Light nuclei in supernova envelopes: a quasiparticle gas model

Stefan Heckel, Philipp P. Schneider, Armen Sedrakian
Institute for Theoretical Physics, J. W. Goethe-University, D-60438 Frankfurt am Main, Germany
(Dated: July 7, 2009)

We present an equation of state and the composition of low-density supernova matter composed of light nuclei with mass number \( A \leq 13 \). We work within the quasiparticle gas model, which accounts for bound states with decay time scales larger than the relevant time scale of supernova and protoneutron star evolution. The mean-field contribution is included in terms of Skyrme density functional. Deuterons, tritons, and \(^4\)He nuclei appear in matter in concentrations that are substantially higher than those of heavier nuclei. We calculate the critical temperature of deuteron condensation in such matter, and demonstrate that the appearance of clusters substantially lowers the critical temperature.

I. INTRODUCTION

A key ingredient of studies of the formation of neutrino signal in supernova explosions and the supernova mechanism itself is the equation of state and composition of matter at the densities \( \rho \leq 10^{12} \text{ g cm}^{-3} \) and within the temperature range \( 0 \leq T \leq 10 \text{ MeV} \). The matter at densities below the nuclear saturation density is composed of a mixture of nuclei and free (unbound) nucleons with a charge neutralizing background of electrons. The state of the art equations of state that are routinely used in the current supernova simulations, include the nucleons, the \( \alpha \) particles, and a heavy nucleus as the independent degrees of freedom. Instead of using one single heavy nucleus as a representative, an ensemble of nuclei with \( A \leq 1000 \) was included in the composition in Refs. \[17\] and \[18\], treating the nuclei as noninteracting Boltzmann gas. These statistical ensemble calculations predict nuclei that are smaller than those obtained in a single (representative) nucleus approximation and they find substantial amounts of light nuclei in the composition. The treatment of light nuclei has been improved by including the interactions among the nucleons and \( \alpha \)'s on the basis of phase shifts (virial expansion). This approach has been extended further to include the three-body bound and scattering states and contributions of all nuclei up to \( A \leq 4 \). Neutrino interactions with light nuclei are also of importance for setting the initial conditions for possible nucleosynthesis process in supernova winds.

In this work we focus our attention primarily on the composition and the equation of state of dilute isospin symmetric and asymmetric nuclear matter. Our goal is to introduce a simple setup for treating increasingly complex many-body problems related to light nuclei in supernova and protoneutron star matter. Our motivation lies in the Bose-Einstein condensation (BEC) of deuterons and \( \alpha \) particles in nuclear matter and under supernova conditions. Furthermore, recent computations of two- and three-body binding energies in nuclear medium at nonzero temperature and density allow us a fully quantum mechanical assessment of these effects beyond the occupied volume approxima-

The implications of the rich and complex composition
of matter on the thermodynamics of matter and its effect on neutrino transport and other aspects of supernova physics are not yet fully understood. The purpose of this work is to advance the study of light clusters in supernovas in the following directions. The composition of matter is extended to include all stable nuclei up to \( A \leq 4 \), a number that is larger than that included in studies of light clusters to date. In doing so the quantum statistics is fully included, i.e., the assumption of Boltzmann gas adopted, for example, in nuclear statistical ensemble studies is relaxed. It follows then that any possible Bose-Einstein condensation (BEC) in clustered matter is automatically included in the theory. Indeed, we find that there is a BEC of deuterons in the supernova environment. The effect of isospin asymmetry on the composition of matter containing nuclei with mass number \( A \leq 4 \) is studied. The formalism to address this issue is based on expressing the thermodynamical potential in terms of a sum over clusters, where each term is expressed through the spectral function of the corresponding cluster. This method, allows one to address a multitude of effects, such as finite decay width, short-lived states, Landau-Pomeranchuk suppression in radiation processes, etc.

To summarize, the novelty of this work lies in the following: first, the formalism presented here has the advantage that it represents the contribution of the clusters to the thermodynamic potential in terms of their spectral functions. Second, we present a complete quantum statistical treatment of clusters up to \( A \leq 4 \). Most previous work treats clusters as Boltzmann particles. Such an approach by default excludes any possible Bose-Einstein condensation. Furthermore, the majority of the previous works were restricted to clusters up to \( A \leq 4 \), whereas we include clusters up to \( A = 13 \). Third, we demonstrate the Bose-Einstein condensation of deuterons in supernova matter. Fourth, we demonstrate the dependence of the \( A \leq 4 \) cluster abundances on arbitrary isospin asymmetry.

This article is organized as follows. In Sec. II we describe the quasiparticle model for a mixture of light nuclei in symmetric and asymmetric nuclear matter. In Sec. III we present the results for the composition, equation of state, and deuteron condensation within the QGM. Section IV studies the effects of the in-medium modifications of the deuteron binding energies and summarizes our results.

II. QUASIPARTICLE GAS MODEL

We consider matter composed of unbound nucleons and light nuclei with mass numbers \( A \leq 13 \) in thermodynamical equilibrium at temperature \( T \) and nucleon number density \( n \). Each nucleus is characterized by its mass number \( A \) and charge \( Z \), which we collectively denote by \( \alpha = (A, Z) \). We expand the thermodynamical potential of the system into a sum of contributions of clusters

\[
\Omega(\mu_n, \mu_p, T) = \sum_{\alpha} \Omega_\alpha(\mu_\alpha, T),
\]

where \( \mu_n \) and \( \mu_p \) are the chemical potentials of neutrons and protons and \( \mu_\alpha \) is the chemical potential of a nucleus, which is completely characterized by the variable \( \alpha \). The chemical equilibrium among the species (baryon number and charge conservation) implies that

\[
\mu_\alpha = (A - Z)\mu_n + Z\mu_p.
\]

At this stage one may either develop a direct perturbation theory for the thermodynamical potential [26] or construct the Green’s functions of the theory from appropriate Martin-Schwinger hierarchy [3] and express the thermodynamical potential in terms of densities. We follow the second path. The Martin-Schwinger hierarchy is truncated with the help of self-energies such that the equation of motion for a nucleus \( \alpha \) decouples from others. Then, the thermodynamic potential for each species is given by

\[
\Omega_\alpha(\mu, T) = -V \int_{-\infty}^{\mu_\alpha} d\mu'_\alpha n_\alpha(\mu_\alpha', T),
\]

where \( n_\alpha(\mu_\alpha', T) \) is the number density of a nucleus \( \alpha = (A, Z) \). By introducing the Fourier transform of the finite temperature Green’s function \( iG^\alpha_\omega(x_1, x_2) = \langle \psi_\alpha(x_1)\psi_\alpha^\dagger(x_2) \rangle \), where \( \psi_\alpha(x_1) \) and \( \psi_\alpha^\dagger(x_1) \) are the creation and annihilation operators of a nucleus \( \alpha \) at the space-time point \( x_1 \), we write the densities of species as

\[
n_\alpha = \frac{V}{(2\pi)^4} \int d\omega d^3 p G^\alpha_\omega(\omega, p^\parallel)
\]

\[
= g_\alpha \frac{V}{(2\pi)^3} S_\alpha(\omega, p^\parallel) f_{F/B}(\omega),
\]

where \( g_\alpha \) is the degeneracy factor for spin and isospin degrees freedom and the Fermi/Bose distribution functions \( f_{F/B}(\omega) \) account for statistical distribution of species with half-integer/integer spin,

\[
f_{F/B}(\omega) = \left[ 1 \pm \exp \left( \frac{\omega}{T} \right) \right]^{-1}.
\]

The spectral function is given by

\[
S_\alpha(\omega, p^\parallel) = \frac{\Gamma_\alpha(\omega, p^\parallel)}{|\omega - E_\alpha(\omega, p^\parallel)|^2 + \Gamma_\alpha^2(\omega, p^\parallel)/A},
\]

where the quasiparticle energy is

\[
E_\alpha(\omega, p^\parallel) = \frac{p^2}{2Am} + B_\alpha + \text{Re}\Sigma_\alpha(\omega, p^\parallel) - \mu_\alpha,
\]

where the quasiparticle energy is
scales of supernova evolution, i.e., $\Gamma_\alpha(\omega, \vec{p}) = 0$. We also assume that the real parts of the self-energies are constants independent of momentum and frequency, in which case they can be absorbed in the chemical potential. Finally, we neglect the effects of medium modification of binding energies; we return to this problem in the concluding section. Under these approximations, the spectral function is given by

$$S_\alpha(\omega, \vec{p}) = 2\pi\delta \left( \omega - \frac{\vec{p}^2}{2Am} - B_\alpha - \text{Re}\Sigma_\alpha + \mu_\alpha \right),$$

and the energy integral in Eq. (4) is straightforward. The defining feature of our model is now transparent - the density is the sum of contributions from infinite lifetime quasiparticles (nuclei) characterized by the value $\alpha$. All relevant thermodynamic quantities can be computed from the thermodynamic potential Eq. (1): the pressure and the entropy are given by

$$P = \frac{\Omega}{V}, \quad S = -\frac{\partial\Omega}{\partial T}. \quad (9)$$

The pressure, entropy and other thermodynamical parameters of the electron gas are obtained from the thermodynamic potential

$$\Omega_e = -g_eT\int \frac{d^3k}{(2\pi)^3} \ln \left[ f^{-1}(-E_e(k) + \mu_e) \right], \quad (10)$$

where electron degeneracy factor $g_e = 2$, the electron energy is $E_e = \sqrt{k^2 + m_e^2}$, where $m_e$ is the electron mass, and $\mu_e$ is the chemical potential. The electron density $n_e$ couples to the density of baryonic matter via the charge neutrality condition

$$n_e = -\sum_\alpha Zn_\alpha = 0, \quad (11)$$

where $n_\alpha = \partial\Omega_e/\partial\mu_\alpha$. The thermodynamical potential of positrons is obtained upon substituting $\mu_e \to -\mu_e$. The thermodynamical potential of neutrinos of a given flavor has the same form as Eq. (10), where the neutrino mass and the chemical potential appear instead of the electron ones and the neutrino degeneracy factor is $g_\nu = 1$. The thermodynamical potential of antineutrinos is obtained in a similar fashion.

III. RESULTS

Under supernova conditions the electron fraction in matter is fixed and the evolution is nearly adiabatic (constant entropy). Here, to set the stage, we first explore the limit where the matter is isospin symmetric and isothermal. This discussion is followed by a study of a more general case of arbitrary isospin asymmetries. Below, the isospin asymmetry is characterized either by the asymmetry parameter $\chi = (n_n - n_p)/n$, where $n_n, n_p$ are the neutron and proton number densities and $n$ is the total number density or by the electron fraction $Y_e = n_e/n$ [see Eq. (11)]. Although large asymmetries are not realized in supernovas, a rapid neutronization process eventually equilibrates when the electron fraction reaches $Y_e \sim 0.05$ in protoneutron stars. The specific conditions prevailing in supernova matter, e.g., finite neutrino chemical potential, will be considered elsewhere.

A. Density functional

We start with a brief summary of the Skyrme density functional. We assume that the nucleons interact via the Skyrme interaction, which is given by

$$V(\vec{r}_1, \vec{r}_2) = t_0 \delta(\vec{r}_1 - \vec{r}_2) + \frac{1}{2} t_1 \left[ \delta(\vec{r}_1 - \vec{r}_2) k^2 + k^2 \delta(\vec{r}_1 - \vec{r}_2) \right] + \frac{1}{6} t_3 \rho \delta(\vec{r}_1 - \vec{r}_2), \quad (12)$$

where $k = (\vec{\nabla}_1 - \vec{\nabla}_2)/2i$ and $k' = -(\vec{\nabla}_1 - \vec{\nabla}_2)/2i$, whereby $n$ is the density of nuclear matter. The parameters $t_0, t_1, t_2$ and $t_3$ are determined phenomenologically. We use the SkIII parametrization [27]; the parameter values are $t_0 = -1128.75$ MeV fm$^3$, $t_1 = 395$ MeV fm$^4$, $t_2 = -95$ MeV fm$^5$, and $t_3 = 1.4 \times 10^4$ MeV fm$^6$. The (on-shell) quasiparticle spectrum for nucleons is given by $\epsilon_i(p) = p^2/(2m_i) + \text{Re}\Sigma(\epsilon_i(p), \vec{p}) - \mu_i$ which we take in the quasiparticle approximation, i.e.,

$$\epsilon_i(p) = \frac{p^2}{2m_i} - \mu_i', \quad (13)$$

where $i = n, p$ is the isospin index ($n$, neutrons; $p$, protons), $\mu_i' = \mu_i - \text{Re}\Sigma(\epsilon_i(p_F,i), p_F,i)$, where $p_F,i$ is the Fermi momentum. The effective mass of a nucleon is computed from

$$\frac{m_{n/p}}{m} = \left[ 1 + \frac{mn}{2}(t_1 + t_2) + \frac{mn}{8}(t_2 - t_1)(1 + \chi) \right]^{-1}, \quad (14)$$

which we use as a correction for the masses of free and bound nucleons. The explicit form of the self-energy is immaterial, because its value at the Fermi surface can be absorbed in the chemical potential; we drop the prime on the chemical potentials hereafter.

B. Isospin symmetric matter ($\chi = 0$)

Our numerical procedure uses the tabulated binding energies for nuclei with mass number $A \leq 13$ with half-decay times that are larger than the relevant dynamical time scales associated with supernova explosions [18]. We first compute the effective masses of nucleons and the mean-field from the Skyrme density functional with the SkIII parametrization. This is followed by a computation
FIG. 1: (Color online) Abundances of nuclei $Y_\alpha = n_\alpha/n$ in dilute isospin symmetrical matter composed of nuclei with mass numbers $A \leq 13$ as a function of matter density, in units of nuclear saturation density $n_0 = 0.16 \text{ fm}^{-3}$, at $T = 10$ MeV. The abundances of clusters decrease with increasing mass number.

FIG. 2: (Color online) Dependence of abundances of light nuclei $A \leq 4$ on matter density, in units of $n_0$, for two temperatures $T = 10$ MeV (solid lines, blue online) and 6 MeV (dashed lines, red online). Because of isospin symmetry, the abundances of protons and $^3$He nuclei, which are shown by squares and triangles, respectively, are nearly identical to those of neutrons and $^3$H nuclei.

of the partial densities from Eq. (4) with the normalization $n = \sum_\alpha n_\alpha$ and constraint (2), which provides us the chemical potentials of the species. Finally, we compute the thermodynamical potential (1) from which we obtain the pressure and the entropy. The effects of mean-field and mass renormalization are small at the relevant densities. Furthermore, the results shown below are insensitive to the choice of Skyrme parametrization.

Figure 1 displays the abundances of light nuclei, defined as

$$Y_\alpha = \frac{n_\alpha}{n},$$

at constant temperature $T = 10$ MeV as a function of density (in units of nuclear saturation density $n_0 = 0.16 \text{ fm}^{-3}$). At low densities the matter is dominated by nucleons with a small (about 10%) admixture of deuterons. At intermediate densities the deuteron fraction becomes larger than that of the free nucleons; even though the population of nuclei becomes more significant, those with $A \geq 4$ contribute less than 1% to the total density. Next to deuterons $^3$H and $^3$He nuclei are the dominant species in matter. The $\alpha$-particle abundance does not exceeds 0.5% percent at any density. Medium modifications of binding energies of nuclei shift the balance between the abundances of nucleons and light nuclei in the high density part of Fig. 1. Recall that as $n/n_0 \rightarrow 1$ nuclei disappear asymptotically, leaving a continuum of nucleons. Note that numerically the abundances of neutrons and protons in mirror nuclei (obtained by an interchange of neutrons and protons) differ slightly because of the differences in their masses and binding energies; however, these differences are insignificant on the scales of the figure.

Figure 2 shows the abundances of dominant species for two different temperatures. Reducing the temperature from $T = 10$ to $T = 6$ MeV increases the abundances of light species, such as deuterons, $^3$H and $^3$He, while the abundance of $\alpha$-particles is suppressed (note that here we assume that $B_\alpha = \text{const.}$, which is a valid assumption only in the low-density limit).

Figure 3 shows the chemical potentials of species under the conditions discussed in Fig. 1. The relative ordering of the chemical potentials follows from Eq. (2). Because $\mu_n \approx \mu_p$, their absolute value scales as $\mu_\alpha \sim A \mu_n$. The negative sign of chemical potentials of bosonic (integer total spin) nuclei implies that these are above their critical temperature and density of Bose-Einstein condensation (see Fig. 4). The condition $\mu_\alpha(T) = 0$ at fixed density is first fulfilled for deuterons (the critical temperature of Bose condensation scales as $T_c \sim M^{-1}$, where $M$ is the boson mass). The critical temperature of BEC of deuterons as a function of density is shown in
FIG. 3: (Color online) Dependence of chemical potentials of $A \leq 13$ mass number nuclei on matter density, in units of $n_0 = 0.16$ fm$^{-3}$, at $T = 10$ MeV. The chemical potentials decrease with increasing mass number.

FIG. 4: (Color online) Dependence of critical temperature of Bose-Einstein condensation of deuterons on matter density for $A \leq 2$ matter (solid line, black online) $A \leq 4$ matter (dashed line, red online), and $A \leq 13$ matter (squares).

FIG. 5: (Color online) Dependence of pressure (upper panel) and entropy (lower panel) on the density of matter for temperatures $T = 10$ MeV (solid line, black online), $T = 8$ MeV (dashed line, red online), and $T = 6$ MeV (dashed-dotted line, blue online). $k_B$ is the Boltzmann constant.

C. Isospin asymmetric matter ($\chi \neq 0$)

In this subsection we study light nuclei in isospin asymmetric nuclear matter. We consider proton-deficient matter, i.e., $0 \leq \chi = (n_n - n_p)/n \leq 1$, or in terms of electron fraction $0 \leq Y_e \leq 0.5$, which is the relevant case in supernovas and neutron stars. The dependence of the abundances of light nuclei on the electron fraction $Y_e$ at fixed
density \( n = 0.041 \text{ fm}^{-3} \) and two temperatures \( T = 10 \text{ MeV} \) and \( T = 6 \text{ MeV} \) is shown in Fig. 6. Consider first deuterons (the arguments below apply equally to \( \alpha \) particles and other nuclei with equal numbers of protons and neutrons). Their abundance is maximal for \( Y_e = 0.5 \). Increasing asymmetry reduces the number of protons that are available for building a deuteron; consequently the number of deuterons reduces with increasing asymmetry and in the limit \( Y_e = 0 \) they are extinct. Asymmetry breaks the degeneracy between the abundances of \( ^3\text{H} \) and \( ^3\text{He} \); the abundance of \( ^3\text{He} \), which requires two protons per neutron, decreases most rapidly. The abundance of triton (\( ^3\text{H} \)) is nonmonotonic: it first increases because excess neutrons can be easily accommodated in nuclei and then decreases because the number of available protons vanishes. These two effects make a compromise when \( Y_e \simeq 0.25 \), where triton abundance is maximal. Note that the ratio of abundances of deuterons to tritons is inverted for large asymmetries; indeed, in symmetric nuclear matter the deuterons are the second most abundant species, while in asymmetric matter their abundances fall below those of tritons for large enough asymmetries. Lower temperatures are seen to increase the proton depletion, \( ^3\text{He} \) and deuteron abundances decrease faster, and the increase in triton abundance at \( Y_e \leq 0.5 \) is more pronounced.

The dependence of chemical potentials of light nuclei on electron fraction at fixed density \( n = 0.041 \text{ fm}^{-3} \) and temperature \( T = 10 \text{ MeV} \) is shown in Fig. 7. The behavior of chemical potentials is understood in analogy
to the behavior of abundances discussed above: the nuclei with equal neutron to proton ratio, as well as those that require proton excess are disfavored by asymmetry and their chemical potentials are negative and large. The chemical potentials of tritons ($^3$H) are nonmonotonic functions of $Y_e$ because excess neutrons are responsible for its increase for $Y_e \leq 0.5$, while the proton extinction for $Y_e \geq 0$ is responsible for its decrease.

The dependence of pressure and the entropy on the electron fraction $Y_e$ is shown in Fig. 8. It is seen that the pressure is lowest in the symmetric case and increases with the asymmetry; like in the symmetric case larger temperatures sustain larger pressures and entropies. The entropy increases with asymmetry starting from the neutron matter limit $Y_e = 0$, an increase associated with the onset of new degrees of freedom (nuclei), which is followed by a decrease as one approaches the isospin symmetric limit.

**IV. SUMMARY AND OUTLOOK**

In this article we set up a quasiparticle gas formalism to compute the equation of state and composition of dilute isospin symmetric and asymmetric nuclear matter for applications to supernova physics. Our key finding is that matter is dominated by the light nuclei, such as deuterons, tritons ($^3$H), and $^3$He isotopes of helium. The $\alpha$-particles ($^4$He) contribute less than 1% to the number density. Furthermore, we find that in a large portion of the density and temperature diagram deuterons form a Bose-Einstein condensate. The effect of heavier clusters is to reduce the critical temperature of Bose-Einstein condensation of deuterons. A novel feature of isospin asymmetric matter is the enhancement of the abundances of neutron-rich nuclei and the corresponding suppression of proton-rich ones. This is clearly manifest in the enhancement of triton abundances with increasing asymmetry, which makes tritons the most abundant species after neutrons in asymmetric nuclear matter. Compared to isospin symmetric matter the relative abundance of deuterons and tritons is inverted in strongly asymmetric matter.

The present setup is a useful platform for further extensions of the theory, which we would like to discuss briefly. The binding energies of light nuclei are generally functions of density and temperature. At high densities and low temperatures the binding energies are reduced and at some critical values of these parameters bound states are dissolved (see Ref. [12] and references therein). Thus, for example, nuclei will disappear in matter at high densities leaving behind a uniform nuclear fluid. The critical extinction line for deuterons and tritons in the phase diagram of symmetric nuclear matter was obtained recently in Ref. [11]. In Fig. 9 we show the effect of incorporating the temperature-density-dependent binding energies of deuterons, computed in Ref. [11], on the composition of matter with mass numbers $A \leq 2$. It is seen that the high-density asymptotic state of abundances is inverted; the abundances of deuterons are larger than the nucleonic abundances for constant, free space, binding energies. However, their relative ratios are inverted when the reduction of the deuteron binding energies at large densities is taken into account. Matter effects will affect the abundances of other light nuclei in a similar way, which will guarantee that the high-density asymptotic state corresponding to the continuum of nuclear fluid at saturation density is recovered.

Apart from the statistical effect of suppression of bound state energies in matter further aspects that should be incorporated in the model include (i) leptons and electromagnetic forces (screening of nuclear charge), (ii) onset of $\beta$ equilibrium during the late time dynamics of supernovas, (iii) elastic scattering among the light nuclei themselves and with nucleons, and (iv) reactions. Of course, larger numbers of nuclei and resonances (nuclei with short-decay times scales) can be easily incorporated within our model.

This work was in part supported by the Deutsche Forschungsgemeinschaft (Grant SE 1836/1-1).

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