# NUCLEAR REACTION RATES AT HIGH DENSITIES

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### ABSTRACT

In this paper we calculate general expressions which are suitable for use in numerical stellar-interior calculations for nuclear reaction rates. We consider the density-temperature combinations which are called the weak-screening, strong-screening, and pycnonuclear regimes. Except in the pycnonuclear case we express our results in the form of "correction factors" with which one multiplies the ordinary thermonuclear reaction rate evaluated at the same temperature and density. By considering the extreme cases of  $Z_1 = Z_2$  and  $Z_1 \gg Z_2$ , where  $Z_1$  and  $Z_2$  are the atomic numbers of the two reacting nuclei, we are able to devise interpolation formulae which are valid for any ratio of charges  $Z_1/Z_2$  throughout the entire weak- and strong-screening regimes. We also discuss strong-screening corrections to resonant nuclear reaction rates, and we give an explicit formula for the important special case of the triple-alpha reaction. Finally, by applying our results to the case of the proton chain, we show that the hydrogen abundance in the white dwarf Sirius B must be less than  $3.5 \times 10^{-6}$ .

#### I. INTRODUCTION

Calculations of rates for thermonuclear reactions involving two charged particles have generally been based on the assumption that the Coulomb interactions with all the other nuclei and electrons can be neglected. At sufficiently low density  $\rho$  and high temperature T this is a good approximation, since the nuclei behave as an almost perfect, classical, ionized gas, and the small corrections due to the electrostatic interaction with the background plasma can be calculated from the Debye-Hückel theory. This leads to the "weakscreening" approximation for the reaction rate. For an intermediate regime of  $\rho$  and T. most of the nuclei are bound in a Coulomb lattice structure, but the reacting pair of highenergy nuclei is still free. The electrostatic effects are then large, but can still be expressed as a multiplicative factor in the reaction rate, called the strong-screening correction factor. These two regimes have been discussed by Schatzman (1948, 1958) and by Salpeter (1954, hereafter referred to as S). At very high density and relatively low temperature, however, even the reacting nuclei are bound in the Coulomb lattice, and quite different methods must be used to evaluate the nuclear reaction rates. This "pycnonuclear" regime was first discussed by Wildhack (1940), by a series of Soviet workers (Zel'dovich 1958; Kirzhnits 1960; Abrikosov 1961; Kopyshev 1965), by Cameron (1959), and most recently by Wolf (1965) and by Van Horn (1965; hereafter referred to as V).

It is the aim of the present paper to consider the relationships among these different regimes, to discuss the pertinent physics, and to derive interpolation formulae for the nuclear reaction rates in forms suitable for use in numerical stellar-interior calculations.

In a completely general treatment of the Coulomb effects we would have to deal with eight different parameters:  $\rho$ , T, and the nuclear charges and atomic weights of each of the two reacting nuclei and of a "typical" nucleus in the medium. Even in the case of a homogeneous medium with nuclei of atomic weight A and charge Z, which is the situation we shall discuss in most detail, we are still dealing with four separate quantities; however, in the survey given in § II we shall see that to a good approximation the results can be expressed in terms of merely two dimensionless parameters. In § III we next discuss the weak- and strong-screening cases, which can be done with fairly good accuracy

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for arbitrary ratios  $Z_2/Z_1$  of the charges of the two reacting particles, and we give an interpolation formula connecting these two cases. In § IV we discuss the borderline region between the strong-screening and the pycnonuclear regimes. This is done separately for a homogeneous medium and for the other limiting case of  $Z_2 \ll Z_1$ , and an interpolation formula for general  $Z_2/Z_1$  is given which is accurate in the strong-screening regime and at least tolerable in the borderline region. The pycnonuclear regime at both zero and finite temperature is considered in § V, but only for the case of a homogeneous medium, as this limit is perhaps of less practical interest than the other regimes. In § VI we discuss resonant reactions and the somewhat special case of the triple-alpha reaction, and, finally, in § VII we give a brief summary and index the equations that contain the main results.

### II. PHYSICAL CONDITIONS IN A HOMOGENEOUS PLASMA

## a) Survey and Definition of Parameters

We consider a plasma at density  $\rho$  and temperature *T* consisting solely of electrons and of bare nuclei with charge +Ze and atomic weight *A*, using  $H = 1.66044 \times 10^{-24}$  g as the physical unit of atomic mass (so that A/Z = 2 for a C<sup>12</sup> nucleus), and let -e and *m* be, respectively, the charge and mass of an electron. In these units the number densities  $N_A$  of nuclei and  $N_e$  of electrons are given by:

$$N_A = \rho/\mu_A H; \quad \mu_A \equiv A(1 + Zm/AH),$$
  

$$N_e = \rho/\mu_e H; \quad \mu_e \equiv \mu_A/Z,$$
(1)

where  $\mu_e(\mu_A)$  is the mean molecular weight per electron (atomic nucleus).

It is convenient to measure lengths and energies in terms of the characteristic quantities  $r^*$  and  $E^*$ , defined, in analogy with the Bohr radius and (twice) the Rydberg energy, as:

$$r^{*} = \frac{\hbar^{2}}{MZ^{2}e^{2}} = \left(\frac{m}{H}\frac{1}{AZ^{2}}\right)\frac{\hbar^{2}}{me^{2}} = \frac{29.030 \text{fm}}{AZ^{2}},$$

$$E^{*} = \frac{Z^{2}e^{2}}{r^{*}} = \left(AZ^{4}\frac{H}{m}\right)\frac{me^{4}}{\hbar^{2}} = AZ^{4}k_{\text{B}}5.7562 \times 10^{8} \,^{\circ}\text{K},$$
(2)

where  $k_{\rm B}$  is Boltzmann's constant and M = AH is *twice* the reduced mass for a pair of nuclei. The density of the plasma may thus be expressed in terms of  $r^*$  and the dimensionless inverse-length parameter  $\lambda$ , which we define by:

$$\lambda \equiv r^* \left(\frac{N_A}{2}\right)^{1/3} = \frac{1}{AZ^2} \left(\frac{1}{\mu_A} \frac{\rho}{1.3574 \times 10^{11} \,\mathrm{g \, cm^{-3}}}\right)^{1/3}.$$
 (3)

As we shall see, in most cases of practical interest the Coulomb effects for the electrons are relatively weak, and throughout this paper we shall therefore consider the electrons merely as a uniform distribution of negative background charge in which the nuclei move. In contrast, the electrostatic interaction energies of the ions can in certain regimes be of sufficient magnitude to cause the nuclei to "freeze" into a Coulomb lattice structure. In analogy with the case of the hypothetical electron solid, which has been well studied in the literature of solid-state physics, we assume this lattice to be a body-centered cubic (bcc) structure, the structure having the greatest binding energy per nucleus. If  $a \equiv (N_A/2)^{-1/3}$  is the bcc lattice constant, the magnitude of the total electrostatic interaction energy per nucleus is given by (Carr 1961):

$$E_{\text{Coul}}^{(\text{bcc})} = 1.81962 \frac{Z^2 e^2}{a} = 1.81962 \lambda E^*$$
 (4)

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For some purposes, however, it is more convenient to replace the true, polyhedral lattice cell by the so-called Wigner-Seitz sphere, which is the sphere of radius  $a_s$  containing a total distributed negative charge -Ze,  $\frac{4}{3}\pi a_s^3 N_e = Z$ , plus one single ion of charge +Ze at the center. In the Wigner-Seitz approximation, the magnitude of the total Coulomb energy thus becomes:

$$E_{\text{Coul}}^{(W-S)} = \frac{9}{10} \frac{Z^2 e^2}{a_s} = \frac{9}{10} \left(\frac{8\pi}{3}\right)^{1/3} \frac{Z^2 e^2}{a} = 1.82788\lambda E^* .$$
(5)

(In the future we shall omit the superscript in referring to  $E_{\text{Coul}}^{(W-S)}$ .) This approximation is in error only by a multiplicative factor of 1.00454 for a homogeneous bcc lattice and has the advantage of being a good approximation for a mixture of isotopes (or an alloy) where the actual lattice structure is in any case not known accurately.

Within the Coulomb lattice the nuclei undergo small oscillations about their equilibrium lattice sites. The oscillation frequency is of the order of magnitude of the ionplasma frequency  $\omega_p$ , defined by

$$\hbar\omega_p = \hbar \left(4\pi \frac{2}{a^3} \frac{Z^2 e^2}{AH}\right)^{1/2} = 4 \left(\frac{\pi}{2}\right)^{1/2} \lambda^{3/2} E^* = 2.7426 \lambda^{1/2} E_{\text{Coul}} \,. \tag{6}$$

If  $\lambda$  is small, the zero-point oscillation amplitude is small at zero temperature. At finite temperature T, higher modes of oscillation of the ion lattice can be excited, and it is convenient to introduce a dimensionless parameter  $\beta$  which measures the degree of the excitation. A dimensionless parameter  $\Gamma$  comparing Coulomb and thermal energies is also useful, and we define

$$\Gamma = \frac{E_{\text{Coul}}}{0.9k_{\text{B}}T} = \frac{Z^2 e^2}{a_s k_{\text{B}}T};$$
  

$$\beta = \frac{|v_s^{(\text{rel})}(0)|}{3\pi 2^{1/3}} \left(\frac{\hbar\omega_p}{k_{\text{B}}T}\right)^{2/3} = 0.18084 \left(\frac{\hbar\omega_p}{k_{\text{B}}T}\right)^{2/3}$$

$$= 0.52972 \left(\frac{\lambda^{3/2} E^*}{k_{\text{B}}T}\right)^{2/3} = 0.032234\lambda\tau^2,$$
(7)

where  $v_s^{(rel)}(0)$  is a dimensionless number of order unity related to the screening potential at zero separation, which is defined and discussed in § IIb.

The physically interesting parameters  $\beta$  and  $\Gamma$  involve both density  $\rho$  and temperature T. It is also useful to define another dimensionless parameter  $\tau$ , which depends only on T (not on  $\rho$ ),

$$\tau^{3} = \frac{27\pi^{2}}{4} \frac{E^{*}}{k_{\rm B}T} = \frac{1}{2} A Z^{4} \frac{7.6696 \times 10^{10} \,^{\circ} \,\mathrm{K}}{T} \,. \tag{8}$$

The parameter  $\tau$  is the natural variable in the thermonuclear regime, but of course any two of the four parameters  $\lambda$ ,  $\tau$ ,  $\Gamma$ , and  $\beta$  specify the physical state of the plasma in any regime.

In all practical cases involving exothermic nuclear reactions between charged particles in stars, *both* of the following inequalities hold:

$$\tau \gg 1, \quad \lambda \ll 1. \tag{9}$$

Physically, the first inequality means that the nuclear Coulomb repulsion dominates the thermal energy and the Coulomb barrier penetration is very slow; the second inequality means that the Coulomb repulsion energy  $E_{\text{Coul}}$  is large compared with the quantum-mechanical zero-point energy  $\hbar \omega_p$ , and the zero-point vibration amplitude is small compared with the lattice spacing. The evolutionary cause of these two inequalities lies in

the fact that time scales for stellar evolution are very much longer than intrinsic nuclear reaction times: If the first (second) inequality were violated for any exoenergetic nuclear reaction at some evolutionary stage, the reaction would be proceeding at an extremely fast rate by means of thermonuclear (pycnonuclear) reactions; in reality, this reaction would already have gone to completion at an earlier evolutionary stage when the density was lower and  $\tau$  and  $\lambda^{-1}$  were large enough for the nuclear reaction rates to be slowed down to astronomical time scales. These arguments would not necessarily apply to endothermic reactions involving the most stable nuclei near Fe<sup>56</sup>. However, for these heavy nuclei the factor  $AZ^2$  in equation (3) is very large and  $\lambda$  is still quite small, even at densities as large as 10<sup>11</sup> g cm<sup>-3</sup>, beyond which inverse  $\beta$ -decays would convert these nuclei into neutron matter, anyway.



FIG. 1.—Temperature-density plane for a pure C<sup>12</sup> plasma showing the various screening regimes discussed in the text. In the hatched region the electron Fermi energy  $E_{\rm F,e}$  and  $k_{\rm B}T$  are both too small for complete ionization.

For the electrons in most stellar interiors we have quite the opposite situation, namely, that typical kinetic energies are large compared with the Coulomb interaction of an electron with the nearest nucleus. This difference is, of course, due to the large mass ratio H/m, so that the electrons can be highly degenerate and have a much larger Fermi energy than the thermal energy of the non-degenerate nuclei. In general, one can show that Coulomb effects for electrons are unimportant for a star of mass large compared with  $Za^{3/2} M_{\rm Ch}$ , where  $a \equiv e^2/\hbar c = (137.037)^{-1}$  and  $M_{\rm Ch} = (2/\mu_e)^2$  1.4587  $M \odot$  is the Chandrasekhar limiting mass. For the charges Z of the main elements undergoing nuclear reactions in a star, this inequality is well satisfied, and we therefore neglect any non-uniformity in the electron density throughout this paper.

Let us now consider the approximations which apply in the various regimes of interest. For a fixed density (and hence a fixed and small value of  $\lambda$ ) one can distinguish four main temperature regimes where the electrostatic interactions have a significant effect upon the nuclear reaction rates. These regions are indicated in Figure 1, which depicts the

log  $\rho$ -log T diagram for a plasma composed wholly of  $C^{12}$  nuclei plus electrons. At sufficiently high temperatures and low densities so that  $E_{\text{Coul}}/0.9k_{\text{B}}T = \Gamma \ll 1$  (giving  $\beta \ll \lambda^{1/3} \ll 1$ ) the nuclei form a gas and weak screening applies, as discussed in S. For  $\Gamma \gg 1$ , on the other hand, the Coulomb forces dominate, and the nuclei form a condensed phase. At sufficiently low temperatures,  $\Gamma \leq \Gamma_m \sim 50$  to 125, one has a genuine lattice with full long-range order (Brush, Sahlin, and Teller 1966; Mestel and Ruderman 1967; Van Horn 1968); but, strictly speaking, for  $1 \ll \Gamma \leq \Gamma_m$  one is dealing with a liquid. Even in the liquid phase, however, one has practically the same short-range order as in a crystalline solid, and since our nuclear reaction rates are mainly affected only by nearby nuclei, we shall assume for calculational purposes that a perfect lattice structure exists whenever  $\Gamma \gg 1$ , even if  $\Gamma/\Gamma_m$  is not large. With this approximation, the bulk of the nuclei are then bound in the lattice structure whenever  $k_{\text{B}}T \ll E_{\text{Coul}}$  (although they may possibly be in highly excited vibrational levels with energies greatly exceeding the zeropoint energy  $\sim \hbar \omega_p$ ).

When the temperature of the Coulomb lattice is still sufficiently high, the energy of the Gamow peak  $E_{\rm pk} \sim \tau k_{\rm B}T$  for the reacting nuclei is much larger than typical thermal energies. In this case  $E_{\rm pk}/E_{\rm Coul} \sim \tau/\Gamma \sim \beta^{-1}$ , so that for  $\beta \ll 1$  the main contribution to the reaction rate comes from nuclei which have sufficient energy still to move relatively freely through the lattice. This is the so-called strong-screening regime. For somewhat lower temperatures, such that  $\beta \gg 1$ , almost all the nuclei are in the vibrational ground state, and even the reacting nuclei are now bound (but not necessarily in the ground state). In this pycnonuclear regime we shall find that, if  $1 \ll \beta^{3/2} \ll \ln \lambda^{-1}$ , the typical reacting nuclei are bound but in highly excited vibrational levels; we shall refer to this as the "T > 0 pycnonuclear" case. These inequalities can be satisfied only for a very narrow range of temperatures, however, and for  $\beta^{3/2} \gg \ln \lambda^{-1} \gg 1$  we finally have the zero-temperature pycnonuclear regime, in which even the reacting nuclei are in the vibrational ground state and in which the nuclear reaction rate becomes dependent only on the density and independent of T.

## b) Approximations for the Screening Potential

Let r be the vector separation between two given nuclei, and let R be the coordinate of their center of mass. If we neglect the interactions with other nuclei and electrons (which is valid in the extreme high-temperature [thermonuclear] limit where  $\Gamma \rightarrow 0$ ), we have only the long-range, repulsive, Coulomb potential  $Z^2 e^2/r$  acting between the two nuclei. For non-zero values of  $\Gamma$ , however, it is necessary also to take into account the interactions with the other particles, and the effective interaction potential for the given pair of nuclei, therefore, also includes a "screening potential" term  $V_s(r)$  arising from the shielding effect of the rest of the plasma. In principle this potential should be evaluated by regarding r as fixed and carrying out a statistical ensemble average over **R** and over the coordinates of the remaining particles. In the weak-screening regime where  $\Gamma \ll 1$ , just such a "potential of mean force" can be evaluated by using the Debye-Hückel approximation that is applicable here, and there are no difficulties in this limit. Even in the intermediate case of the strong-screening regime, where  $\Gamma \gg 1$  but  $\beta \ll 1$ , little ambiguity arises, since the two reacting nuclei are unbound and the classical turning point is reached only for separations r much less than the lattice spacing a. Thus  $V_{s}(r)$  can be assumed spherically symmetric in the region of interest and can be evaluated by straightforward and simple arguments in this regime, also. The determination of the potential in these two regimes is discussed in S and will not be considered further here.

When  $\Gamma \gg 1$  and  $\beta \gg 1$ , however (i.e., in the pycnonuclear regime), the coupling of the motions of the different particles is so strong that no independent-particle model is an adequate approximation, the ensemble average cannot be carried out, and *no* simple

approximation for the potential is fully justified. In this case, two alternative prescriptions seem plausible for replacing the many-body problem by an effective potential  $V_s(r)$ : (1) The "fully relaxed" approximation, in which we regard r as fixed and allow the remaining lattice points to polarize into the fully relaxed positions appropriate to the given value of r. This prescription overestimates the magnitude of  $V_s$ . (2) The "static lattice" approximation, in which all other nuclei plus the center of mass of the reacting pair are considered "frozen" at their respective equilibrium positions. This prescription underestimates the magnitude of  $V_s$ . The difference between these two prescriptions thus gives a measure of the present uncertainty in these pycnonuclear calculations (see the end of §§ IV and V). In this paper, however, we shall use mainly the fully relaxed prescription, since it is the one that applies in the strong-screening regime and is thus of the most practical interest.

The screening potential can be evaluated in cases where  $\Gamma \gg 1$  in the following way: The exact expression for the potential is given in a useful form (involving a sixfold sum over the displacements from equilibrium of all of the nuclei in the lattice) by Carr (1961). In the static approximation, as shown in V, this expression reduces simply to a triple "lattice sum" parametrized by r. For  $|r_{12} - r|/r_{12} \ll 1$ , where  $r_{12}$  is the vector separation between nearest-neighbor equilibrium lattice sites, the lattice sums can in fact be evaluated analytically, and the total potential for the relative motion of the two nuclei reduces to the anisotropic harmonic oscillator potential

$$u^{-1} + v_s \approx 2.8642(u_{12} - u_z)^2 + 1.7095(u_x^2 + u_y^2), \qquad (10)$$

where we have subtracted off the (constant) value of the potential at the equilibrium position. In this equation  $v_s$  is the screening potential  $V_s(r)$  expressed in units of  $\lambda E^*$ , u is the vector separation r expressed in units of a, with  $u_z$  parallel to  $r_{12}$  and with  $u_x$ ,  $u_y$  perpendicular to it, and  $u_{12} = 0.8660 r_{12}/r_{12}$  is the vector separation between nearest-neighbor equilibrium sites expressed in units of a. The energy-level spacings which result from this potential are  $\hbar\omega_z = 0.6752\hbar\omega_p$  for vibrations in the z-direction and  $\hbar\omega_{x,y} = 0.5216\hbar\omega_p$  for vibrations in the x- or y-direction.

For values of  $|r_{12} - r|$  which are not small compared with  $r_{12}$ , we have evaluated the lattice sums numerically (still in the static approximation) for a number of values of  $u_z$  with  $u_x = u_y = 0$ . The results depend only on the parameter  $\eta \equiv u_z/u_{12} = 1.1547u_z$  and can be approximated with an absolute error less than  $\pm 0.0002$  for all  $\eta$  between 0 and 1 by the simple polynomial

$$v_{s}^{(\text{stat})}(\eta) = -1.1547 - 1.1602(1-\eta) + 1.0394(1-\eta)^{2} - 0.4001(1-\eta)^{3} + 0.0692(1-\eta)^{4}.$$
(11)

In principle, the first three terms in this expression could have been chosen to agree with the oscillator potential in equation (10), and the last two coefficients could have been obtained by requiring the correct difference in Coulomb energies between "initial" and "final" configurations,  $v_s^{(\text{stat})}(0) = -1.6064$ , plus the absence of a term linear in  $\eta$ (symmetry of  $v_s$  about  $\eta = 0$ ). In practice, however, we chose very slightly different values for the coefficients in equation (11) which provided a somewhat better approximation for intermediate values of  $\eta$ . The form of the total potential function over the entire range of separations in this static-lattice approximation is shown schematically in Figure 2.

In a later section we shall also need the derivatives of the screening potential; these were calculated in exactly the same way as equation (11), although to lesser absolute accuracy, and are given by:

$$\frac{\partial v_s^{(\text{stat})}}{\partial u_z} = -1.3333\eta^{-2} + 5.3333(1+\eta)^{-2} - 5.148(1-\eta) + 8.7676(1-\eta)^2 - 20.6702(1-\eta)^3 + 19.5412(1-\eta)^4 - 9.4842(1-\eta)^5; \qquad (12) \left(\frac{\partial^2}{\partial u_x^2} + \frac{\partial^2}{\partial u_y^2}\right) v_s^{(\text{stat})} = -1.5396\eta^{-3} + 4.1888 + 6.1584(1+\eta)^{-3} + 0.9398(1-\eta) - 6.3698(1-\eta)^2 + 9.9108(1-\eta)^3 - 8.9930(1-\eta)^4.$$

In the fully relaxed approximation, an accurate calculation of the lattice sums would be very involved, but fortunately a fairly good approximation can be obtained easily as follows. For  $\eta \sim 1$ , all of the nuclei are very close to their equilibrium lattice sites, and one would expect little difference between the static and relaxed approximations. We therefore assume that the first three terms in a five-term polynomial expression for the relaxed screening potential  $v_s^{(rel)}$  are the same as those in equation (11), since the coefficients of these terms are the ones which are determined by conditions near  $\eta = 1$ . The two remaining coefficients are then determined by the symmetry condition which still applies at  $\eta = 0$ , and by the difference in Coulomb energies between  $\eta = 1$  and  $\eta = 0$ . This can be calculated approximately by the Wigner-Seitz method discussed in S: As remarked before, the Wigner-Seitz approximation to the Coulomb energy  $E_{\text{Coul}}$  per lattice cell—equation (5) for a spherical "cell"—is extremely close to the correct value for an



FIG. 2.—Schematic diagram showing the relation of the screened potential to the pure Coulomb potential. The screening potential  $V_s(r)$  and the total energy E are also shown, and the effect of screening in reducing the width of the potential barrier is apparent.

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actual lattice structure. Thus the total electrostatic energy for the two unperturbed lattice cells  $(\eta = 1)$  is accurately given by  $-2E_{\text{Coul}}$ . On the other hand, when the two nuclei are close together  $(\eta = 0)$ , the lattice cell surrounding the nuclear pair in the fully relaxed case must also possess a high degree of symmetry and can therefore be approximated by a Wigner-Seitz sphere of radius  $2^{1/3}a_s$ , as discussed in S. The total electrostatic energy of this cell of charge 2Z is then  $-2^{5/3}E_{\text{Coul}}$ , so that the energy difference between "initial" and "final" configurations for the fully relaxed case is, in units of  $\lambda E^*$ ,

$$-v_0 \equiv v_s^{(rel)}(0) = -\frac{9}{10} \left(\frac{8\pi}{3}\right)^{1/3} (2^{5/3} - 2) = -2.1474.$$
(13)

In analogy with equation (11), we then have

$$v_{\bullet}^{(rel)}(\eta) = -1.1547 - 1.1602(1 - \eta) + 1.0394(1 - \eta)^{2} - 2.5690(1 - \eta)^{3} + 1.6971(1 - \eta)^{4}.$$
(14)

#### III. WEAK AND STRONG SCREENING

#### a) General Considerations

In this section we shall consider the case of a pair of interacting nuclei with charges  $Z_1 \ge Z_2$  and atomic weights  $A_1$ ,  $A_2$  immersed in a background-plasma mixture that contains  $X_i$  grams of species *i* (nucleus of atomic weight  $A_i$  plus  $Z_i$  electrons) per gram of material. The number densities of ions and electrons are then given in terms of the mass density by equation (1), but with the mean molecular weights now defined by:

$$\frac{1}{\mu_A} \equiv \sum_i X_i \frac{1}{A_i} / \left( 1 + \frac{Z_i}{A_i} \frac{m}{H} \right);$$

$$\frac{1}{\mu_a} \equiv \sum_i X_i \frac{Z_i}{A_i} / \left( 1 + \frac{Z_i}{A_i} \frac{m}{H} \right).$$
(15)

The ratio  $\mu_A/\mu_e \equiv \langle Z \rangle$  thus defines the mean atomic charge of the nuclei in the plasma. We generalize the definitions of the various characteristic parameters introduced in the previous section, essentially by the replacement of A by  $2A_1A_2/(A_1 + A_2)$  and of  $Z^2$  by the product  $Z_1Z_2$  in equations (2), (3), and (8) and in the definition of  $\Gamma$ . Our generalized parameters then become

$$r^{*} = \frac{A_{1} + A_{2}}{2A_{1}A_{2}Z_{1}Z_{2}} \frac{\hbar^{2}}{\mathrm{H}e^{2}}, \quad E^{*} = \frac{Z_{1}Z_{2}e^{2}}{r^{*}},$$

$$\lambda = r^{*} \left(\frac{N_{e}}{2Z_{1}}\right)^{1/3} = \frac{A_{1} + A_{2}}{2A_{1}A_{2}Z_{1}Z_{2}} \left(\frac{1}{Z_{1}\mu_{e}} \frac{\rho}{1.3574 \times 10^{11} \mathrm{ g \ cm^{-3}}}\right)^{1/3},$$

$$\tau^{3} = \frac{27\pi^{2}}{4} \frac{E^{*}}{k_{B}T} = \frac{A_{1}A_{2}Z_{1}^{2}Z_{2}^{2}}{A_{1} + A_{2}} \frac{7.6696 \times 10^{10} \,^{\circ} \mathrm{K}}{T}, \quad (16)$$

$$\Gamma_{\epsilon} = \frac{Z^{2}e^{2}}{a_{e}k_{B}T} = Z^{5/3} \frac{e^{2}}{k_{B}T} \left(\frac{4\pi}{3} N_{e}\right)^{1/3},$$

$$= Z^{5/3} \frac{5.7562 \times 10^{8} \,^{\circ} \mathrm{K}}{T} \left(\frac{1}{\mu_{e}} \frac{\rho}{6203 \times 10^{10} \mathrm{ g \ cm^{-3}}}\right)^{1/3},$$

where we have introduced in the definition of  $\Gamma$  the explicit dependence upon the charge Z contained in a Wigner-Seitz sphere. In these units we have  $E \ll 1$  for all cases of interest, the "classical turning-point"  $r_{\rm tp}$  is always close to its value  $E^{-1}$  for a pure Coulomb potential, and we have the double inequality  $r_n \ll r_{\rm tp} \gg 1$ , where  $r_n$  is the so-called nuclear interaction radius.

In the present section we shall evaluate (as in S) a simple correction factor with which one multiplies the ordinary thermonuclear reaction rate to take account of the electrostatic screening of the nuclear Coulomb **po**tential. This reaction probability (per second) is the product of (i) the probability of the two nuclei penetrating through the potential barrier to the nuclear radius  $r_n$  (ii) the nuclear "cross-section factor" S(E), defined by Burbidge *et al.* (1957), which gives the probability that penetration to  $r_n$  actually leads to the desired exothermic nuclear reaction, and (*iii*) a statistical-mechanics weight factor which gives the probability for the two nuclei to approach each other with energy between E and E + dE and which is directly proportional to the Boltzmann factor,  $\exp(-E/k_{\rm B}T) = \exp(-4\tau^3 E/27\pi^2)$ , and inversely proportional to the partition function.

The barrier-penetration probability (i) is given by the square of the wave function evaluated at the nuclear radius, which can be derived from the WKB approximation (see § VI of Van Horn and Salpeter 1967, hereafter referred to as VS). This approximation gives the wave function at the nuclear radius,  $\psi(r_n)$ , (asymptotically a plane wave of unit amplitude and energy E) in the form of multiplying factors (which depend on the angular-momentum quantum numbers l, m, as well as  $r_n$  and E) times a simple and dominant exponential factor:

$$|\psi(r_n)|^2 \propto \exp\left\{4r_n^{1/2} - 2\int_0^{r_{\rm tp}} \sqrt{[r^{-1} + V_s(r) - E]}dr\right\},$$
 (17)

where  $V_s(r)$  is the effective screening potential and  $r_{tp}$  is the turning radius, at which the integrand vanishes. The strongly energy-sensitive part of the nuclear-reaction-rate integral thus becomes

$$\int_{0}^{\infty} dES(E)e^{-g(E)}; \quad g(E) \equiv 2\int_{0}^{r_{\rm tp}} \sqrt{[r^{-1} + V_s(r) - E]}dr + \frac{4}{27\pi^2}\tau^3 E, \quad (18)$$

where we have included the Boltzmann factor.

In all practical cases the wave function at the nuclear surface is very small, and the integral in equation (17) is correspondingly very large. Since also  $\tau \gg 1$ , the factor exp [-g(E)] thus has a sharp maximum at the energy  $E_{pk}$  (the Gamow peak) where g(E) is a minimum. In many cases the nuclear cross-section factor S(E) varies slowly enough with energy so that one can use the non-resonant approximation for the reaction rate integral:

$$\int_{0}^{\infty} dES(E) e^{-g(E)} \approx (\pi/2g''_{\rm pk}) S(E_{\rm pk}) e^{-g(E_{\rm pk})} , \qquad (19)$$

where  $g''_{pk}$  is the second derivative of g(E) at  $E = E_{pk}$ . For a pure Coulomb potential  $(V_s = 0)$  one thus finds explicitly

$$2\int_{0}^{\tau_{\rm tp}} \sqrt{\left(\frac{1}{r} - E\right)} \, dr = \frac{\pi}{E^{1/2}}; \quad E_{\rm pk} = \left(\frac{2}{3\pi\tau}\right)^2 E^* = \frac{1}{3}\tau k_{\rm B}T; \quad g(E_{\rm pk}) = \tau.$$
(20)

In some cases, however, S(E) has a large and sharp maximum at a resonance energy  $E_r$ . In such cases one evaluates an additional "resonant reaction rate," for which the dominant exponential factor is exp  $[-g(E_r)]$ . This factor is negligibly small unless  $E_r$  is

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within a factor of 2 or 3 of  $E_{pk}$ , and we shall therefore assume that  $E_r$  and  $E_{pk}$  are of the same order of magnitude. Except in § VI, however, we shall deal exclusively with the non-resonant case throughout this paper.

### b) Screening Correction Factors

We summarize first the case of weak screening, where  $\Gamma_{Z1} \ll 1$  so that the Coulomb interaction energy, even for the larger of the charges  $Z_1$ , is small compared with thermal energies. In this case *all* ions are free and carry Debye-Hückel screening charge clouds which freely interpenetrate. The effect of the plasma is then to introduce an additional "potential of mean force"  $k_{\rm B}TU_w(r)$  between the reacting nuclei, where  $U_w \to 0$  for  $r \gg \lambda_{\rm D}$  and  $U_w^{(r)} \to U_w(0) \equiv U_w$  for  $r \ll \lambda_{\rm D}$ , and where  $\lambda_{\rm D} = [k_{\rm B}T/4\pi e^2 N_e(1 + \langle Z \rangle)]^{1/2}$ is the Debye screening length. As is clear from the preceding discussions, we are mainly concerned with radii of the order of  $r_{\rm tp}$  in calculating the reaction-rate integral. Since  $\lambda_{\rm D} \sim a_s \Gamma_{Z1}^{-1/2} \gg a_s \gg r_{\rm tp}$ , however, we have  $U_w(r) \approx U_w(0) \equiv U_w$  for all relevant energies, and the whole effect of the weak screening is simply to multiply the thermonuclear reaction rate by exp  $U_w$ . As shown in S the multiplicative weak-screening correction factor exp  $U_w$  for the most general chemical composition is given by:

$$U_{w} = \sqrt{3} \frac{Z_{2}}{Z_{1}} \left(\frac{\mu_{e}}{Z_{1}}\right)^{1/2} \zeta \Gamma_{Z1}^{3/2} ,$$

$$\zeta^{2} \equiv \sum_{i} X_{i} \frac{Z_{i}^{2}}{A_{i}} / \left(1 + \frac{Z_{i}}{A_{i}} \frac{m}{H}\right) + \frac{f'}{f} \frac{1}{\mu_{e}} ,$$
(21)

where f'/f is the logarithmic derivative of the Fermi-Dirac distribution function f with respect to its argument and is unity for non-degenerate and zero for fully degenerate electrons.

We consider next the strong-screening regime where  $\Gamma_{Z_1} \gg 1$  so that most nuclei are bound, but where also  $\Gamma_{Z_1}Z_2/Z_1 \ll \tau$  (i.e.,  $E_{pk} \gg E_{Coul}$ ) so that the reacting nuclear pair is unbound. Because of the second inequality, we again have  $r_{tp} \ll a_s$ , and the screening potential  $V_s(r)$  can again be replaced by  $V_s(0)$  for energies of the order of  $E_{pk}$ . The main effect is then a multiplying factor exp  $[-V_s(0)/k_BT]$ , which is simply the Boltzmann factor for the Coulomb energy difference between the "initial" and "final" configurations. For the case of the homogeneous lattice discussed in § II, this factor becomes simply exp  $(v_0\Gamma_Z/2.0310) \equiv \exp(\beta\tau)$ , where  $\beta$  is given by equation (7) for a homogeneous lattice. Since the Wigner-Seitz approximation does not depend on the actual lattice structure, however, we may immediately write this factor in a form appropriate for arbitrary values of the charges  $Z_1$ ,  $Z_2$ . From equations (5) and (16) we have, as shown in S,

$$- V_{s}(0)/k_{\rm B}T \equiv U_{s_0} = 0.9(\Gamma_{Z1+Z2} - \Gamma_{Z1} - \Gamma_{Z2}) = \beta\tau , \qquad (22)$$

where we have redefined the parameter  $\beta$  for the general case as:

$$\beta \equiv \frac{U_{s_0}}{\tau}$$

$$= \frac{\left[(Z_1 + Z_2)^{5/3} - Z_1^{5/3} - Z_2^{5/3}\right]}{\left[Z_1^2 Z_2^2 A_1 A_2 / (A_1 + A_2)\right]^{1/3}} \left(\frac{4.2579 \times 10^7 \,^\circ \text{K}}{T}\right) \left(\frac{\rho/\mu_e}{1.6203 \times 10^{10} \,\text{g cm}^{-3}}\right)^{1/3}.$$
(23)

In addition to the factor exp  $U_{s_0}$ , which gives the correction due to the difference in Coulomb energies, in the strong-screening regime we must also take into account the difference in the partition functions between the initial and final configurations, which we do in the following approximate way. For small displacements  $xa_s$  of a nucleus from

the center of its Wigner-Seitz sphere, the potential can be approximated by the harmonic oscillator potential  $\frac{1}{2}Z^2e^2x^2/a_s$ , and the partition function for the sphere is then (relative to the partition function for a perfect gas)

$$\int_{0}^{1} 3x^{2} dx \exp\left(-\frac{1}{2}\Gamma_{Z}x^{2}\right) \approx \left[1 + \frac{3}{10}\Gamma_{Z} + \frac{1}{3}\left(\frac{2}{\pi}\right)^{1/2}\Gamma_{Z}^{3/2}\right]^{-1}, \quad (24)$$

where the latter approximation is entirely adequate for our purposes. With this approximation for the two initial spheres and one final sphere, our prescription for the complete strong-screening correction factor  $e^{U_*}$  is then given by:

$$U_{s} = U_{s_{0}} + U_{s_{1}}$$

$$\exp U_{s_{1}} \equiv \frac{(1 + 0.3\Gamma_{Z_{1}+Z_{2}} + 0.266\Gamma^{3/2}_{Z_{1}+Z_{2}})}{(1 + 0.3\Gamma_{Z_{1}} + 0.266\Gamma_{Z_{1}}^{3/2})(1 + 0.3\Gamma_{Z_{2}} + 0.266\Gamma_{Z_{2}}^{3/2})},$$
(25)

which includes the logarithmic correction factor  $U_{s_1}$  in addition to the dominant term  $U_{s_0}$  originally derived by Salpeter (1954).

For the special case of  $Z_1 \gg Z_2$  and abundances  $X_1 \ll X_2$ , the screening factor has been evaluated in S also for intermediate values of  $\Gamma_{Z_1}$  and agrees fairly well with the simple interpolation formula  $e^{U_{sw}}$ , where

$$U_{sw} \equiv U_s U_w / \sqrt{(U_s^2 + U_w^2)} .$$
 (26)

For cases with  $Z_1 \sim Z_2$  as well as  $\Gamma_{Z_1} \sim 1$  no accurate expressions exist at the moment, but we shall use equation (26) throughout the weak- and strong-screening regimes for all values of  $Z_1$  and  $Z_2$ ; the uncertainty in  $U_{sw}$  is probably  $\sim \pm 30$  per cent when  $U_s \sim U_w \sim 1$ . In the typical strong-screening case, where the double inequality  $1 \ll U_s \ll \tau$  holds,  $U_{sw}$  is very close to  $U_s$  and probably uncertain by less than 5 per cent.

## IV. PYCNONUCLEAR CORRECTIONS TO STRONG SCREENING

In the strong-screening regime the dominant thermonuclear factor  $e^{-\tau}$  in the reaction rate formula is replaced by exp  $(-\tau + U_{s_0}) = \exp [-\tau(1-\beta)]$ . As we have seen, the derivation of this result is based on the assumption that  $\beta \ll 1$ . In § V we shall discuss the typical pycnonuclear cases with  $\beta \gg 1$ , but in the present section we derive a polynomial in  $\beta$  which multiplies  $\tau$  in the exponential factor to give approximately the correct reaction rate when  $\beta \leq 1$  (but not necessarily  $\beta \ll 1$ ).

We consider first the case of a homogeneous lattice, for which equation (23) becomes  $\beta = \tau^2 \lambda |v_s^{(rel)}(0)| \times 4/27\pi^2$ . As discussed earlier, we shall use only the fully relaxed approximation for the screening potential  $V_s(r)$ ; i.e.,  $V_s = \lambda E^* v_s^{(rel)}(\eta = r/r_{12})$ , with  $v_s^{(rel)}$  given by equation (14). In this case, the WKB integral in equation (17) becomes:

$$2\int_{0}^{r_{\rm tp}} \sqrt{[r^{-1} + V_s(r) - E]} dr = \sqrt{3\lambda^{-1/2}} \int_{0}^{\eta_{\rm tp}} \sqrt{[1.1547\eta^{-1} + v_s(\eta) - \epsilon]} d\eta$$
  
$$\equiv \lambda^{-1/2} J(\epsilon) , \qquad (27)$$

where  $\eta_{\rm tp} \equiv r_{\rm tp}/r_{12}$ , and equation (18) can be rewritten as

$$\frac{1}{\tau} g(\lambda E^* \epsilon) = \frac{1}{(\tau^2 \lambda)^{1/2}} J(\epsilon) + \left(\frac{4}{27\pi^2} \tau^2 \lambda\right) \epsilon , \qquad (28)$$

so that g depends only on the parameter  $\epsilon \equiv E/\lambda E^*$  and on the combination  $\tau^2 \lambda \propto \beta$  (not on  $\tau$  and  $\lambda$  separately). The integral  $J(\epsilon)$  depends only on the dimensionless quan-

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tity  $\epsilon$ , and we have evaluated this integral as well as  $dJ/d\epsilon$  for a number of different values of  $\epsilon$ , with the results listed in Table 1. For each of several different values of  $\beta$ , we then found the value  $\epsilon_{pk}$  of  $\epsilon$  at which  $dg/d\epsilon$  vanishes and evaluated the minimum value  $g(E_{pk})/\tau$  for each  $\beta$ . We shall present below an approximate interpolation formula for this tabular function of  $\beta$ , but for illustrative purposes we discuss first an analytical limit for  $\beta \ll 1$ .

For  $\eta \ll 1$ , the function  $v_s(\eta)$  can be approximated by  $[v_s(0) + b\eta^2]$ , with b a positive

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BARRIER PENETRATION INTEGRALS  $J(\epsilon)$  FOR EQUAL CHARGES  $Z_1 = Z_2$  OF REACTING NUCLEI IN STATIC AND RELAXED APPROXIMATIONS, AND FOR  $Z_1 = \langle Z \rangle \gg Z_2$ 

	$Z_1 = Z_2$				Z1=	$Z_1 = Z_2$	
E	Static	Relaxed	$Z_1 \gg Z_2$	E	Static	Relaxed	$Z_1 \gg Z_2$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2 6436 2 6390 2 6258  2 5946  2 5094  2 3340 	2 5224 2 5176 2 5034  2 4698  2 3784  2 1962 	 1.9506  1.9472 1.9428  1.9344 1.9258 1.9146 1.8940  1.8732 1.8462  1.7982	$\begin{array}{c} 0 \ 4307 \\ 0 \ 5 \dots \\ 0 \ 6091 \\ 0 \ 7 \dots \\ 0 \ 9 \ \dots \\ 1 \ 0 \\ 1 \ 1 \\ 1 \ 5 \ \dots \\ 2 \ 2 \ \dots \\ 3 \ 3 \ \dots \\ 5 \ 0 \ \dots \\ 7 \ 5 \\ 10 \ 0 \ \dots \\ 15 \ 0 \ \dots \\ 20 \ 0 \\ 30 \ 0 \end{array}$	$\begin{array}{c} & \ddots & \ddots \\ & 2 & 2022 \\ & \ddots & \ddots \\ & 2 & 0944 \\ & 2 & 0028 \\ & 1 & 9778 \\ & 1 & 9234 \\ & 1 & 7906 \\ & 1 & 6142 \\ & 1 & 4198 \\ & 1 & 2228 \\ & 1 & 0412 \\ & 0 & 9222 \\ & 0 & 7710 \\ & 0 & 6758 \\ & 0 & 5588 \end{array}$	2 0.60 1 9636 1 8786 1 8786 1 8410 1 8060 1 6868 1 5298 1 3570 1 1798 1 0134 0 9024 0 7590 0 6678 0 5542	1 7492  1 6836 

constant. If  $b/[\epsilon - v_s(0)]^3 \ll 1$ , the integrand in equation (27) can be linearized in b, and the integral evaluated to give

$$J(\epsilon) \approx \frac{\pi}{\sqrt{[\epsilon - v_s(0)]}} \left\{ 1 + \frac{5}{12} \frac{b}{[\epsilon - v_s(0)]^3} \right\}, \tag{29}$$

accurate to first order in  $b/[\epsilon - v_s(0)]^3$ . Using this expression and equation (28), together with the definition of  $\beta$ , we find for  $\beta \ll 1$ 

$$\epsilon_{\rm pk} \approx |v_s(0)| \left(\frac{1}{3\beta} - 1\right), \quad \frac{1}{\tau} g(\epsilon_{\rm pk}) \approx 1 - \beta + \frac{15}{2} \frac{b}{|v_s(0)|^3} \beta^3. \tag{30}$$

With b and  $v_s(0)$  of order unity, the error in this expansion for  $g(\epsilon_{pk})/\tau$  is only of order  $\beta^6$ . The first term represents the ordinary thermonuclear rate, the term  $-\beta$  is the strong-screening factor, and the term in  $\beta^3$  is a new correction.

As a generalization of equation (30) we have fitted a ratio of polynomials with two adjustable parameters to some of our numerical evaluations of  $g(\epsilon_{pk})/\tau$  as a function of  $\beta$ . Our proposed generalization of equation (22) for the homogeneous case is then to replace  $U_{s_0} = \beta \tau$  by  $U_{sp}$  for values of  $\beta$  up to about 0.6, where

$$U_{sp} \equiv \tau - g(\epsilon_{pk}) \approx \tau \left(\beta - \frac{2.15\beta^3 + 47.8\beta^9}{1 + 17.1\beta^3}\right).$$
 (31)

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The purely numerical error in this polynomial fit to our numerical values for  $(\tau - g)$  is about 1 per cent or less for all  $\beta \leq 0.6$ . The uncertainty in  $(\tau - g)$  due to having used the fully relaxed potential in the evaluation of  $J(\epsilon)$ , however, is considerably greater, as can be seen by comparing the static and relaxed cases in Table 1. For this reason the polynomial in equation (31) could be in error by 20 per cent or so at the largest values of  $\beta$  for which this equation is applicable, compared with only about 5 per cent for  $\beta$ itself.

In equation (31) the pychonuclear correction term in  $U_{sp}$  was derived only for the special case of equal charges of the reacting nuclei  $(Z_2 = Z_1)$ . In the opposite limiting case where  $Z_2/Z_1 \ll 1$ , one can also carry out an explicit calculation quite simply. To first order in  $Z_2/Z_1$  we need consider only the interaction of the smaller point-charge  $Z_2$  with the larger point-charge  $Z_1$  and its Wigner-Seitz sphere (the rearrangement energy of the background charge of the smaller sphere is only of order  $Z_2^{5/3}$ ). We then get for the screening potential in either the fully relaxed or the frozen approximation

$$V_s(r) = \frac{Z_1 Z_2 e^2}{a_s} \left[ -\frac{3}{2} + \frac{1}{2} \left( \frac{r}{a_s} \right)^2 \right], \tag{32}$$

where  $a_s \propto Z_1^{5/3}$  is the radius of the larger Wigner-Seitz sphere. With this potential  $J(\epsilon)$ ,  $\epsilon_{\rm pk}$ , and  $g(\epsilon_{\rm pk})$  were evaluated numerically for a number of values of  $\epsilon$  and  $\beta$  with the results given in the third column of Table 1, and a good polynomial fit, analogous to equation (31), to the resulting values of  $(\tau - g)$  was found to be

$$U_{sp} \approx \tau \left(\beta - \frac{0.84\beta^3}{1 + 1.45\beta^3}\right),\tag{33}$$

for values of  $\beta$  up to about 0.5.

We do not have any explicit calculations for intermediate values of  $Z_2/Z_1$ , but we shall adopt the following interpolation formula between equations (31) and (33). For any  $Z_2 \leq Z_1$ , and  $\beta \leq 0.5$ , we take

$$U_{sp} = \tau \left[ \beta - \frac{(0.84Z_1 + 3.46Z_2)\beta^3 + 95.6Z_2\beta^9}{(Z_1 + Z_2) + (1.45Z_1 + 32.8Z_2)\beta^3} \right].$$
 (34)

While this prescription is somewhat ad hoc, it is a simple formula, and the ratio of polynomials is unlikely to be in error by as much as a factor of 2 even for intermediate values of  $Z_2/Z_1$ . This expression used in place of  $U_{s_0}$  in equations (25) and (26) thus leads to a single formula for the screening correction for all values of  $\beta$  up to about 0.5.

#### V. PYCNONUCLEAR REACTION RATES

In this section we discuss the calculation of pycnonuclear reaction rates, i.e., cases with  $\beta \gg 1$ , but only for the simplest case of a perfectly homogeneous lattice. We explicitly neglect any effects of dislocations or other lattice defects (see § Vc, however). In the pycnonuclear regime, one cannot simply derive correction factors to the thermonuclear formulae but must calculate the rates *ab initio* as a function of the excitation energy E of the reacting pair of nuclei, which are now bound. Details of the calculation are given in V and we only summarize them here.

Since the classical turning point  $r_{tp} \gg r_n$ , where  $r_n$  is the nuclear radius, the probability per second p of a reaction between two given nuclei can, as shown in V, be written in the form

$$p = \frac{8S}{\hbar(r^*)^2} (r^*)^3 r_n^{1/2} \exp\left(-4r_n^{1/2}\right) |\psi_E(r_n)|^2, \qquad (35)$$

where S is the usual cross-section factor (Burbidge *et al.* 1957) and  $r_n$  is in units of  $r^*$ . The wave function  $\psi_E(r_n)$  in this equation is the full, *normalized* wave function for the relative motion of the two reacting nuclei in the lattice, with excitation energy E, evaluated at the nuclear radius. The general, temperature-dependent pycnonuclear reaction rate for a bcc lattice (each nucleus has eight nearest neighbors, and we neglect reactions with all other nuclei) is then given by

$$P = \frac{8}{2} \frac{\rho}{\mu_A \mathrm{H}} \langle p \rangle_{\mathrm{Av}} \text{ reactions } \mathrm{cm}^{-3} \mathrm{sec}^{-1} , \qquad (36)$$

where  $\langle p \rangle_{Av}$  denotes the thermal average of the pairwise reaction probability.

## a) Pycnonuclear Rates at Zero Temperature

We consider first the case in which the temperature is so low that even the two reacting nuclei are in the ground state, and the thermal average in equation (36) reduces simply to the ground-state term (for limits of this regime see § Vb). Since we always have  $\lambda \ll 1$ , the zero-point vibration energy  $E_0 \sim \hbar \omega_p \ll E_{\text{Coul}}$ , and each nucleus is restricted to a very small region about its equilibrium lattice position:  $r_{\text{tp}} \sim r_{12}$ . Under these conditions, the wave function at the nuclear surface can be calculated by the three-dimensional WKB approximation discussed in VS, which leads to

$$\psi_{E_0}(r_n) = 0.553\lambda^{7/8}(r^*)^{-3/2}r_n^{-1/4} \exp\left[-\frac{1}{2}\lambda^{-1/2}(J-\lambda^{1/2}K) + 2r_n^{1/2}\right].$$
(37)

The WKB integrals J and K have been calculated numerically for densities in the range  $1.7 \times 10^{-5}$  g cm<sup>-3</sup>  $\leq \rho/\mu_A A^3 Z^6 \leq 1.7 \times 10^4$  g cm<sup>-3</sup>, and the results are given (with an absolute uncertainty of  $\pm 0.004$ ) by the expressions

$$J - \lambda^{1/2} K = \begin{cases} 2.638 - 3.6\lambda^{1/2} \\ 2.516 - 3.8\lambda^{1/2} \end{cases}.$$
(38)

In both equations (38) and (39) the upper line refers to computations in which the static approximation for the potential function was used, and the lower line, to computations in which the relaxed approximation was used. With these results, the general expression for the zero-temperature pycnonuclear reaction rate becomes

$$P_{0} = \frac{\rho}{\mu_{A}} A^{2} Z^{4} S \begin{pmatrix} 3.90 \\ 4.76 \end{pmatrix} 10^{46} \lambda^{7/4}$$

$$\times \exp\left[-\lambda^{-1/2} \begin{pmatrix} 2.638 \\ 2.516 \end{pmatrix}\right] \text{ reactions } \text{cm}^{-3} \text{ sec}^{-1},$$
(39)

where  $\rho$  is in g cm<sup>-3</sup> and the cross-section factor S is in units of MeV barns. The nuclear energy generation rate in ergs g<sup>-1</sup> sec<sup>-1</sup> is obtained directly from equation (39) by multiplying by  $\frac{1}{2}(Q/\rho)$ , where Q is the energy release per reaction.

## b) Pycnonuclear Reactions at Non-Zero Temperatures

At finite temperatures, when reactions between nuclei in excited states of the lattice become important,  $(r_{12} - r_{tp})$  is no longer small compared with  $r_{12}$ , and the oscillator wave function is not a good approximation in the forbidden region (although we shall still use the oscillator potential in the allowed region). In this case, the three-dimensional WKB wave function must be used for all r, and the transition between the allowed and forbidden regions requires the use of the connection formulas given in VS. Since we are mainly interested in highly excited states of the lattice whenever the temperature dependence is important at all, we shall use a quasi-classical normalization of the WKB wave function in the allowed region, taking  $|\psi_E(r)|^2 d^3r$  as the fraction of the total

$$\begin{aligned} |\psi_{E}(r_{n})|^{2} &= \frac{16}{\pi^{1/2}} \left( \frac{\omega_{x} \omega_{y} \omega_{z}}{\omega_{p}^{3}} \right) \frac{\lambda^{5/2}}{(r^{*})^{3}} \epsilon^{-1} r_{n}^{-1/2} \exp \left[ 4r_{n}^{1/2} - \lambda^{-1/2} J(\epsilon) + K(\epsilon) \right], \\ \frac{1}{2} J(\epsilon) &= \int_{0}^{u} \sqrt[v_{p}] [v(u) - \epsilon] du, \quad \frac{1}{2} K(\epsilon) = \int_{u}^{u_{12}} H^{+} du + \frac{1}{2} \ln u, \end{aligned}$$
(40)

where the "curvature coefficient" of the WKB wave function  $H^+$  is in units of  $a^{-1}$ ,  $r_n$  is in units of  $r^*$ ,  $\epsilon = E/\lambda E^* \leq 1$  is the dimensionless energy parameter, and the oscillator frequencies  $\omega_{x,y,z}$  are defined in § IIb.

We have evaluated the WKB integrals J, K numerically over the range  $0.001 \le \epsilon \le 30$ , with the results listed in Table 1. These results were approximated by the following polynomial expressions:

$$\frac{1}{2}J_{\text{stat}} = \frac{\epsilon \ln \epsilon}{6.772} + 1.3235 - 0.3575\epsilon + 0.0225\epsilon^2, \qquad (41)$$
$$\frac{1}{2}J_{\text{rel}} = \frac{\epsilon \ln \epsilon}{6.772} + 1.2619 - 0.3809\epsilon + 0.0446\epsilon^2, \qquad \frac{1}{2}K = 0.3 \ln \epsilon - 0.2.$$

For  $\epsilon \leq 0.3$ , equation (41) represents the values of the *J*-integrals to within an absolute uncertainty of  $\pm 0.001$  and the *K*-integral to about 10 per cent accuracy for  $\epsilon < 0.9$ .

The general, temperature-dependent pycnonuclear reaction rate can now be calculated from equations (35), (36), (40), and (41). The thermal average of the reaction probability p is

$$\langle p \rangle_{A_{v}} = \Sigma_{n} \exp \left[ - (E_{n} - E_{0})/k_{B}T \right] p(E_{n})/\Pi(T) ,$$

$$\Pi(T) \equiv \Sigma_{n} \exp \left[ - (E_{n} - E_{0})/k_{B}T \right] ,$$

$$(42)$$

where  $\Pi$  is the partition function, and the sums extend over all quantum states *n* of the "relative particle." To evaluate the sums, we approximate the energy levels by the energy levels of the anisotropic harmonic oscillator (equation [10]) and (since the energy of the Gamow peak is large) the sums by integrals. We then obtain

$$\Pi^{-1} = (1 - e^{-\hbar\omega_{x}/k_{\rm B}T})(1 - e^{-\hbar\omega_{y}/k_{\rm B}T})(1 - e^{-\hbar\omega_{z}/k_{\rm B}T}),$$

$$\Sigma e^{-(E_{n}-E_{0})/k_{\rm B}T} p(E_{n}) \approx p(E_{0}) \qquad (43)$$

$$+ \frac{1}{\pi^{2}\sqrt{2}} \frac{S}{\hbar(r^{*})^{2}} \lambda e^{+E_{0}/k_{\rm B}T} \int_{0}^{\infty} \exp\left(-\epsilon \frac{\lambda E^{*}}{k_{\rm B}T} - \lambda^{-1/2}J + K\right) \epsilon d\epsilon.$$

Note that the effective level spacing for vibrations transverse to the line of centers is twice the true level spacing, since odd-parity wave functions do not contribute to the reaction rate. As in thermonuclear calculations, the integral in equation (43) can be evaluated by the saddle-point method, giving

$$\int_{0}^{\infty} \exp\left[-\epsilon \frac{\lambda E^{*}}{k_{\rm B}T} - \lambda^{-1/2}J + K\right] \epsilon d\epsilon \approx \left[\frac{2\pi\lambda^{1/2}}{J^{\prime\prime}(\epsilon_{\rm pk})}\right]^{1/2} \epsilon_{\rm pk}$$

$$\times \exp\left[-\epsilon_{\rm pk} \frac{\lambda E^{*}}{k_{\rm B}T} - \lambda^{-1/2}J(\epsilon_{\rm pk}) + K(\epsilon_{\rm pk})\right], \qquad (44)$$

$$\epsilon_{\rm pk} \approx \binom{4.141}{4.853} \exp\left(-3.386 \frac{\lambda^{3/2}E^{*}}{k_{\rm B}T}\right) = \binom{4.141}{4.853} \exp\left(-8.783\beta^{3/2}\right),$$

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where  $J''(\epsilon_{pk})$  is the second derivative of J with respect to  $\epsilon$  at  $\epsilon_{pk}$ , and the upper and lower lines in the definition of  $\epsilon_{pk}$  apply to the static and relaxed approximations, respectively. This approximation for  $\epsilon_{pk}$  is accurate to 10 per cent in the exponent over the entire range of validity of equation (41) for J, and better than that for the smaller values of  $\epsilon_{pk}$ .

With the help of equation (44), the ratio of the full, temperature-dependent pycnonuclear rate to the zero-temperature rate can be written as

$$\frac{P(T)}{P_0} - 1 = {\binom{0.0430}{0.0485}} \lambda^{-1/2} \left[ 1 + {\binom{1.2624}{2.9314}} e^{-8\ 7833\beta^{3/2}} \right]^{-1/2} \times \exp\left\{ -\ 7.272\beta^{3/2} + \lambda^{-1/2} {\binom{1.2231}{1.4331}} e^{-8\ 7833\beta^{3/2}} \left[ 1 - {\binom{0.6310}{1.4654}} e^{-8\ 7833\beta^{3/2}} \right] \right\},$$
(45)

where, as usual, the upper and lower lines refer to the static and relaxed approximations, respectively. The first term in the main exponential factor in equation (45) is just the Boltzmann factor for the contributions from the excited states (relative to the ground state). The remaining terms in the exponent represent the increase of the rate above its zero-temperature value due to the additional contributions from energies in the vicinity of  $E_{\rm pk}$ . These terms are only of order unity even when  $\lambda^{-1/2} \exp(-8.78\beta^{3/2}) \geq 1$ , i.e., when  $E_{\rm pk} \geq E_0$ , but are included here for completeness. As equation (45) clearly shows, the temperature dependence of the pycnonuclear reaction rate is important only over a rather limited range of temperatures; for  $\beta^{3/2} > (\ln \lambda^{-1/2})/8.78$ , the zero-temperature rate is entirely adequate, while for  $\beta \leq 1$ , equation (31) applies.

### c) Effects of Lattice Imperfections

The pycnonuclear rates above apply only in the limit of a perfect, crystalline lattice. In practice, any real lattice structure will possess a sizable concentration of defects, which strongly affect the actual nuclear reaction rates. We emphasize that these effects will be important *only* for the pycnonuclear regime, however. In all other cases, the reacting nuclei are not bound but can move freely through the plasma, and the reaction rates are completely unaffected by defects or impurities.

Consider first a lattice homogeneous in chemical composition but containing structural defects. In this case, the nuclear reaction rate is considerably greater than the rate given by equation (45) because roughly half of the nuclei involved in the defects are crowded into regions of increased density (or  $\lambda$ ). According to equations (39) and (45), the local rate at the defect is then increased by a factor of approximately exp (+1.3  $\lambda^{-1/2} \delta \lambda / \lambda$ ), where  $\delta \lambda$  is the local excess of the parameter  $\lambda$  above the mean. The pycnonuclear reaction rate immediately after formation of the crystal will thus be strongly time-dependent, even for a *fixed* density and temperature. Initially the rate is dominated by reactions in the defect regions (if sufficient numbers of defects exist), but as the dislocations "anneal out" due to the preferential reactions, the rate gradually decreases to the expression for a perfect lattice.

The formation of product nuclei, generated by the reaction under investigation, can have another consequence. Relaxation of the reacting particles about a newly generated product nucleus may result in an increase of 40 to 100 per cent in the local density  $(\delta\lambda/\lambda \text{ equals 0.2 to 0.5})$ , which *strongly* enhances the probability of subsequent reactions among these particles. In this case, also, our rates therefore represent a lower limit.

For very low concentrations of reacting nuclei (themselves imperfections in a lattice of non-reacting elements) we have the opposite situation, as has been discussed by Kirzhnits (1960) and by Kopyshev (1965) for the first reaction in the proton chain. Under these conditions, the proton pair has to overcome an "activation energy" W,

thermally or by barrier penetration, due to the repulsion from interposed "host nuclei," and the rate per proton pair is much lower than in a pure-hydrogen lattice.

### VI. RESONANT RATES AND THE TRIPLE-ALPHA REACTION

Throughout most of this paper we have dealt only with the case of "non-resonant" nuclear reactions. In this section we shall discuss briefly the effect of the electrostatic corrections on the contribution to the reaction rate from a sharp resonance in the compound nucleus, but only for the case of strong screening, where  $\Gamma_z > 1$  and  $\beta \leq 0.5$ . The relevant resonance energy  $E_r$  (relative to the two nuclei  $Z_1, Z_2$  at infinite separation) is comparable to the energy  $E_{\rm pk}$  of the Gamow peak in situations of interest, as discussed in § III, but of course does not depend on the temperature.

We shall distinguish two classes of resonances, depending on whether the incident reaction channel dominates or not. We consider first the most common class, where the partial width due to the incident channel is a small fraction of the total width of the resonant state in the compound nucleus because of the small probability of Coulomb barrier penetration in the incident reaction channel. In such cases, we merely have to substitute for the usual barrier-penetration integral the full expression given by equation (27) evaluated at the resonant energy and including the effect of the screening potential  $V_s(\mathbf{r})$ . Because of the different energy zero-point for  $E_r$  and for the incident energy  $\lambda E^* \epsilon$  of the "relative particle" in the plasma, we have to substitute  $\epsilon'_r = [\epsilon_r + v_s(0)] = (\epsilon_r - v_0)$  for  $\epsilon$  in equation (28), where  $\epsilon_r = E_r/\lambda E^*$ . Note that while  $E_r$  is a property solely of the compound nucleus, the parameter  $\epsilon_r$  depends also upon the density.

For a homogeneous lattice, the numerical evaluation of  $J(\epsilon)$  is given in Table 1. We have fitted a simple polynomial expression to this tabular function of  $\epsilon$  for  $\epsilon > 1$  and have used this expression to write the strong-screening effects for the resonant rate in the form of a multiplying factor exp  $(U_{sr})$  with

$$U_{sr} = U_{s_0} - \frac{\pi}{\sqrt{(\lambda\epsilon_r)}} \left[ \frac{1.22}{\epsilon_r^3} - \frac{3.1}{\epsilon_r^6} + \frac{75}{\epsilon_r^9} \right].$$
(46)

The first term,  $U_{s_0} = \beta \tau$ , defined in equation (22), comes from the change of energy zero-point and is simply the Boltzmann factor of our previous strong-screening potential; this factor is independent of the resonance energy  $E_r$ . The second term in equation (46) comes from the polynomial fit to  $J(\epsilon)$  and takes the place of the second term in equation (31) for the non-resonant rate; it depends on  $\epsilon_r$  (and thus on the density) but is independent of the temperature.

For arbitrary values of the charges  $Z_1, Z_2$  of the reacting nuclei,  $\lambda$  is given by equation (16), and  $\epsilon_r$  becomes

$$\epsilon_r = \frac{1}{Z_1 Z_2} \left( \frac{Z_1 \mu_e 1.3574 \times 10^{11} \text{ g cm}^{-3}}{\rho} \right)^{1/3} \frac{E_r}{49.600 \text{ keV}} \,. \tag{47}$$

For the special case of  $Z_1 \gg Z_2$  we have also carried out the numerical evaluation of  $J(\epsilon)$ , with the results again listed in Table 1. This case leads to an approximation like equation (46), but with the bracket replaced by  $[1.30\epsilon_r^{-3} + 28.2\epsilon_r^{-6}]$ . For any value of the two charges (but with  $Z_1 \ge Z_2$ ) we then propose the simple ad hoc generalization

$$U_{sr} = U_{s_0} - \frac{\pi}{\sqrt{(\lambda \epsilon_r)}} \left[ \frac{1.30Z_1 + 1.14Z_2}{(Z_1 + Z_2)\epsilon_r^3} + \frac{28.2Z_1 - 34.4Z_2}{(Z_1 + Z_2)\epsilon_r^6} + \frac{150Z_2}{(Z_1 + Z_2)\epsilon_r^9} \right].$$
(48)

In principle the expression  $U_{s_1}$  given by equation (25) should be added to  $U_{sr}$ , but  $U_{sr}$  is usually much the more important of the two.

If the resonance energy  $E_r$  is unusually large, or if the radiative partial widths for the outgoing channels of the resonant state are particularly small, one has the opposite

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extreme class of resonances in which most of the total width of the compound nucleus state is contributed by the incident channel. In these cases, the partial width of the ingoing channel (*including* the screening factor in the barrier penetration) drops out of the resonant rate completely upon integrating the Breit-Wigner cross-section over energy, and the second term in equation (48) must be replaced by zero. The first term, however, comes entirely from statistical mechanics (and the difference in energy zero-points discussed before) and remains. For this class of resonances, therefore,  $U_{sr}$  is simply replaced by  $U_{s_0}$  given in equation (22). Although this expression does not depend explicitly on the value of  $\epsilon_r$ , these results as well as equation (48) are valid only if  $(\epsilon_r - v_0) \gg \epsilon_0$ , since the energy of the resonant state is otherwise lower than the ground state energy  $\epsilon_0$  of the lattice. Since  $\epsilon_0 \ll v_0$ , this condition can be written approximately as

$$\epsilon_r > \frac{3.04Z_1 + 1.26Z_2}{Z_1 + Z_2} \,. \tag{49}$$

We finally turn to the triple-alpha reaction, the net effect of which is the conversion of three He<sup>4</sup> nuclei into one C<sup>12</sup> nucleus. This is accomplished in two steps: the formation of the "Be<sup>8</sup> ground state" at a resonance energy  $E_r = 94$  keV, followed by the reaction between the Be<sup>8</sup> and the third He<sup>4</sup> nucleus through a resonant state in the C<sup>12</sup> compound nucleus at energy  $E_r = 278$  keV. In *each* of these two reactions the partial width for the incident channel strongly dominates the total width (in the first reaction there is no radiative channel, and in the second the radiative widths are small and the *a*-particle width is large). The screening effects increase the ingoing widths further and merely strengthen the inequality, so that we may use equation (22) for each of the two successive reactions, as discussed in the preceding paragraph. For the total triple-alpha rate we thus obtain a multiplying correction factor exp ( $U_{s3a}$ ), where

$$U_{s3a} = 2.916\Gamma_2 - 3\ln\left(1 + 0.3\Gamma_2 + 0.266\Gamma_2^{3/2}\right) + \ln\left(1 + 1.87\Gamma_2 + 4.15\Gamma_2^{3/2}\right)$$
(50)

and  $\Gamma_2$  is the Coulomb-thermal parameter for He<sup>4</sup> nuclei, as defined by equation (16). Since inequality (49) must hold for each of the two reactions, and since this requirement is the more stringent for the first reaction, we require only  $\rho < 6.9 \times 10^9$  g cm<sup>-3</sup> for the validity of equation (50).

### VII. SUMMARY

We have discussed in this paper the changes in the rates of thermonuclear reactions in cases where the density is so high that it becomes necessary to take account of screening corrections to the Coulomb interaction potential between a pair of reacting nuclei andin the extreme case—of the zero-point energies of the nuclei. For sufficiently high temperatures and low densities such that  $E_{\text{Coul}} \ll k_{\text{B}}T$ , electrostatic corrections are quite small and the screening is "weak." In this case, the true reaction rate is simply equal to the usual thermonuclear reaction rate (calculated for the same temperature and density) multiplied by the weak-screening correction factor  $e^{U_w}$ , with  $U_w$  defined by equations (15), (16), and (21). At somewhat lower temperatures (or higher densities) where  $E_{\text{Coul}} \gg$  $k_{\rm B}T$  but where we still have  $E_{\rm pk} \gg E_{\rm Coul}$ , the electrostatic interactions are strong enough to cause the formation of a condensed phase. In this regime the reaction rate is given by the strong-screening correction factor  $e^{U_s}$  times the thermonuclear rate, where  $U_s$  is given by equations (15), (16), (22) or (23), and (25). In the intermediate cases where  $E_{\rm Coul} \sim$  $k_{\rm B}T$ , we suggest the simple interpolation formula (26) for the logarithm of the correction factor. At the other extreme limit where  $E_{\rm pk} \sim E_{\rm Coul} \gg k_{\rm B}T$ , we approach the boundary of the "pycnonuclear" regime. In this intermediate region we suggest another simple interpolation formula given by equations (23) and (34) for general values of the charges of the two reacting nuclei.

When the temperature is so low that  $E_{\rm pk} < E_{\rm Coul}$ , even the two reacting nuclei are bound in the Coulomb lattice. In this regime it is possible to distinguish two subcases, depending on whether  $E_{\rm pk}$  is large compared with  $E_0$  or not. In the former case, the temperature is so low that the energy required to penetrate the Coulomb barrier comes entirely from the zero-point motion of the nuclei in the lattice, and the reaction rate given by equations (15), (16), and (39)—becomes independent of the temperature. In the temperature range  $E_0 < E_{\rm pk} < E_{\rm Coul}$  the temperature-dependent part of the reaction rate must also be included, and this is given by equations (15), (16), (23), (39), and (45).

We have also considered the problem of calculating resonant as well as non-resonant reaction rates in the important strong-screening regime. For reactions in which the incident channel width is only a small fraction of the total width of the resonance in the compound nucleus, the resonant correction factor  $e^{U_{sr}}$  is given by equation (48), with  $\epsilon_r = E_r/\lambda E^*$  where  $E_r$  is the resonance energy. This replaces the factor  $e^{U_{so}}$  in the strongscreening correction formula. For resonances in which the incident channel dominates, however,  $U_{sr}$  reduces merely to the term  $U_{s_0}$  given by equation (22). Both of these cases are subject to the restriction expressed by equation (49). A particularly important example of the latter class of cases is the triple-alpha reaction, for which we give the explicit expression for the correction factor in equation (50).

Finally, as an example of the application of these calculations, we compute a limit for the hydrogen content of the white dwarf Sirius B. From the mass and luminosity of 1.05  $M_{\odot}$  and 2.8  $\times$  10<sup>-3</sup>  $L_{\odot}$  given by Harris, Strand, and Worley (1963) we compute the extreme lower limits of central temperature and density by assuming a composition of pure He<sup>4</sup> and using equation (7) of Van Horn (1968) and the tables of Hamada and Salpeter (1961). These values are  $\rho_c = 2.2 \times 10^7$  g cm<sup>-3</sup>,  $T_c = 8 \times 10^6$  °K, and the corresponding values of the parameters  $\tau$ ,  $\lambda$ , and  $\beta$  are  $\tau = 16.87$ ,  $\lambda = 0.0341$ ,  $\beta =$ 0.313. Under these conditions, the center of Sirius B is in the borderline region between the strong-screening and pycnonuclear regimes, the pycnonuclear correction to  $\beta$  given by equation (31) is -0.043, and the correction factor becomes  $e^{U_{sp}} = 94$ . Since the strong-screening formula for the reaction rate is affected by the hydrogen abundance only in the multiplicative factor of  $X_{\rm H}^2$  and not in the exponent, as mentioned previously, an upper limit to the mean hydrogen content of Sirius B can be evaluated simply by equating the screened thermonuclear energy generation rate to the rate necessary to support the observed luminosity. The result is  $X_{\rm H} < 3.5 \times 10^{-5}$  if the composition is mainly helium; if the star is composed primarily of heavier elements, as seems more likely, the central temperatures and densities are higher, and the upper limit on  $X_{\rm H}$  is even further decreased. We stress again that this limit is *not* dependent on the hydrogen concentration, so that the high concentrations found by Kirzhnits (1960) are not permissible.

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