag{18}
\]

The equation of motion then follows:

\[
-\nabla^2 \Phi + \ell^{-2} \Phi = 0, \\
\ell = \sqrt{\frac{1 + 2\Delta_\phi/(Z^{3/2}\Gamma)}{1 + 1/Z}}. \tag{19}
\]

In dimensional units, the corrected screening length is

\[
\Lambda_{QC} = \sqrt{\frac{k_B T \left[ 1 + 2\Delta_\phi/(Z^{3/2}\Gamma) \right]}{4\pi(Z^2 + Z)ne^2}} \tag{20}
\]

Note that without quantum corrections, the screening length is about 0.281 Å. Quantum fluctuations increase the screening length by \(\approx 2\%\) at solar conditions, defined earlier. The classical enhancement factor of the fusion rate is 1.17. It is reduced slightly to 1.16 via quantum corrections. The next higher order quantum correction to the rate from our theory [expanding eq. (16) to \(O(\Delta_\phi^3)\)] turns out to be approximately 0.4%.

The numerical values obtained for the screening length and the Salpeter rate enhancement factor have been encapsulated for solar conditions in Table 1. Hence, the leading-order quantum correction decreases the fusion rate by about 2.1% for the conditions chosen. The numerical estimates provided above are in good agreement with those found in the literature (Salpeter 1954; Gruzinov & Bahcall 1998).

3. CONCLUSION

Systematic quantum corrections to screening in thermonuclear fusion were derived in powers of \(h^2\) and estimated for solar conditions. Leading-order corrections were shown to be about 2.1% under solar conditions, while the next leading-order term is \(\approx 0.4\%\). Our corrections are consistent with those previously obtained by Gruzinov & Bahcall (1998). They complement the results of Brown et al. (2006), who show that classical, nonlinear effects on screening are small.

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