The equation of state and composition of hot, dense matter in core-collapse supernovae.

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Abstract

The equation of state and composition of matter are calculated for conditions typical for pre-collapse and early collapse stages in core collapse supernovae. The composition is evaluated under the assumption of nuclear statistical equilibrium, when the matter is considered as an 'almost' ideal gas with corrections due to thermal excitations of nuclei, to free nucleon degeneracy, and to Coulomb and surface energy corrections. The account of these corrections allows us to obtain the composition for densities a bit below the nuclear matter density. Through comparisons with the equation of state (EOS) developed by Shen et al. we examine the approximation of one representative nucleus used in most of recent supernova EOS's. We find that widely distributed compositions in the nuclear chart are different, depending on the mass formula, while the thermodynamical quantities are quite close to those in the Shen's EOS.

keywords: Nuclear reactions, nucleosynthesis, abundances – Stars: neutron – supernovae: general

1 Introduction

A proper description of the equation of state (EOS) for subnuclear and supernuclear densities is of vital importance for current studies on the explosion mechanism of core-collapse supernovae (Bethe 1990; Suzuki 1994; Janka et al. 2007). The success of the prompt shock propagation in the supernova mechanism depends on the size of the homologously contracting inner part of a collapsing core. The larger is Y_{e} (the number of electrons per nucleon) at the time of bounce, the smaller part of matter will be dissociated and the stronger will be the prompt shock wave. Therefore, all factors which influence Y_{e} must be thoroughly studied.

One factor is the mass fraction of the free protons, X_{p}, in the dense matter of supernova core. Since the rate of electron capture on a free proton is much higher than that on a nucleus, free protons play an important role in establishing the value of $Y_{\rm e}$ at the neutrino trapping. The abundance of free protons depends sensitively on the nuclear models of dense matter. The variations of $X_{\rm p}$ amount to more than order of magnitude in the studies of supernova EOS so far (Cooperstein 1985; Cooperstein & Baron 1990; Hillebrandt & Wolf 1985; Hillebrandt 1991; Lattimer et al. 1985; Lattimer & Swesty 1991; Shen et al. 1998a,b) and can affect the initial strength of shock wave (Bruenn 1989a; Swesty et al. 1994; Sumiyoshi et al. 2004, 2005). As shown by Bruenn (1989a,b), the free proton fraction may be largely different depending on the nuclear interaction and its model. Another factor is the composition of various nuclei, which exist under the nuclear statistical equilibrium. The total rate of electron captures on nuclei can dominate that on free protons, if the number of the free protons is small (Hix et al. 2003), and nuclei may affect the dynamics in this way as well. Therefore, it is crucial to evaluate the composition of dense matter in a precise manner.

Another astrophysical problem, where an accurate chemical composition is important, is the nucleosynthesis of heavy elements. The studies of various models of the explosive nucleosynthesis as well as the rapid neutron capture process (see, e.g. Ptitsyn & Chechetkin 1982; Woosley & Hoffman 1992; Nadyozhin et al. 1998; Arnould et al. 2007, and references therein) require knowledge of the chemical composition close to the nuclear statistical equilibrium (NSE) as an initial condition for nuclear reaction network calculations. Neutron star mergers and collapsar models for gamma-ray bursts may contain similar conditions as well.

The thermodynamic properties of hot, dense matter have been investigated in various approaches: Saha-like equations (Mazurek et al. 1979; El Eid & Hillebrandt 1980; Murphy 1980; Ishizuka et al. 2003; Nadyozhin & Yudin 2004), Hartree-Fock approaches (Bonche & Vautherin 1981; Wolff 1983; Hillebrandt & Wolf 1985; Lassaut et al. 1987), compressible liquid-drop model (Baym et al. 1971; Lattimer et al. 1985; Lattimer & Swesty 1991), and the relativistic mean field theory (Sutaria et al. 1999) with local density approximation (Shen et al. 1998a,b). The review of those approaches, beginning from Bethe et al. (1970), can be found in the context of cold neutron star matter in Rüster et al. (2006) and Haensel et al. (2007). In most of the sets of EOS used for recent supernova simulations, the approximation of one species of nuclei (in addition to neutrons, protons and alpha particles) has been adopted (Hillebrandt & Wolf 1985; Lattimer & Swesty 1991; Shen et al. 1998b). However, the advance in recent studies of electron capture rates on nuclei for a wide mass range (Langanke & Martínez-Pinedo 2003) necessitates the evaluation of multi-composition of nuclei to determine the total electron capture rate. Although the treatment with one nuclear species should be a good approximation to derive overall thermodynamical properties of dense matter (Burrows & Lattimer 1984), it is necessary to take into account the multi-composition at high densities $\sim 10^{12}$ g/cm^3 near the neutrino trapping regime, where nuclear interaction and multi-compositional treatment may become more influential to determine the equation of state. The description of the EOS with the multi-composition is, of course, crucial to predict the abundance of nuclei and free protons, see e.g. Murphy (1980).

In spite of an extensive use of the Saha equation in the literature, not all relevant physics was included in the published work within this approach from the very beginning. For example, Murphy (1980) has not taken into account the effects of non-ideal nucleon gas. El Eid & Hillebrandt (1980) have consistently taken into account finite temperature effects in nucleon interactions following El Eid & Hilf (1977), but they have omitted the Coulomb corrections. Later Hillebrandt & Müller (1981), Bravo & García-Senz (1999) and Nadyozhin & Yudin (2005) included them in different approximations and solved the implicit set of Saha equations. Moreover, Hillebrandt & Müller (1981) have taken into account an 'excluded-volume' effect due to the finite size of nuclei. It was noted by Hillebrandt (1991) that the number of nuclear species included in the Saha treatment strongly affects the mass fraction of free protons, which may change the effective adiabatic index through electron captures.

In this paper we describe our code suitable for studying the properties of dense matter relevant to core-collapsing supernova conditions, and we put an emphasis on the composition of nuclei. Our code is originally rather old: we have compared our NSE results with the kinetic approach already in the paper (Panov et al. 2001), but the code has not been described in detail. Another motivation for our work is the availability of new mass formulae like (Koura et al. 2005) and (Möller et al. 1995) and detailed EOS tables like (Shen et al. 1998b). Our aim is to develop and to test a practical and reliable tool for predictions of NSE composition at subnuclear densities.

Following most closely the conventional Saha approach (Clifford & Tayler 1965) and the method by Mazurek et al. (1979), we extend this approach in the following points:

- We take into account, at a certain level of approximation, the influence of free nucleon gas on the surface and Coulomb energies of nuclei. We retain some terms which were omitted by Mazurek et al. (1979). However, we do not take into account the 'excluded-volume' effect, not pretending to reach very high densities.
- We have an option to include various results for nuclear partition functions like those of Fowler et al. (1978) and newer partition functions by Engelbrecht & Engelbrecht (1991) and Engelbrecht et al. (1990).
- Our network is appreciably larger than the one used previously. The atomic mass table is updated using recent theoretical compilations of atomic masses. It covers ∼20000 nuclides (Koura 2007) for the KTUY mass formula (Koura et al. 2005) and ∼9000 nuclides for the FRDM mass formula (Möller et al. 1995) as an extra option.

To examine the basic properties of the equation of state for supernovae in the current formulation, we calculate the properties of dense matter covering a wide range of density, ρ, electron fraction, $Y_{\rm e}$, and temperature, T. We report here the results at the equilibrium for the nuclear and electromagnetic processes, i.e. the NSE, for fixed values of $Y_{\rm e}$ without imposing beta equilibrium. The beta-equilibrium is easily incorporated in the Saha approach as in Mazurek et al. (1979) and El Eid & Hillebrandt (1980), and our code has such an option. A brief discussion of account of the beta equilibrium is also given below. We show the global features of the dense matter (thermodynamical quantities and compositions) for the supernova environment. In order to assess the dependence of the nuclear mass, we make the comparisons among several choices. We also examine the similarity and difference from the single nuclear species treatment by comparisons with the Shen EOS table (Shen et al. 1998b).

We explain the formulation of nuclear statistical equilibrium in §2.1 with the detailed description of spin of nuclei in §2.2. We describe briefly the atomic mass data used for the calculations in §2.3, the Shen equation of state in §2.4 and the beta equilibrium in §2.5. We show the properties of dense matter in the current framework in §3. The summary and discussions will be given in §4.

2 Thermodynamics of interacting nuclides

2.1 Inclusion of nuclear and Coulomb contributions

The basis is the equation of nuclear statistical equilibrium (NSE) with respect to strong and electromagnetic processes for the chemical potentials of nuclei:

$$\mu_i = Z_i \mu_{\rm p} + (A_i - Z_i)\mu_{\rm n} \ . \tag{1}$$

We denote $i = 1 = p$ for proton and $i = 2 = n$ for neutron. We use the index i mostly for nuclei (A_i, Z_i) with $A > 1$, but we include nucleons $(i = 1, 2)$ in the summation over all species. To find the correct expressions for μ_i we suppose that the free energy of the set of $\{N_i\}$ nuclides is

$$F_{\rm nuc} = \sum_i N_i \Phi_i(T, \{n_k\}) \ . \tag{2}$$

Here Φ_i is the free energy per nucleus i and it may depend not only on the concentration,

$$n_i = N_i/V \ , \tag{3}$$

of the i-th nucleus but also on concentrations of some other nuclei n_k. Then we have by definition

$$\mu_i = \frac{\partial F_{\rm nuc}}{\partial N_i}\bigg|_{T,V} = \Phi_i + \sum_k n_k \frac{\partial \Phi_k}{\partial n_i}\bigg|_T \ . \tag{4}$$

Thus we find for the pressure

$$P_{\rm nuc} = -\frac{\partial F_{\rm nuc}}{\partial V}\bigg|_{T,\{N_k\}} = \sum_k \mu_k n_k - F_{\rm nuc}/V \tag{5}$$

which is consistent with the definition of the grand thermodynamic potential, PV. We have to give these elementary details here since we find that some terms are omitted in the expressions for μ_i, e.g. by Yakovlev & Shalybkov (1989).

For example, let us start with the Coulomb contribution to $F_{\rm nuc}$. As usual we introduce

$$\Gamma_i = \frac{1}{k_{\rm B}T}\left(\frac{e^2 Z_i^2}{a_{Z_i}}\right) = \frac{e^2 Z_i^2}{k_{\rm B}T}\left(\frac{4\pi}{3} n_i\right)^{1/3} \tag{6}$$

with a_{Z_i} being the radius of the ion sphere:

$$\frac{4\pi}{3} a_{Z_i}^3 = n_i^{-1} \ . \tag{7}$$

If Q_i denotes the Coulomb correction to the free energy and has the functional form

$$Q_i \equiv k_B T f_0(\Gamma_i) \tag{8}$$

then we find the Coulomb contribution to the chemical potential as

$$\mu_i^{\rm Coul} = k_B T \left[f_0(\Gamma_i) + \frac{1}{3}\frac{\partial f_0}{\partial \ln \Gamma_i} \right] \tag{9}$$

contrary to Eq.(17) of Mazurek et al. (1979) and to Eq.(97) of Yakovlev & Shalybkov (1989) who find $\mu_i = k_B T f_0(\Gamma_i)$, but their expressions lead to zero correction to $P_{\rm nuc}$ in Eq. (5). On the other hand, our expression Eq. (9) gives the expected correction to $P_{\rm nuc}$ after substitution into Eq. (5). Basically the formulae in Yakovlev & Shalybkov (1989) are correct, since one is free to separate Coulomb contributions, ascribing them either to electrons or ions, but one has to avoid confusion with this separation. In the book by Haensel et al. (2007) they mostly rely on free energy F instead of μ_i. Actually, the expression which is equivalent to (9) appeared already in Dewitt et al. (1973), however, the argument on the role of the chemical potentials and debates on approaches to them still persists. For example, Brown et al. (2006) discuss the difference of their use of chemical potentials with that of Dewitt et al. (1973). Essentially, Brown et al. (2006) found that the Coulomb correction found by Dewitt et al. (1973) for a classical plasma is applicable to quantum plasma as well. (See also Brydges & Martin 1999, for a detailed review on modern perspective on Coulomb systems).

We closely follow Mazurek et al. (1979) in the assumed form of the free energy but with some modifications. The main results presented below use the Coulomb correction as in Eq.(8), as was also taken by Mazurek et al. (1979). In the end we check the effect of the additional term in Eq.(9). Thus, we put

$$\Phi_{\rm p} = \Phi_{\rm p}^{(0)} + W + Q_{\rm p} + B_{\rm p} \ , \tag{10}$$

$$\Phi_{\rm n} = \Phi_{\rm n}^{(0)} + W + B_{\rm n} \ . \tag{11}$$

Here $\Phi_{\rm p}^{(0)}$ and $\Phi_{\rm n}^{(0)}$ are the Fermi-Dirac expressions for the free energy of non-relativistic nucleons and they are expressed through the Fermi integrals of half-integer index. To calculate them we use the code by Nadyozhin (1974a,b). (The superscript zero indicates that an expression is for non-interacting particles). For the bulk interaction energy of free nucleons we take the zero temperature expression from Mazurek et al. (1979) where they have used the expression of Baym et al. (1971) with minor corrections from Mackie (1976):

$$W = W(k, \beta) \tag{12}$$

with $k^3 = 1.5\,\pi^2(n_{\rm p}+n_{\rm n})$ and $\beta = n_{\rm p}/(n_{\rm p}+n_{\rm n})$. We have used the same values of parameters entering in Eq. (12) as Mazurek et al. (1979): $k_0 = 1.34$ fm^{-1}; $W_0 = 15.5$ MeV; $s = 27.1$ MeV; $K = 268$ MeV.

For nuclei ($i > 2$) we assume:

$$\Phi_i = \Phi_i^{(0)} + Q_i + B_i \; . \tag{13}$$

The binding energy in Eqs. (10), (11) and (13) is

$$B_i = M_i - \frac{A_i}{A_m} M_m \; , \tag{14}$$

with M_i being the mass of a nucleus number i, which depends on the choice of the reference nucleus m. We use ^{56}Fe as the reference nucleus in our calculations. In calculating the total energy we exclude electron mass $m_{\rm e}$ from the electron energy, then we have

$$B_i = \Delta M_i - \frac{A_i}{A_m} \Delta M_m \; . \tag{15}$$

where ΔM_i is the atomic mass excess, which accounts for the mass of electrons. To compare with Lattimer & Swesty (1991) one has to take into account that they assume $B_{\rm n} = 0$, where $m = 2 = {\rm n}$ in our notation, and $B_i = \Delta M_i - A_i \Delta M_{\rm n}$.

Considering the Coulomb corrections we follow Lattimer et al. (1985) and take for the total Coulomb energy of a nucleus

$$E_i^{Coul} = \frac{3}{5}\frac{Z_i^2 e^2}{r_A}\big[1 - \frac{3}{2}\frac{r_A}{a_Z} + \frac{1}{2}(\frac{r_A}{a_Z})^3\big] \; . \tag{16}$$

Here r_A is the nuclear radius, $r_A = 1.2 \cdot 10^{-13} A^{1/3}$ cm. So the Coulomb correction is

$$Q_i = \frac{3}{5}\frac{Z_i^2 e^2}{r_A}\big[-\frac{3}{2}\frac{r_A}{a_Z} + \frac{1}{2}(\frac{r_A}{a_Z})^3\big] \; . \tag{17}$$

In the leading term, which is what we need at high density, this is just $-0.9\,\Gamma_i$ with Γ_i defined in Eq.(6) when the form (8) is used. With the modification as in Eq.(9) it will be $-1.2\,\Gamma_i$ – very close to the numbers in Eqs. (56) and (57) found by Dewitt et al. (1973) by two different methods.

The Boltzmann expression for the chemical potential satisfies the relation

$$\exp(\mu_i^B / k_{\rm B} T) = \frac{n_i}{\Omega_i}\left(\frac{h^2 N_0}{2\pi k_{\rm B} T A}\right)^{3/2} \; . \tag{18}$$

One has to introduce the corrections Δ_i in addition to $\mu_i^{\rm B}$:

$$\mu_i = Z\mu_{\rm p}^{\rm B} + (A - Z)\mu_{\rm n}^{\rm B} + \Delta_i \; , \tag{19}$$

where

$$\Delta_i = \Delta_i^{\rm deg} + \Delta_i^{\rm Coul} + \Delta_i^{\rm nuc} + \Delta_i^{\rm sur} \; . \tag{20}$$

The corrections for degeneracy are:

$$\Delta_i^{\rm deg} = Z(\mu_{\rm p}^0 - \mu_{\rm p}^{\rm B}) + (A-Z)(\mu_{\rm n}^0 - \mu_{\rm n}^{\rm B}) \; , \tag{21}$$

and for the Coulomb part:

$$\Delta_i^{\rm Coul} = ZQ_p - Q_i \; . \tag{22}$$

For nuclear interactions we have:

$$\begin{aligned}\Delta_i^{\rm nuc} = \quad & -B_i^0 + AW + (X_{\rm p}+X_{\rm n})\left[Z\tfrac{\partial W}{\partial X_{\rm p}} + (A-Z)\tfrac{\partial W}{\partial X_{\rm n}}\right] \\ & + \left[-\chi_i + Z\textstyle\sum_{A',Z'>1} \tfrac{X_{A',Z'}}{A'}\cdot\tfrac{\partial \chi_{A',Z'}}{\partial X_{\rm p}} + (A-Z)\textstyle\sum_{A',Z'>1}\tfrac{X_{A',Z'}}{A'}\cdot\tfrac{\partial \chi_{A',Z'}}{\partial X_{\rm n}}\right]\end{aligned} \tag{23}$$

Mazurek et al. (1979) have argued that these expressions can often be simplified. We take relation Eq. (23) in full which requires an additional loop of NSE iterations.

We assume the following correction to the surface energy:

$$\Delta_i^{\rm sur} = W_{\rm sur}A^{2/3}\left(1-\frac{W}{W_{\rm nuc}}\right)^{1/2}\left[1-(X_{\rm p}+X_{\rm n})\frac{\rho}{\rho_{\rm nuc}}\right]^{4/3} \; . \tag{24}$$

The expression actually used in the mass formula for the surface energy may be much more complicated than just $W_{\rm sur}A^{2/3}$, but since the term in braces tends to zero for vanishing ρ this correction does not influence the vacuum values of nuclear masses.

2.2 Spin of ground state

To find the spin of ground states of exotic and experimentally unknown nuclei we have used the simple shell model with the Woods-Saxon potential for defining the scheme of levels and nuclear systematics. It is well known from experiments and calculations using up-to-date versions of shell model with residual interaction that the spin of ground states of even-even nuclei is equal to zero. The spin of nuclear ground states of odd–A nuclei is determined generally by the spin of the uncoupled nucleon (exceptions: $^{19}\mathrm{F}_9$, $^{23}\mathrm{Na}_{11}$, $^{55}\mathrm{Mn}_{25}$). That is why in the present paper we defined the ground state spin of odd–A nuclei by the spin of an uncoupled proton or neutron according to experimental data and shell model calculations with phenomenological coupling.

The spin of ground state of odd-odd nuclei is defined by the spins of the uncoupled proton, j_p, and neutron, j_n, and could not be calculated precisely even on the base of the microscopic models of atomic nuclei. That is why we have used, in the odd-odd case, the simple phenomenological Nordheim rules (Nordheim 1950).

In the case of opposite spins of proton and neutron ($j_n = l_n \pm 1/2,\ j_p = l_p \mp 1/2$) the spin of an odd-odd nucleus is equal to

$$I = j_n - j_p \; . \tag{25}$$

In the other case ($j_n = l_n \pm 1/2,\ j_p = l_p \pm 1/2$) it is rather difficult to find the right value of ground state spin because it can fall into the wide range:

$$j_n - j_p \le I \le j_n + j_p \; . \tag{26}$$

But it is well known from systematics that $I \approx j_n + j_p$ mainly. For simplicity we have chosen $I = j_p + j_n$.

The value of the ground state spin should not strongly influence the results of NSE calculations because in our model the nuclei are mostly in the excited states. We have done a calculation using another approach of the ground state spin calculation (Engelbrecht & Engelbrecht 1991) to check the influence. It is also based on the simple shell model level scheme, and significantly differs from ours only in the case of odd-odd nuclei, for which the spin is defined as: $I = (j_p + j_n + 1)/2$.

We find that the calculated results depend weakly on the different approaches to ground state spin calculation only in the region with the significant amount of "heavy" nuclei, where the role of odd-odd nuclei rises. Since the most abundant nuclei are even-even and odd–A ones under NSE conditions, one can use any simple estimation of the ground state spin of nuclei under these conditions. For $T_9 < 10$ and low ρ one should prefer our model of ground state spin evaluation, or an "exact" calculations of nuclear characteristics from first principles.

As for the role of the excited states, we agree with the conclusions of Liu et al. (2007) that the effect is not very large. They used a reliable method of nuclear partition function calculation, based on the Fermi gas formula. However, the question deserves further investigation, especially with account of new data from Rauscher et al. (1997); Rauscher & Thielemann (2000); Rauscher (2003). The used in Liu et al. (2007) is related to an energy-dependent level density parameter with microscopic correction to a nuclear mass model (Rauscher et al. 1997; Rauscher & Thielemann 2000; Rauscher 2003). Our code may incorporate various options for the partition functions.

2.3 Nuclear masses

We adopt the table of nuclear masses (KTUY) by Koura et al. (2005) for our EOS calculations. The prediction of nuclear masses by Koura et al. (2005) is based on the mass formula composed of macroscopic and microscopic terms (Koura et al. 2000), which treat deformation, shell and even-odd energies. It covers ∼9000 species of nuclei (Z $\geq$ 2 and N $\geq$ 2) in the nuclear chart. We use the extended mass table containing ∼20000 species (Koura 2007) to cover the neutron- and proton-rich regions in the nuclear statistical equilibrium. The root-mean-square deviation from experimental masses is 666.7 keV. We examine the dependence on the nuclear mass by adopting other tables of the nuclear masses by Hilf et al. (1976). The mass data by Möller et al. (1995) will be implemented in the code. Those mass tables predict the experimental masses very well around the stability line in the nuclear chart, however, they provide different predictions in neutron-rich region away from the stability. It would be interesting to examine whether these differences appear in the composition of dense matter in supernova core.

2.4 Shen equation of state

We adopt the table of EOS by Shen et al. (1998a,b) to investigate the influence of mixture of nuclei on the equation of state. The Shen EOS is a set of thermodynamical quantities of dense matter under the wide range of density, proton fraction and temperature for supernovae. It has been widely used for numerical simulations of core-collapse supernovae (Sumiyoshi et al. 2005, 2006; Janka et al. 2005; Burrows et al. 2006) and other astrophysical phenomena (Rosswog & Liebendörfer 2003). The equation of state is calculated by the relativistic mean field theory (Serot & Walecka 1986), which is based on the relativistic Brückener Hartree Fock theory (Brockmann & Machleidt 1990) and is constrained by the experimental data of neutron-rich nuclei (Sugahara & Toki 1994). The nuclei in dense matter is described within the local density approximation assuming one species of nucleus surrounded by neutrons, protons and alpha particles in the Wigner-Seitz cell. The basic behaviour of the Shen EOS in supernova core as well as the comparison with the another set of EOS by Lattimer & Swesty (1991) can be found in Sumiyoshi et al. (2004, 2005).

2.5 Beta-equilibrium

Although we fix the value of Y_e in the current calculations, we can impose the condition of beta equilibrium in the Saha approach. We add the formulation here for the applications to proto-neutron stars.

The condition of beta-equilibrium is governed by the relation

$$\mu_{\rm p} + \mu_{\rm e} = \mu_{\rm n} + \mu_{\nu} \ . \tag{27}$$

Therefore, one has to calculate chemical potentials of neutrinos and electrons in an additional loop of iterations.

For calculating lepton chemical potentials one can use simple relations derived by Nadyozhin (1974a,b) (see also Blinnikov 1987; Blinnikov & Rudzsky 1988):

$$n - \tilde{n} = \left.\frac{\partial P}{\partial \mu}\right|_T \quad = \frac{g}{6\pi^2}\left(\mu^3 + \pi^2 \mu T\right) \ . \tag{28}$$

Here n is a fermion number in the unit volume, i.e., the fermion concentration, $\tilde{n}$ is an anti-fermion concentration. $n - \tilde{n}$ is a charge of the unit volume, for example, for the electrons and it is a lepton charge for neutrinos ($g = 2$ for electrons and $g = 1$ for neutrinos). It is possible to express the lepton chemical potentials μ through the radicals if $n - \tilde{n}$ and T are given. In actual calculations it is faster to do this by Newton iterations.

3 Results

We report the numerical results in a set of selected conditions for density, ρ, electron fraction, $Y_{\rm e}$, and temperature, T. We show the properties of dense matter at typical conditions (ρ=10^{10}–10^{13} g/cm^3) during the core collapse, where the composition of nuclei and free protons are crucial to determine the electron capture. We remark that the present framework is generally applicable in the wide range of conditions, which are necessary for core-collapse supernova simulations. However, it is limited up to $Y_{\rm e}$ ∼0.3 due to the coverage of nuclear mass models at neutron-rich region. The limited range of low T ∼2 MeV and high ρ ∼10^{13} g/cm^3 is due to the consideration of nuclear interaction and the convergence of iterations.

We show, at first, the general behaviour of equation of state in the current framework with the mass formula by Koura et al. (2005) in §3.1. Next, we compare the equation of state obtained by the current Saha-approach with that of Shen EOS (Shen et al. 1998b) in §3.2. We examine the difference between the two nuclear mass models. We also compare with the results calculated in the formulation of Mazurek et al. (1979). In §3.3, we show the composition of nuclei in the nuclear chart in the situations of supernova core.

3.1 General behaviour

We show, in Figs. 1, 2, 3 and 4, the global features of dense matter at $Y_{\rm e} = 0.316$ for a wide range of density and temperature relevant to collapsing supernova cores. We have calculated also the cases with $Y_{\rm e} = 0.398$ and $Y_{\rm e} = 0.473$, which are not shown here. The values of $Y_{\rm e}$ are selected so as to match with the values in the original table of Shen EOS. We see very smooth variations of calculated quantities in the range of density and temperature shown in the plot. There are some wiggles in the plots of the average of mass number, A, and proton number, Z in Figs. 2, 3 due to the shell effects. One can recognise the appearance of nuclei at low density $\sim 10^{10}$ g/cm^3 at the lowest temperature. This is different from the Shen EOS as we will see in the next subsection.

3.2 Comparisons among models

We compare the current results with those in the Shen EOS to see the effect of multi-composition with respect to the one-species treatment, which has been used in most of the supernova EOS's. We examine also the dependence on the nuclear mass models by comparing the cases by Koura et al. (2005) and Hilf et al. (1976). We set here $Y_{\rm e} = 0.316$ and T=2 MeV which roughly corresponds to the neutron-rich supernova core. This T value also corresponds to the lower T boundary in the figures shown above.

We show that the mass fractions of nuclei, free protons and alpha particles as a function of density in Figs. 5 and 6. As the density goes higher, we have found the nuclei appear earlier than the Shen EOS does. This is because the nuclei other than alpha particles appear abundantly in the treatment of multi-composition. In the Shen EOS, on the other hand, alpha-particle appear more in this density region $\sim 10^{11}$ g/cm^3 as seen in Fig. 6. Figure 7 elucidates clearly this difference further. From $\sim 10^9$ g/cm^3, the Saha-treatment provides nuclei of average mass number $A \sim 10$. At densities higher than $\sim 3\times10^{11}$ g/cm^3, the average mass number is smaller than that of representative nuclei in the Shen EOS. The one-species treatment may overestimate the mass number in this respect. We note that the average mass number in the Saha-treatment does not include the contribution of alpha particles, which are separately treated in the Shen EOS.

The thermodynamical quantities, i.e. entropy and pressure of nuclear contribution, are shown in Fig. 8. The entropy of the Shen EOS is in accord very well with the current result. The pressure of the Shen EOS has trough around 10^{13} g/cm^3 because of the decrease of nuclear part of free energy. As it has been already reported in Shen et al. (1998a), this is due to the increasing binding energy of nuclei. We note that one should add lepton and radiation contributions in addition, therefore, the total pressure is always positive.

In Fig. 9, we show the average mass number and proton number of nuclei for $Y_{\rm e} = 0.473$ and T=0.63 MeV, which is more closer to the condition at centre of the initial progenitors. We can see that mass number (proton number also) in the current treatment is larger at low density and smaller at high density. This is quite similar to the case of more neutron-rich and higher temperature, $Y_{\rm e} = 0.316$ and T=2 MeV in Fig. 7.

We comment here on the difference from the calculated EOS using the treatment by Mazurek et al. (1979). The calculation done without the second line in Eq. (23), which express the dependence of binding energy of nucleus on the nucleon fractions, are shown by dash-dotted lines in Figs. 5 to 8. In general, the treatment without iterations gives similar results to the one with iterations to calculate consistently the modified binding energy due to the presence of nucleons at this condition. In Fig. 10, we show the mass fraction of free protons as a function of density for $Y_{\rm e} = 0.398$ and T=2 MeV. We have found the treatment by Mazurek et al. (1979) provides similar results to those of the Shen EOS and our treatment gives lower proton fraction by large factors. This may influence the electron capture rate in collapsing supernova cores.

We remark on the dependence of mass models. The calculations by two mass models are similar to each other and one can hardly see the difference. Only in the prediction of mass number and proton number, there are slight differences between the two lines. In this respect, the derivation of bulk quantities, such as entropy and pressure, can safely be calculated without the uncertainties of mass formulae. We note, however, that the detailed composition depends on the adopted mass formula as we will show below.

3.3 Nuclear composition

We explore the calculated composition using the mass formula by Koura et al. (2005) in Figs. 11, 12 and 13 for three typical conditions of supernova core. We took the conditions from the numerical simulation of core-collapse from a 15M$_\odot$ star by Sumiyoshi et al. (2005).

At ρ=10^{11} g/cm^3, where electron captures goes on during the gravitational collapse from the initial Fe core, nuclei up to $A \sim 100$ appear mostly with the peak abundance at $Z \sim 34$ and the magic number N=50. By the time the density reaches ρ=10^{12} g/cm^3, electron capture is about to cease and $Y_{\rm e}$ becomes smaller. Because of higher temperature due to the collapse, the distribution becomes wider, reaching $A \sim 132$ at the double magic nuclei, ^{132}Sn. Neutron-richness (small $Y_{\rm e}$) makes the peak position at more neutron-rich but at N=50. At high density of 10^{13} g/cm^3 and high temperature of 3 MeV, which corresponds to the moment just before the core bounce, the distribution extends from nucleons to $A \sim 160$ continuously. We see the effect of magic numbers for neutron number 50 and 82 and even-odd numbers, which exist in nuclear mass data.

In order to demonstrate the difference of composition due to the mass models, we show the case of ρ=10^{12} g/cm^3 with the mass data by Hilf et al. (1976) in Fig. 14. Through the comparison with Fig. 12, the distribution is narrower both in N and $A = N + Z$ directions. The peak position is quite close each other in the two models. We see similar differences also in the case of ρ=10^{11} g/cm^3 and ρ=10^{13} g/cm^3, especially on the strength of magic numbers. Neutron-richness at high density causes larger differences among them.

3.4 Difference in Coulomb corrections

As we have discussed above, there is some controversy on the form of Coulomb corrections in the literature. We compare in Fig.15 the effect of changing corrections as in formula (8) and in (9) on the proton fraction. The effect is visible only at highest density but still very small. A bit more pronounced effect is obvious in Fig.16 for the average mass of heavy nuclei again at highest density when the NSE model is near the border of applicability. However, a more detailed study is needed here along the lines undertaken recently by Nadyozhin & Yudin (2005).

4 Summary and discussions

We have studied the properties of hot and dense matter at the conditions relevant to supernova cores in the extended Saha approach. The multi-composition of nuclei is taken into account by solving the chemical equilibrium among nuclei, neutrons and protons. The contributions to chemical potentials due to the degeneracy of nucleons, Coulomb effects, nuclear effects, surface effects are included in the Saha formulation. The modification of binding energies of nuclei due to the existence of nucleons outside nucleus is solved self-consistently. This is different from the treatment of Mazurek et al. (1979). Cf. Nadyozhin & Yudin (2005) were the difficulty of self-consistent treatment is pointed out. We have adopted the recent mass formula by Koura et al. (2005), covering $\sim$20000 nuclides, and compared the results with the ones by Hilf et al. (1976).

We have calculated extensive grids of density and temperature for several choices of Y_{e}. We found that the obtained quantities behave in general very smoothly. When we compared with the values in the Shen EOS, which is a popular set of EOS for supernova simulations, they coincide with each other closely for thermodynamical quantities. This may suggest that the one species treatment of nuclei adopted in most of modern supernova EOS's is a good approximation in this regard. However, the appearance of nuclei starts at lower density than in the Shen EOS and the mass fractions of alpha particles and nuclei are different in two codes. The average mass and proton numbers of nuclei are larger at low density and smaller at high density than those obtained from the Shen EOS. The former arises from the appearance of light nuclei around $A \sim 10$ in addition to alpha particles which are only included in Shen EOS. We explore also the composition in supernova core in the nuclear chart. We found that the distribution extends widely for high density and temperature and it depends on the choice of mass formula, which provides different shell effects.

Our approach is rather simple and may be compared with more sophisticated modern treatment of nuclear reactions based on the statistical multi-fragmentation model (SMM): see Botvina & Mishustin (2008). Recently an exploration on the difference between the treatments under single and multi nuclear species approximations with phenomenological mass formulae has been carried out to demonstrate the overestimation of mass number in the single nuclear species Souza et al. (2008).

The current finding assists understanding of the gravitational collapse of massive stars for supernova explosions. The difference of composition from the one species treatment in the Shen EOS suggests that the proper treatment in multi-composition of nuclei is important and may significantly affect the dynamics of core collapse. Since the electron capture on nuclei and free protons is crucial to determine the size of bounce core, i.e. the location of initial launch of shock wave, one should take into account the composition properly. Such efforts have been made to evaluate the total electron capture rates on nuclei by averaging the distributions (Hix et al. 2003). One should, however, work carefully to predict the composition, since the mass and the nuclear effects may affect the detailed abundance. It is also necessary to calculate the equation of state, thermodynamical quantities and compositions in a consistent manner. We are aiming to apply the extended Saha treatment to provide EOS sets for supernova simulations in future.

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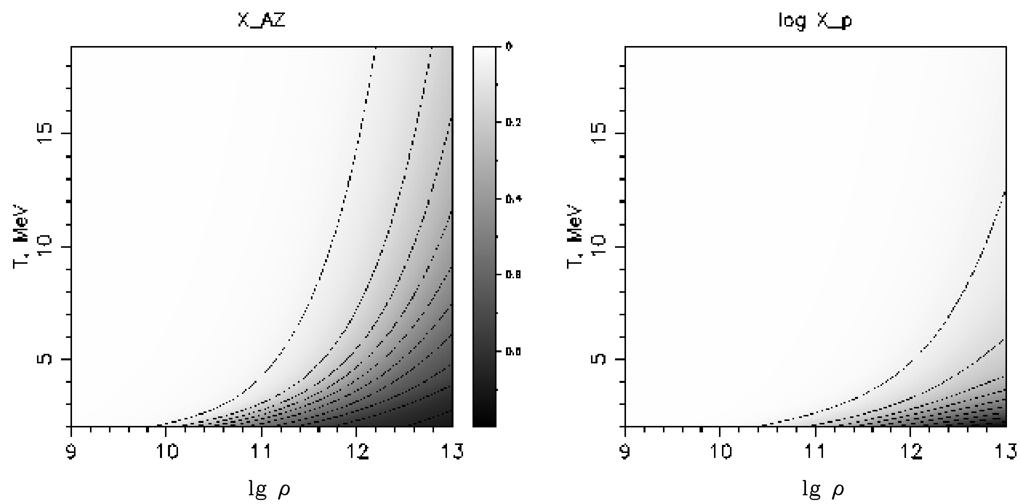

Figure 1: The isocontours of the mass fraction of heavy nuclei, X_{AZ}, (left) and free protons, X_p, (right) for $Y_\mathrm{e} = 0.316$ are shown in the plane of density and temperature.

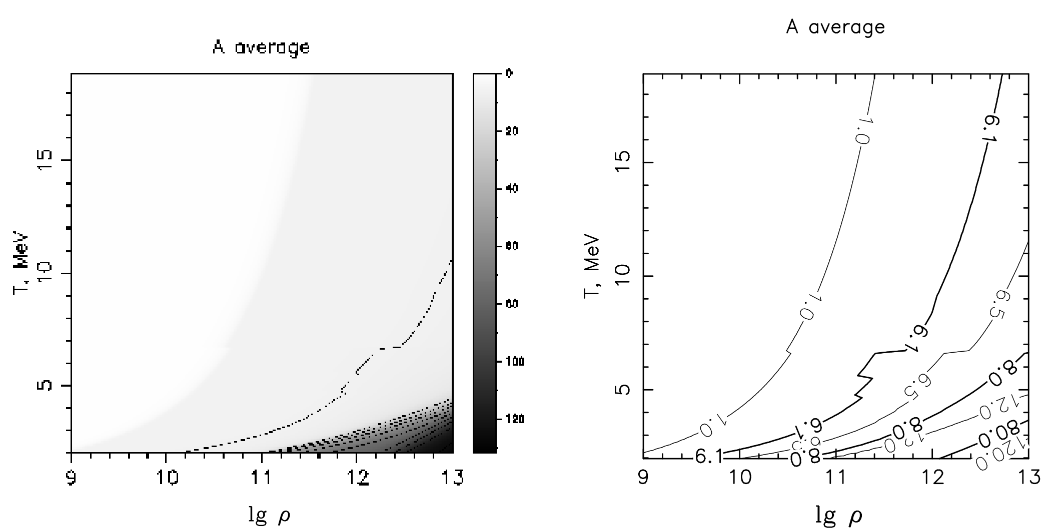

Figure 2: The isocontours of the average mass number, A, of heavy nuclei, for $Y_\mathrm{e} = 0.316$.

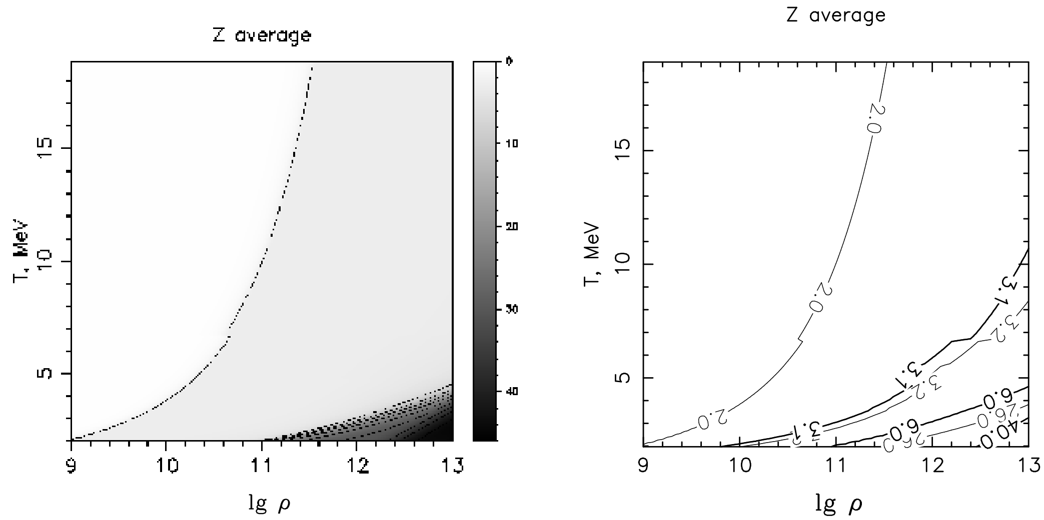

Figure 3: The isocontours of the average proton number, Z, of heavy nuclei, for $Y_{\mathrm{e}} = 0.316$.

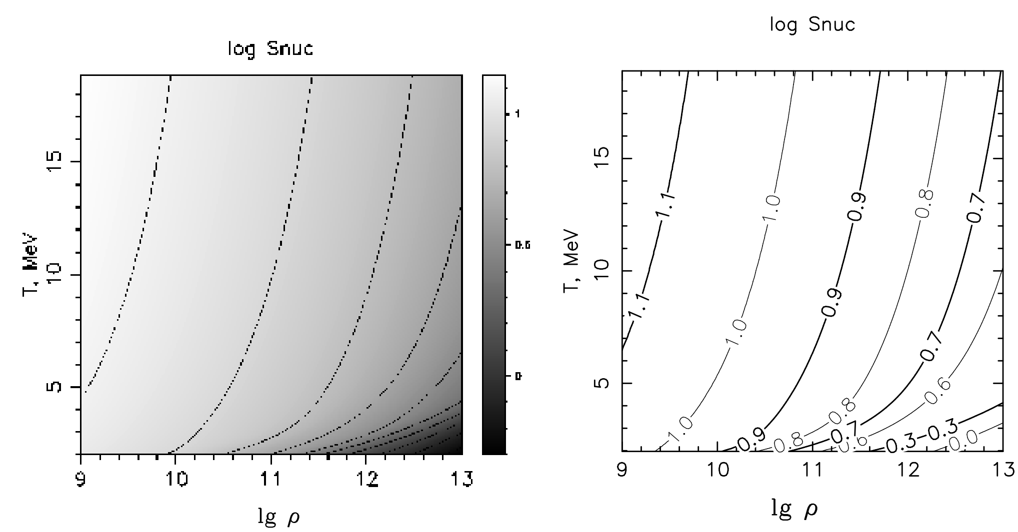

Figure 4: The isocontours of the nuclear contribution to entropy, S_{nuc}, for $Y_{\mathrm{e}} = 0.316$ in the plane of density and temperature.

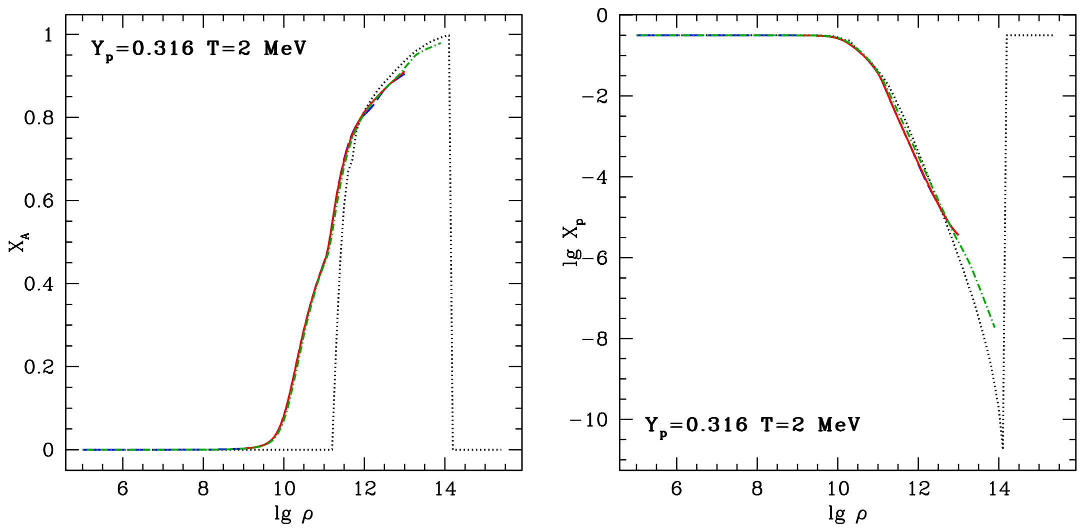

Figure 5: The mass fraction of nuclei, X_A, (left) and free protons, X_p, (right) as a function of density for $Y_{\rm e} = 0.316$ and $T = 2$ MeV. The solid and dashed lines denote the NSE calculation with mass-formulae by Koura (2007) and Hilf et al. (1976), respectively. The dash-dot lines are obtained using Koura (2007), but with a simplified treatment of relation Eq. (23) as has been done by Mazurek et al. (1979). The dotted lines are the results from Shen et al. (1998b).

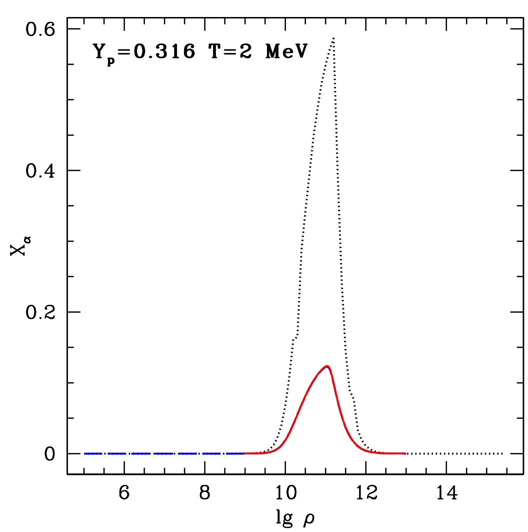

Figure 6: The mass fraction of alpha-particles, X_α, as a function of density for $Y_{\rm e} = 0.316$ and $T = 2$ MeV. The notation is the same as in Fig. 5.

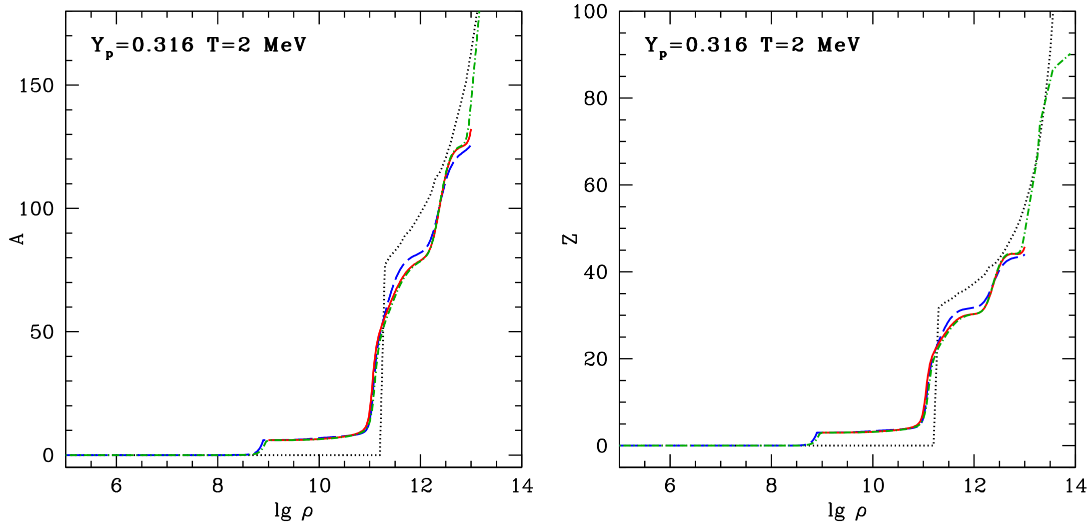

Figure 7: The average mass number, A, (left) and average proton number, Z, (right) of nuclei as a function of density for $Y_\mathrm{e} = 0.316$ and $T = 2$ MeV. The notation is the same as in Fig. 5.

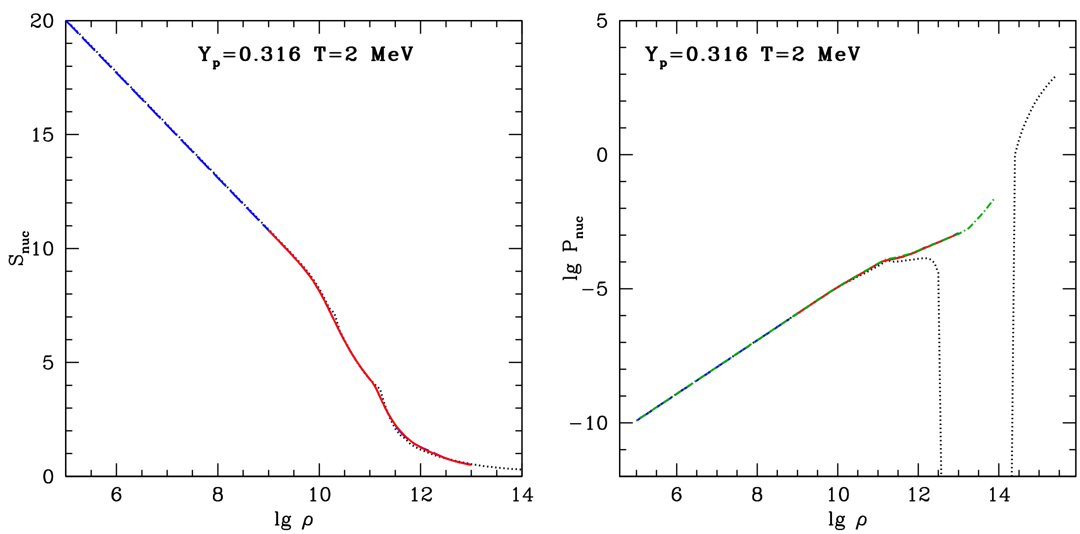

Figure 8: The entropy, S_nuc (left), and pressure P_nuc (right), of nuclei as functions of density for $Y_\mathrm{e} = 0.316$ and $T = 2$ MeV. The notation is the same as in Fig. 5.

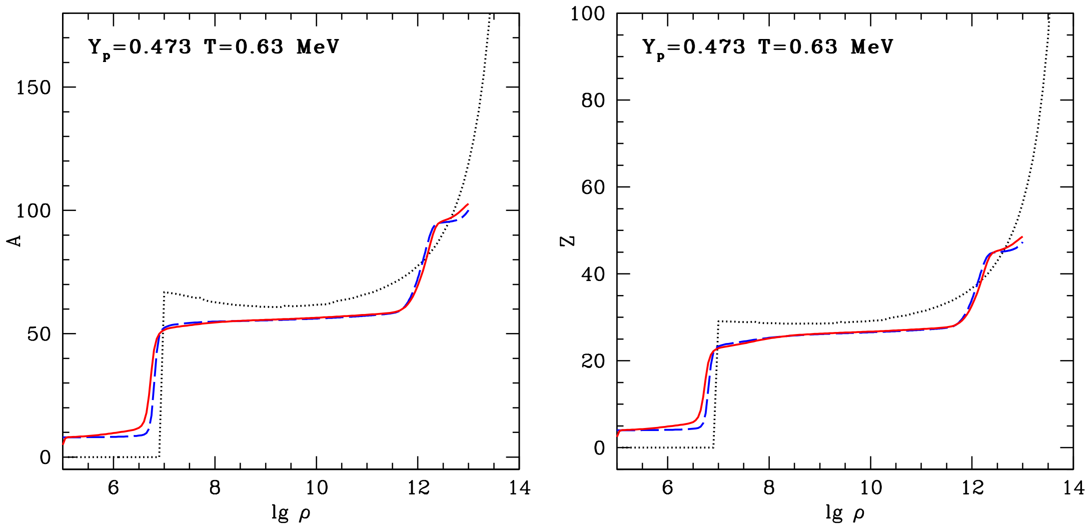

Figure 9: The average mass number, A, (left) and average proton number, Z, (right) of nuclei as a function of density for $Y_\mathrm{e} = 0.473$ and $T = 0.63$ MeV. The notation is the same as in Fig. 5.

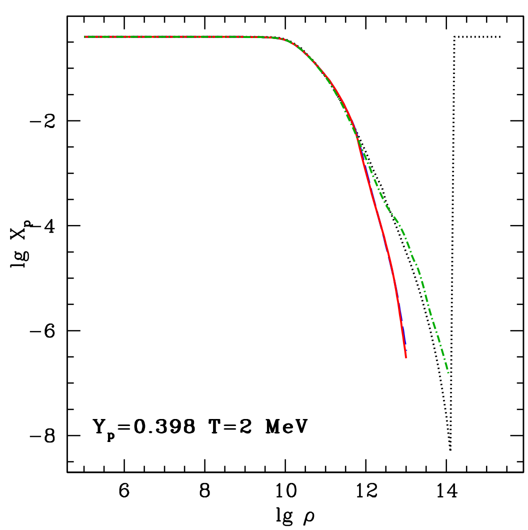

Figure 10: The mass fraction of free protons, X_p, as a function of density for $Y_\mathrm{e} = 0.398$ and $T = 2$ MeV. The notation is the same as in Fig. 5.

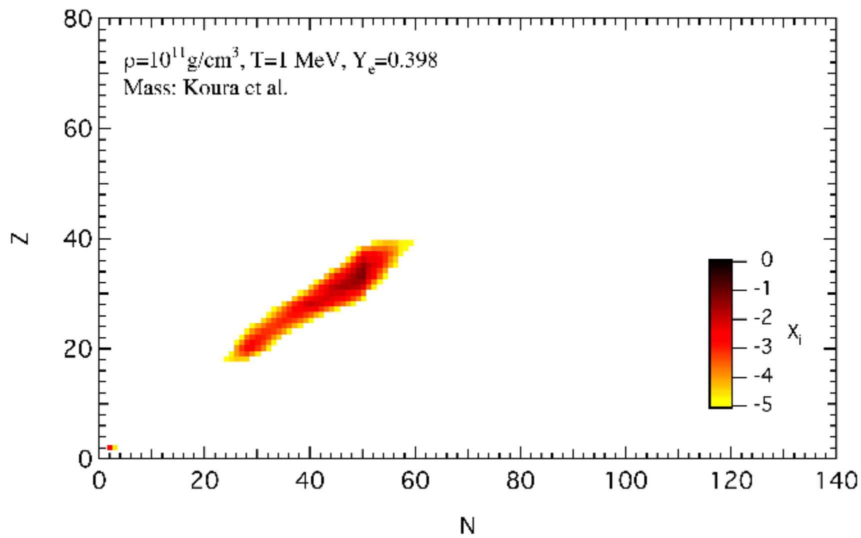

Figure 11: The mass fraction of nuclei, X_A, having proton number, Z, and neutron number, $N = A - Z$ in the nuclear chart for $\rho = 10^{11} g/cm^3, Y_{\rm e} = 0.398$ and $T = 1$ MeV.

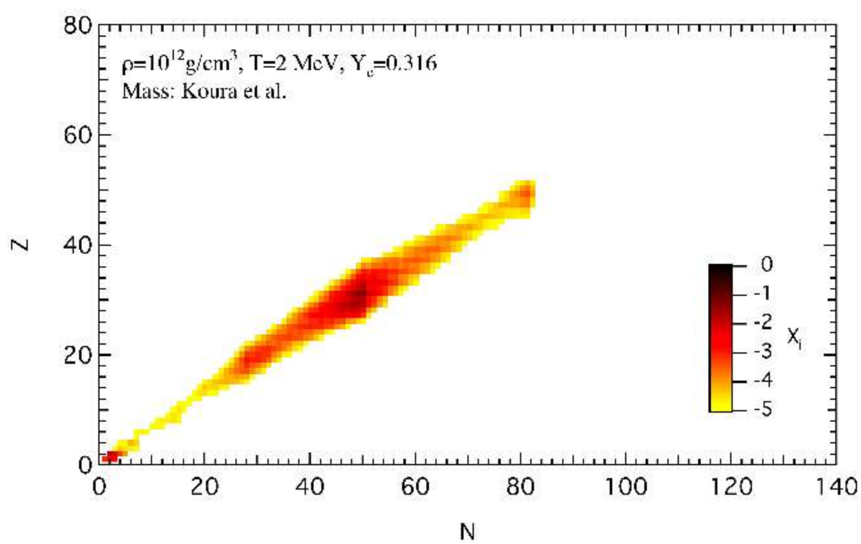

Figure 12: The mass fraction of nuclei, X_A, having proton number, Z, and neutron number, $N = A - Z$ in the nuclear chart for $\rho = 10^{12} g/cm^3, Y_{\rm e} = 0.316$ and $T = 2$ MeV.

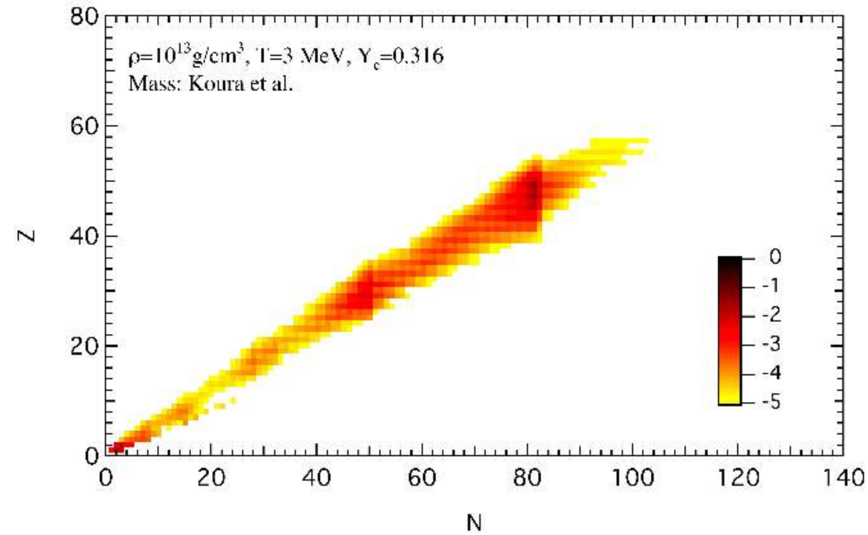

Figure 13: The mass fraction of nuclei, X_A, having proton number, Z, and neutron number, $N = A - Z$ in the nuclear chart for $\rho = 10^{13} g/cm^3, Y_\mathrm{e} = 0.316$ and $T = 3$ MeV.

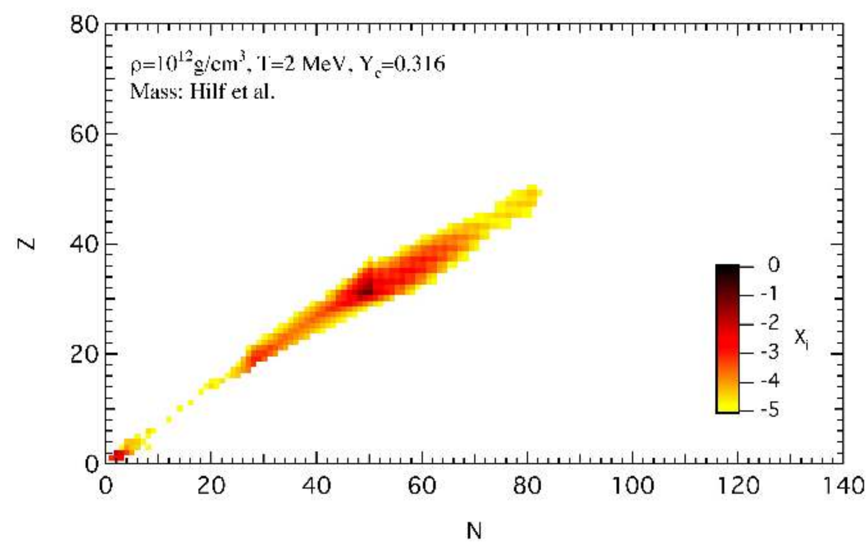

Figure 14: Same as Fig. 12 but for Hilf et al. (1976)

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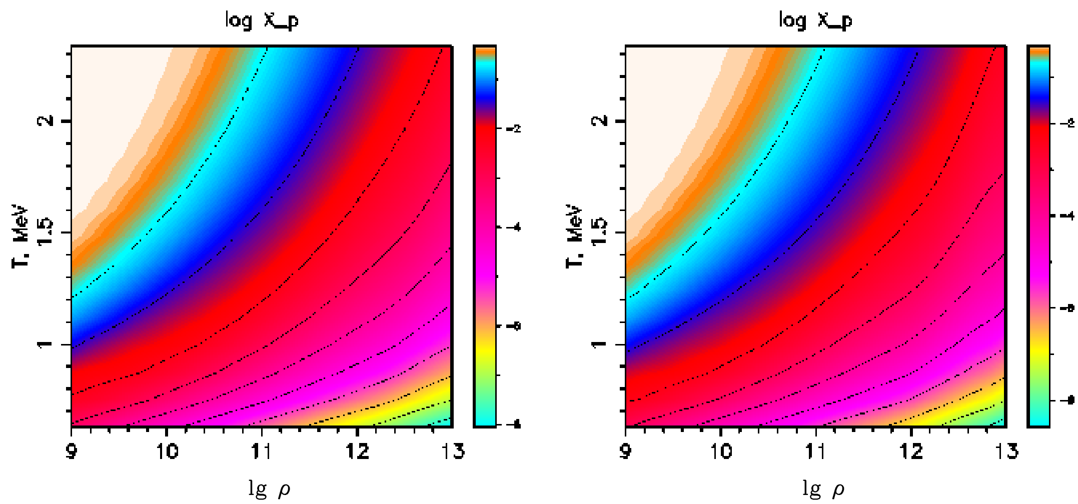

Figure 15: The isocontours of the proton fraction, X_p, for $Y_\mathrm{e} = 0.473$. Left panel: the Coulomb correction is taken as in Eq.(8). Right panel: as in Eq.(9)

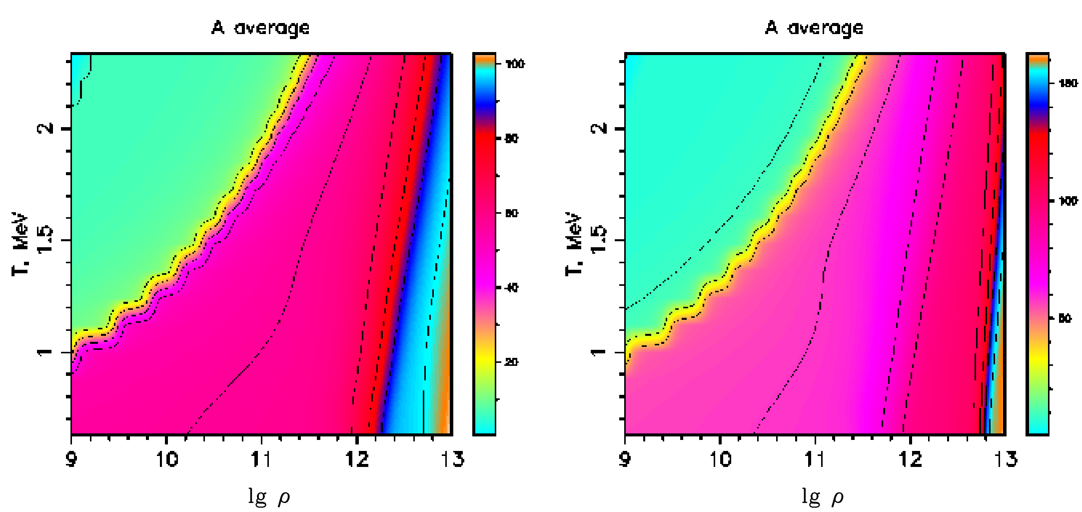

Figure 16: The isocontours of the average mass number, A, of heavy nuclei, for $Y_\mathrm{e} = 0.473$. Left panel: the Coulomb correction is taken as in Eq.(8). Right panel: as in Eq.(9)