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THE EFFECT OF ELECTRON GAS POLARIZATION ON THERMONUCLEAR REACTION RATES IN DENSE STARS

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ABSTRACT

In dense stars the nuclear reaction rates are influenced by screening effects arising from both ions and electrons. In this paper we calculate the enhancement factors due to electron polarization in the high-density, degenerate and relativistic regime, for nonresonant nuclear reaction rates. In an earlier analysis, Sahrling had proposed the possibility that the polarized electrons would lower the reaction rate instead of enhancing it. This analysis was based on Monte Carlo simulations with only one choice of density, temperature, and charge. Here we extend the analysis to a wider range of densities, temperatures, and charges and calculate analytical expressions for the enhancement factors. We concentrate on carbon and oxygen ions and show that at very high densities high order quantum effects will be important and act to reduce the zeroth-order classical value for the enhancement factor. We show that, in any case, the total electron contribution remains weak, namely, an enhancement in the reaction of about a factor 2, contrary to what had been claimed by some authors in previous calculations. We examine the astrophysical implications of these results on the final stages of massive white dwarfs near the carbon-ignition curve.

Subject headings: dense matter — nuclear reactions, nucleosynthesis, abundances — polarization — stars: interiors — supernovae: general — white dwarfs

1. INTRODUCTION

The rate of nuclear reactions plays an important role in many fields of astrophysics. It sets the timescale for various processes, such an energy release in the core of stars. It is also a crucial factor in determining the fate of accreting white dwarfs in binary systems (see, e.g., Isern & Hernanz 1994). In dense matter, the surrounding ions screen the Coulomb barrier between the two reacting nuclei and thus increase the reaction rate compared to the infinitely dilute plasma, as shown originally by Schatzman (1948). One usually assumes that the electrons can be treated as a uniform, *rigid* background, the so-called one-component plasma (OCP) or binary ionic mixture (BIM) model. This approximation has been studied extensively by many authors and for recent discussions see, e.g., Yakovlev & Shalybkov (1989), Sahrling (1994b). In general, electron polarization effects are small since the Thomas-Fermi screening length is larger than the mean distance between the ions. Moreover, people have generally concentrated on the so-called classical or zeroth-order contribution to the reaction rate (see, for example, Mochkovitch & Hernanz 1986; Ichimaru & Utsumi 1983; Yakovlev & Shalybkov 1989; Ichimaru & Ogata 1991; Sahrling 1994b), although the quantum mechanical, or higher order, contributions are discussed to some extent in these papers. Sahrling (1994b) found that the quantum corrections give a much smaller contribution to the reaction rate than suggested by some previous calculations. He also proposed that the electrons would reduce the reaction rate, and this could affect the late stages of stellar evolution. The investigation was based on a mean (or screening) potential that was calculated for only one choice of density, temperature, and charge for the ionic plasma. In this paper, we examine in details the effect of electron gas polarization in the high-density regime corresponding to degenerate, relativistic electrons. We extend the previous calculations to a wider range of densities, charges, and temperatures, and we calculate the quantum correction to the classical enhancement factor.

In § 2 we describe how the polarization of the electron gas is taken into account, and we derive analytical formulae for the corresponding correction to the reaction rate. The astrophysical consequences are described in § 3 followed by the conclusion in § 4.

2. REACTION RATE DUE TO ELECTRON GAS POLARIZATION

This section is divided into three subsections. In § 2.1, we briefly review the theory of reaction rates in dense matter, and we describe the calculations of the correction arising from the electron gas polarization. We concentrate on densities and temperatures where the electrons are degenerate and relativistic since, as we argue below, we expect quantum effects to be most significant in that region. Section 2.2 describes the calculations of the mean potential, and analytical fitting formulae for these potentials are given at the end of the subsection. The enhancement factors due to a polarized electron gas are calculated in § 2.3, and analytical fitting formulae are also provided for these factors.

2.1. *Basic Formalism*

When investigating nonresonant reaction rates in dense matter one usually discusses enhancement factors, where one normalizes the reaction rate in the correlated plasma to its value in an infinitely dilute gas. The advantage of this procedure is that the matrix element describing the actual nuclear reaction, which is considered to be independent of the neighbor ions and electrons, is canceled out and one is left with a simpler expression (see, e.g., Alastuey & Jancovici 1978). For a recent discusion of some of the basic approximations and assumptions see Sahrling (1994a, 1994b). One assumes usually that the electrons are uniformly and homogeneously distributed in the plasma, the so-called rigid

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background approximation. This yields the well-studied OCP model (or BIM for a binary mixture) to describe the thermodynamic properties of dense matter. In this paper, we examine the case where such an approximation is no longer valid and where the *inhomogeneous* electron gas is polarized by the external field due to the surrounding nuclei.

The plasma is described by N ions of mass m and charge Z_e moving in a volume V. The density ρ and temperature T are such that the electrons are degenerate and completely stripped off the atoms, so that the electroneutrality yields $N_e = N \times Z$, where N_e is the number of free electrons. We restrict the present study to the region below the neutronization threshold. For ions such as C^{6+} and O^{8+} all these conditions correspond to $10^5 < \rho < 10^{10}$ g cm^{-3} and $10^7 < T < 10^9$ K. The physical state of the one-component plasma is described universally by two parameters. The coupling parameter Γ is simply the ratio of the mean Coulomb energy to the average kinetic energy of the ions,

$$\Gamma = \beta \frac{(Ze)^2}{a}, \quad \beta = \frac{1}{k_B T}, \tag{1}$$

where k_B is the Boltzmann constant. The Wigner-Seitz radius a is defined as $a = [3V/(4\pi N)]^{1/3}$. Above $\Gamma \simeq 172$, the crystal becomes stable and the matter is solid (Dubin 1990). Since we consider presently reaction rates in the fluid phase, we require $\Gamma < 172$. Relativistic effects on the electrons velocity are measured by the parameter

$$x = \frac{p_F}{m_e c}, \tag{2}$$

where p_F is the Fermi-momentum of the electrons and m_e denotes their mass. To measure quantum effects we use the parameter δ, which is defined as

$$\delta = \frac{b_0}{a} = \left[\frac{16\hbar^2\beta^2(Ze)^2N}{3\pi mV}\right]^{1/3} \sim x^{1/3}\Gamma^{2/3} \sim \left(\frac{Z}{A}\right)^{2/3} T^{-2/3}\rho^{1/3}, \tag{3}$$

where b_0 is the classical turning point at the Gamow peak incident energy for the infinitely dilute plasma. The parameter δ corresponds to the more widely used combination $\delta = 3\Gamma/\tau$, where τ is the penetration probability of the Coulomb barrier for the infinitely dilute plasma. Quantum effects become increasingly important as δ gets larger, i.e., for small temperatures and high densities. In this paper we will examine densities of the carbon/oxygen plasma where the electrons are highly relativistic ($x \gg 1$), as commonly encountered in the core of massive white dwarfs. However, in order to avoid exchange effects between the *ions*, we will restrict the calculations to the region in the (ρ, T)-plane where the ionic thermal de Broglie wavelength is smaller than the mean interionic distance, i.e., $\lambda = (2\pi\hbar^2/mk_B T)^{1/2} \ll a$. In terms of Γ and δ this condition can be written $\lambda/a \simeq 3.9(\delta^3/\Gamma)^{1/2}$,

$$\delta < 0.4\ \Gamma^{1/3}. \tag{4}$$

For carbon and oxygen ions under white dwarf central density conditions, $\delta \sim 2$ when $\Gamma \sim 180$ so the condition (4) is valid below the line of solidification, i.e., in the entire fluid phase. The lowest order correction to the final reaction rate at this limit, in λ/a, is about 50% (Sahrling 1994b).

The effective interionic potential $V^e(\rho, r)$, which takes into account polarization effects of the electron gas, is given by

$$V^e(\rho, r) = \frac{(Ze)^2}{2\pi^2} \int d\boldsymbol{k}\, \frac{1}{k^2\epsilon(\rho, k)} \exp(i\boldsymbol{k}\cdot\boldsymbol{r}), \tag{5}$$

where $k = |\boldsymbol{k}|$ is the wavenumber (Hubbard & Slattery 1971; Galam & Hansen 1976; Yakovlev & Shalybkov 1989; Chabrier 1990). For $\epsilon(k)$ we use the static dielectric function of relativistic degenerate electrons (Jancovici 1962). We exclude the vacuum polarization part of ϵ since that will not affect the rate by more than a few percent (Gould 1990).

Let us now assume that two particles are moving toward each other. The probability of a nuclear reaction between them is given by the pair distribution function $g(d)$, where d is of nuclear dimensions. Since in Coulombic matter d is much smaller than a, one can evaluate the pair distribution at $d = 0$ (Alastuey & Jancovici 1978). If the nuclear reaction itself is independent of the neighbor ions, one can normalize the rate to the infinitely dilute plasma. The enhancement factor E is then given by

$$E = \frac{g(0)}{g_0(0)}, \tag{6}$$

where

$$g(0) = g(r = 0) = \langle \mathbf{0} | \exp(-\beta H) | \mathbf{0} \rangle \tag{7}$$

and

$$H = -\frac{\hbar^2}{m}\Delta + V^e(\rho, r) + w(r). \tag{8}$$

Value $g_0(r)$ is the pair distribution function with $w = 0$ and $r = |\boldsymbol{r}|$ is the distance between the reacting particles. The potential felt by the reacting pair from the neighbor ions is approximated by a mean potential $w(r)$, defined by,

$$e^{-\beta w(r)} = \int_V^{N-1} \int \exp\{-\beta[W(\boldsymbol{r}, \boldsymbol{R}, \alpha) - F]\} \frac{d\alpha d\boldsymbol{R}}{V^{N-1}}, \tag{9}$$

where α denotes the coordinates of all neighbor ions in the volume V and $\boldsymbol{R}$ is the center-of-mass coordinate of the reacting pair. $W(\boldsymbol{r}, \boldsymbol{R}, \alpha)$ denotes the sum of all pair interactions except the one between the reacting pair. F is the Helmholtz free energy of the system. The accuracy of the mean-potential approach has been explored in details by Jancovici (1997), Alastuey & Jancovici (1978), Jändel & Sahrling (1992), and Sahrling (1994a).

The right-hand side of equation (7) denotes a quantum mechanical matrix element which can be calculated, for instance, by the path integral formalism (Feynman & Hibbs 1965). Keeping only the classical action in the functional integral yields the following expression:

$$E = \frac{\int_0^\infty \exp(-S(E')/\hbar)dE'}{\int_0^\infty \exp(-S_0(E')/\hbar)dE'} \{1 - O[(\lambda/a)^2]\}, \tag{10}$$

where

$$S(E')/\hbar = \frac{2}{\hbar}\int_0^b \{m[V^e(\rho, r) + w(r) - E']\}^{1/2} dr + \beta E'. \tag{11}$$

The function S_0 in equation (10) is the same as S but for the bare Coulomb potential $V(r) = (Ze)^2/r$ and $w = 0$. The first term in the integrand of S in equation (11) is the penetration probability through the combined potential $V^e(\rho, r) + w(r)$, and the second term is simply the thermal weight. For details of the derivation, see Alastuey & Jancovici (1978) and Sahrling (1994a, 1994b).

2.2. *Mean Potentials*

We have calculated the mean potential in equation (9) for various combinations of the density and temperature for carbon and oxygen ions. We employ the Monte Carlo so-called "minimum-image convention" (Brush, Sahlin, & Teller 1966). According to this scheme, a particle in the basic box is allowed to interact only with each of the $N - 1$ other particles in the basic box or with the nearest "image" of this particle in one of the neighboring cells. In other words, each particle interacts with the $N - 1$ particles that happen to be located in a cube centered at the particle at any time. This method is not useful for long-range interactions, such as the bare Coulomb interaction. In our case the *screened* effective potential is Yukawa-type, i.e., short-range type. We found that we needed at least 2000 particles in the basic Monte Carlo box in order to avoid border effects for $0 < r/a \leq 2$. In general, we require the accuracy in w/Γ to be better than 10^{-3}. This leads to an uncertainty in w less than 20%. In Figure 1 we show the result for $\Gamma = 120$, $x = 10$, and $Z = 6, 8$.

It is too time consuming to use equation (5) explicitly to calculate the interaction between each pair of particles in the Monte Carlo simulation. We therefore calculate $V^e(\rho, r)$ at 10,000 points between $[0, L]$ and use the result as an input vector to the Monte Carlo code where we interpolate the vector linearly. The accuracy in w/Γ of this procedure was found to be better than 10^{-3} by comparing with runs using 20,000 points. For each combination of density, temperature, and charge, we used 10^7 configurations where we started from a random configuration. We ignored the initial 10^6 configurations because they have not reached equilibrium. We also made sure that this number of configurations was adequate by comparing with runs using 2×10^7 configurations. The code we use is based on a code kindly supplied by W. L. Slattery for the OCP (Slattery, Doolen, & DeWit 1980).

TABLE 1

CONSTANTS IN THE MEAN POTENTIAL EQUATION (12)

Z	A^e	B^e	D^e
6.....	1.055	−0.541	0.071
8.....	1.053	−0.566	0.080

The variation of the mean potential equation (9) with x is smaller than 10% for $x > 10$. There is however, a strong dependence on Z which is consistent with the analysis of Yakovlev & Shalybkov (1989). We have constructed the following fitting formula for the screening potential:

$$\frac{\beta w(r)}{\Gamma} = \begin{cases} -\dfrac{h_0^e}{\Gamma} + h_1^e r^2 + h_2^e r^4 , & r < r_0 , \\ -A^e - B^e r - D^e r^2 , & r_0 \leq r < 2 , \end{cases} \tag{12}$$

where the constants A^e, B^e, and D^e are given in Table 1.

The absolute error in the fit is less than $\simeq 10^{-3}$ above $r = r_0$. Below $r = r_0$ the error is in principle not known. Yakovlev & Shalybkov (1989) calculated the value of the classical contribution from polarized electrons $C_Z^e(\Gamma)$, using the so-called linear mixing law, the accuracy of which has been demonstrated recently (Rosenfeld 1994, 1996; DeWitt, Slattery, & Chabrier 1996). However, Yakovlev & Shalybkov's calculations are based on an expansion scheme of the free energy due to the electron polarization with respect to the reference rigid background energy, thus

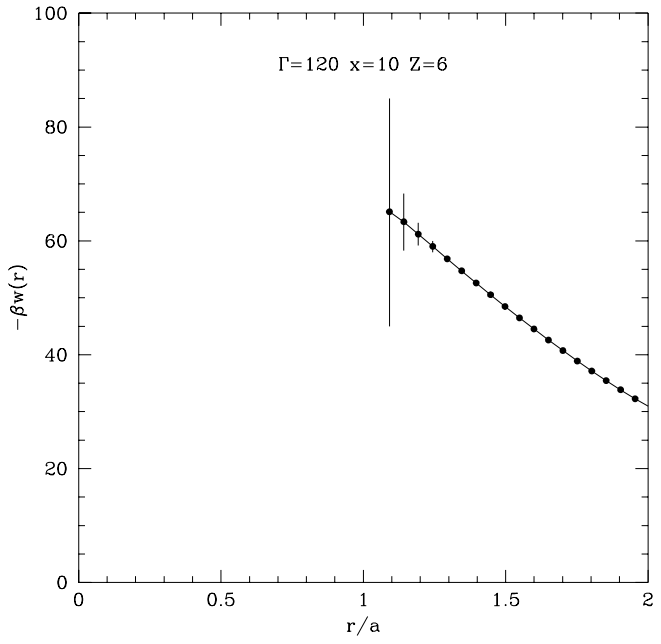

FIG. 1*a*

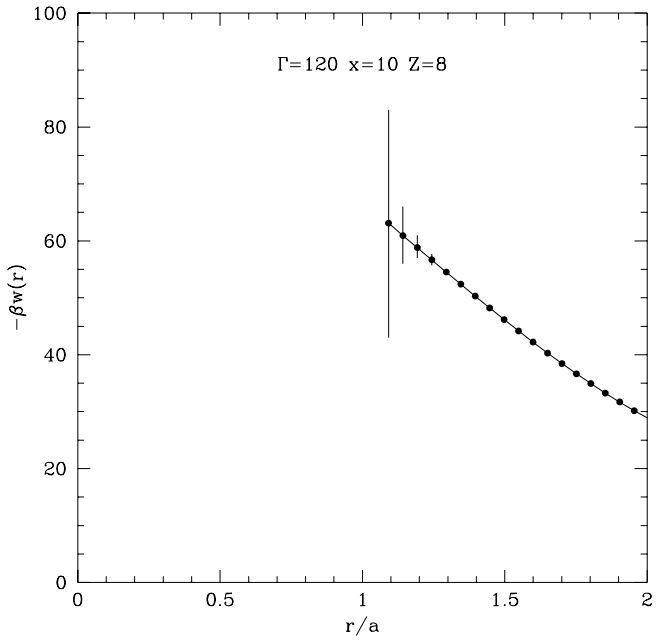

FIG. 1*b*

FIG. 1.—(*a*) Screening potential for $\Gamma = 120$, $x = 10$, $Z = 6$. The solid line corresponds to the fitting formula in eq. (12). The dots indicate the Monte Carlo result. The systematic error in the Monte Carlo dots is $\simeq 10^{-4}$ unless explicitly shown by vertical bars. (*b*) Same as (*a*) but with $Z = 8$.

reducing the validity of the calculations to the weak screening (small x or r_s) regime. Chabrier (1998) extended these calculations to regimes of stronger screening by calculating explicitly the electron contribution from equation (5). The equations were solved within the framework of the so-called hyper-netted chain (HNC) theory of the N-body problem. The HNC results are found to agree remarkably well ($<1\%$) with the Monte Carlo results (see, e.g., Chabrier 1990; DeWitt et al. 1996). Given the rapidity of the HNC calculations compared to lengthy numerical MC simulations, we were able to explore a wide density and temperature range, corresponding to different values of the relativistic parameter. We used these calculations of $C_Z^e(\Gamma)$ and the small-r behavior of $V^e(\rho, r)$ to calculate $\beta W(0) = -h_0^e = -C_Z^e(\Gamma) - \lim_{r\to 0}[\beta V^e(\rho, r) - \Gamma/r]$. The constants h_1^e, h_2^e, and r_0 are found by extrapolating the Monte Carlo results in a way similar to Rosenfeld (1992) and Sahring (1994b). The expressions for these constants are quite complicated and will not be given explicitly.

2.3. *Enhancement Factors*

We have calculated the enhancement factors due to the electron gas polarization. The correction with respect to the rigid-background calculations, for the one-component case, is given by

$$E^e = \frac{E}{E^{\rm OCP}} = \exp\left[C_Z^e - \frac{3\Gamma}{\delta} fz(\delta)\right], \tag{13}$$

where $C_Z^e(\Gamma)$ denotes the classical contribution from the polarized electrons and the second term is the quantum correction. We use equation (10) to calculate E for $Z = 6$ and 8. For the rigid background (OCP) result we use a similar expression but with the potentials derived in Rosenfeld (1992, 1994). For C_Z^e the results calculated at $x = 10$ can be parameterized by

$$\begin{aligned} C_6^e(\Gamma) &= 0.0123\ \Gamma + 0.0125\ \Gamma^{1/4} - 0.00554\ , \\ f_6(\delta) &= 5.26\ 10^{-3}\delta - 8.76\ 10^{-4}\ \delta^2 + 3.94\ 10^{-5}\ \delta^3\ , \\ C_8^e(\Gamma) &= 0.0160\ \Gamma + 0.0350\ \Gamma^{1/4} - 0.0326\ , \\ f_8(\delta) &= 5.38\ 10^{-3}\ \delta - 4.51\ 10^{-4}\ \delta^2 + 4.96\ 10^{-6}\ \delta^3\ . \end{aligned} \tag{14}$$

As mentioned above, the x-dependence of the screening potential, and thus of C_Z^e is weak over the density range of interest. We found that these expressions for C_Z^e are valid in the regime $2 < x < 20$, $\Gamma \le 60$ with an absolute rms error less than 0.05.

The functions f_Z have been calculated using a root-mean-square fit to 30 points in the interval $0 < \delta \le 3$. There is actually a weak dependence on Γ in f, but f in equation (14) has been averaged to give a total error in $E^e \lesssim 20\%$ for the density and temperature range explored presently. In Table 2 we compare these new results for the contribution arising from polarized electrons with the ones obtained in Sahrling (1994b). Within the accuracy of the present formulae, the electrons will essentially *increase* the reaction rate. It is clear from the table that the extrapolation error made in Sahrling (1994b) is most severe for the charge Z but also that a careful analysis of different densities and temperatures is important. It is noteworthy that quantum effects (high δ) act to reduce the enhanced reaction rate caused by the lowering of the Coulomb barrier, as given by C_Z^e. For high values of δ and Γ, quantum effects can be very important for $Z = 8$. In all cases, the contribution of the electrons to the enhancement factors of nuclear reactions in dense stellar plasmas remains of the order of the unity, at most a factor ~ 10 if quantum corrections are not included. This is much smaller than the classical *ionic* contribution $E^{\rm OCP} \approx e^{\Gamma}$ under similar thermodynamic conditions. Confusion had been brought by Ichimaru and collaborators (Ichimaru & Utsumi 1983; Ichimaru & Ogata 1991) who obtained electron enhancement factors of several orders of magnitude. These results are based on erroneous calculations which involve the difference between two very large numbers (eqs. [17] and [9] of the aforementioned references, respectively), whereas a direct resolution of equation (10) with the potential (5) can be done easily, as in the present calculations.

TABLE 2

COMPARISON WITH PREVIOUS ESTIMATES OF E^e

Z	Γ	δ	x	Sahrling 1994b	E^e	exp (C_Z^e)
8.....	113.8	0.8	5.0	0.62	1.2	6.69
8.....	36.4	0.37	5.0	1.2	1.1	1.89
8.....	72.6	0.74	10.0	0.82	1.14	3.42
8.....	145.2	1.18	10.0	0.38	1.34	11.1
8.....	46.0	0.69	20.0	0.93	1.1	2.21
6.....	70.4	0.8	5.0	0.75	0.93	2.45
6.....	22.5	0.37	5.0	1.1	0.97	1.35
6.....	44.9	0.74	10.0	0.89	0.96	1.78
6.....	89.8	1.18	10.0	0.56	0.98	3.12
6.....	142.9	2	20.0	0.38	1.3	5.99
6.....	28.5	0.69	20.0	0.96	0.97	1.45

[a] The last column shows the *classical* contribution to the enhancement factor calculated by Chabrier 1998. The numerical error in the calculation of C^e is of the order of 10%–15% for $\Gamma \gtrsim 70$.

3. CARBON IGNITION CURVE

In the late stages of stellar evolution for intermediate-mass stars, the core consists of a mixture of carbon and oxygen ions and degenerate electrons. As density and temperature increase, they will eventually reach thermodynamic conditions where the energy release from the nuclear reactions equals locally the neutrino energy loss. The points in the $\rho - T$ plane where this occurs define the carbon ignition curve. This fact is of prime importance in particular for accreting white dwarfs, for it determines the fate of the object. Small changes in the enhancement factors of nuclear reactions can make a spectacular difference in the outcome, the star becoming either a Type I supernova or collapsing into a neutron star (Isern & Hernanz 1994). This demonstrates the importance of accurate calculations for these factors. With the enhancement factor $E = E^{\rm OCP}E^e$ in equation (13), the generalization to mixtures according to Rosenfeld (1992; 1994), the perfect gas reaction rates of Caughlan & Fowler (1988), and the neutrino rates calculated by Itoh et al. (1989, 1992), one gets the curves shown in Figure 2 for different oxygen abundances. Note that although the expressions for the electron screening differ by up to a factor 2 with respect to the results of Sahrling (1994b), the corresponding change in the carbon ignition curve is only about 10% at a given temperature around $\Gamma = 180$.

Note also that the effect of the electron screening on the carbon ignition curve remains small, as expected from the value of E_e close to unity, contrarily to what has been claimed by Ichimaru & Ogata (1991). These latter calcu-

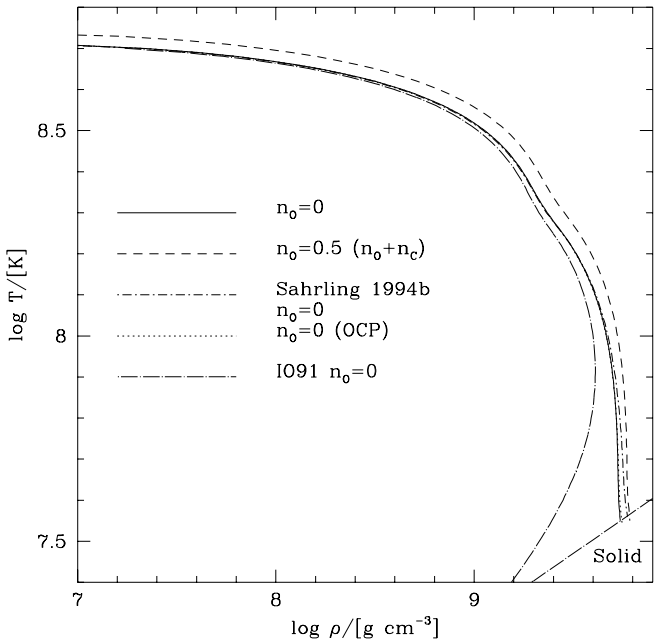

FIG. 2.—Carbon ignition curve for pure carbon and a 50% carbon-oxygen mixture. For comparison we also show the curves obtained for pure carbon by Ichimaru & Ogata (1991), Sahrling (1994b), and within the OCP (*rigid background*) approximation.

lations were based on the aforementioned erroneous electron enhancement factors. As shown in Figure 2, the full and dotted lines (pure carbon with and without polarization, respectively) are nearly superimposed. As shown by Chabrier (1993), quantum effects in the structure of the ionic stellar plasma might also affect the plasma melting curve, and thus the WD cooling and the ignition curve. Work in this direction is under progress.

4. CONCLUSIONS

We have calculated enhancement factors for nonresonant nuclear reaction rates due to polarized electrons over a wide range of temperatures and densities characteristic of dense stellar plasmas. The calculations have been conducted for large values of the electron relativistic parameter and thus are not restricted to weak screening. The analysis is based on a new set of mean (or screening) potentials calculated using standard Monte Carlo techniques and N-body theory calculations. We have focused on carbon and oxygen ions since one expects high-order quantum effects to be most important for these nuclei. The calculations can be easily applied to similar mixtures as oxygen-neon-magnesium, for example. We find that quantum high-order corrections to the classical enhancement factor will be important for low temperatures and high densities and will *reduce* the zeroth-order (classical) contribution. In an earlier work we discussed the possibility that polarized electrons would reduce the nuclear reaction. This work was based on a mean potential calculated for carbon only and just one density and temperature, so the extrapolation error was expected to be large. The present work has removed this extrapolation error and we have shown that polarized electrons yield a small ($\sim$1–2) enhancement of the nuclear reaction rate, contrary to what had been claimed in previous studies. These results have been used to derive more accurate carbon ignition curves for the ultimate stages of intermediate-mass stars and accreting white dwarfs.

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