

Probability Distribution of Equations of State for Astrophysical Simulations

A Dissertation Presented for the
Doctor of Philosophy
Degree

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Abstract

The detection of gravitational wave during the neutron star merger event GW170817 [53] greatly enhanced our ability to probe the interiors of neutron stars. Future measurements of similar events will put further constraints to the equation of state (EOS) of nuclear matter. Also, uncertainties in the EOS create variations in the results of astrophysical simulations of core-collapse supernovae and neutron star mergers. In order to quantify the uncertainties, we construct a probability distribution of equations of states (EOSs). The EOS respects experimental, observational and theoretical constraints on the nature of matter in various density and temperature regimes. It matches (i) the virial coefficients expected from nucleon-nucleon scattering phase shifts, (ii) experimental measurements of nuclear masses and charge radii, (iii) observations of neutron star radii, (iv) theory results on the equation of state of neutron matter near the saturation density, and (v) theory results on the evolution of the EOS at finite temperatures near the saturation density. At sub-nuclear density, inhomogeneous phase tends to form, where in general a full ensemble of nuclei emerged in nucleonic gas exist. In this regime, we add selected light nuclei including deuteron, triton ^3He , ^4He , ^4Li and a full ensemble of heavy nuclei in nuclear statistical equilibrium using an excluded volume approach. We present our results in tabular form in typical conditions that are found for the early stages of core-collapse supernova and neutron star mergers.

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Chapter 1

Introduction

1.1 Formation of neutron stars

Stars generate energy through thermonuclear fusion. The Big bang nucleosynthesis took place in the interval from roughly 10 seconds to 20 minutes after the Big bang left us a universe with 75% of hydrogen and 25% of helium. Most of the hydrogens exist in forms of molecules in interstellar clouds. As the cold clouds collapse under the influence of its own gravity, hydrogen atoms are heated up and gravitational potential is converted to kinetic energy. Once the temperature (kinetic energy) is large enough to overcome the Coulomb repulsion, the fusion begins. Stars in lower mass limit around $0.08 M_{\odot}$ or $80 M_{\text{Jupiter}}$ are barely able to support fusion to deuterium. These failed stars are called brown dwarfs.

More massive stars will successfully ignite and burn hydrogen into helium and then heavier elements. This basic process involves converting four hydrogens to helium and losing 0.7% of its initial mass. The mass loss yields 26.73 MeV, where Einstein's equation $E = mc^2$ comes into play, and powers up the burning of stars ranging from millions to billions of years. The actual reaction is a little bit more complicated. For stars with masses less than $1.0 M_{\odot}$, the dominant reaction is p-p chain, whereas, for stars heavier than $1.3 M_{\odot}$, it is CNO cycle.

Stars with different masses usually have different lifespans. Low mass stars (below $8 M_{\odot}$) burn at a slower rate and usually live more than 10 billion years. Progressively heavy elements are created and accumulated in the core until carbon and oxygen are reached. At the final stage, the outer mantle is ejected slowly over hundreds or thousands of years. Stars with low

masses form the so-called “planetary nebula”. Planetary nebulae consist of carbon/oxygen white dwarfs at the center roughly the size of earth with glowing shells of ionized gas. These tiny fossils have masses around 0.5 to 1.0 $M_{\odot}$ and are supported by electron degenerate pressure.

More massive stars have shorter lifespans but much more spectacular deaths. These stars reach higher temperatures, therefore enable carbon burning to neon, magnesium, and then to silicon, sulfur, calcium and argon, then to iron and its isotopes near the peak of the nuclear binding energy curve. The iron group nuclei are the final products of fusion in stars since the reaction to elements after iron is endothermic. When a star with mass between 8 $M_{\odot}$ and 2 $M_{\odot}$ burns out its fuel after millions of years of evolution, the iron core of star gradually cools down. The pressure from degenerate electrons is not able to support the gravitational attraction, so the star begins to collapse within one second. During this process, the iron core falling freely at the speed of one fourth of the speed of light. From the size of the earth, it soon collapses to a proto-neutron star of only 30 km. Nothing stops the process until its core reaches saturation density where the strong force in nuclear matter prevents the nucleons from getting closer to each other. Once it’s halted at the core, the wave front bounces back which creates a strong shock wave. The shock wave carries away the mantle of the massive star and somehow triggers a supernova explosion. These are called core-collapse or Type-II supernova. Typical type-II supernovae will radiate 10% of its rest mass, releasing some $\sim 3 \times 10^{53}$ ergs, where almost 99 percent are radiated in terms of neutrinos [9, 93]. The remaining 1% is converted to the kinetic energy of the mantle. However, one major unsolved problem in most supernova simulations for the last 40 years is that the shock wave stalls because of photo-disintegration and neutrino loss, causing failed explosions [8, 55]. The possible solution seems to be related to the neutrino driven wind. The neutrinos generated in neutrino-sphere are partially trapped. It means they are absorbed and re-emitted again due to the cross-section of weak reaction $p + \bar{\nu} \rightarrow n + e^+$ and $n + \nu \rightarrow p + e^-$. The neutrino mean free path is on the orders of meters at moderate density ($n_B = 10^{11}$ g/cm³ or 6×10^{-5} fm⁻³) and temperature ($T = 5 - 10$ MeV) [12]. The neutrinos in the core must propagate and deposit their energy at outer layers, reviving the shock and revitalizing the explosion. Since the energy released in the explosion is dominated by neutrino loss, the efficiency of

the absorption and re-emission depend on the properties hot and dense medium which are described by the equation of state (EOS) of the nuclear matter. One purpose of this work is to systematically quantify the uncertainty of the EOS, which enable us to pin down the extent to which these uncertainties contribute to the supernova explosion mechanism. Other contributors to the explosion mechanism include revisions to neutrino physics, fluid stability, rotations, magnetic fields and convection in multidimensional simulations that will probably reduce neutrino losses. There is approximately one supernova in our galaxy around every 30 to 50 years and perhaps 100 million supernova explosions during the lifetime of our galaxy. However, except for 200 known in the Milky way, most of the remnants faded and are too dim to be detected. During the last one thousand years, six supernovae have been observed and recorded in human history. Some of them are visible to the naked eye, such as Crab, Tycho, Kepler and Cas A.

Not all the supernova explosions are the result of the collapse of the stellar core. If a white dwarf happens to have a binary companion, for example, a giant star in its late phase of evolution, the white dwarf could accrete matter from the companion when its outer shell exceeds the dwarf's Roche lobe. Upon reaching the "Chandrasekhar" mass near $1.4 M_{\odot}$, the carbon/oxygen core of the white dwarf is re-incinerated, leading to a drastic explosion. This scenario is often referred to as Type Ia supernova. Type Ia supernovae are about ten times brighter than core-collapse supernovae. However, they are also ten times less prevalent. Because type Ia supernovae have light curves belong to a one-parameter family, they can be used it as 'standard candles' to measure the Hubbard constant of the universe. Observationally, astronomers classify supernovae by their spectrum. Type II has hydrogen lines while type I does not. In contrast to type II, type I supernovae explosion completely blow up the star, leaving nothing behind.

The enormous amount of energy released in the supernova explosion also enables the creation of approximately half of the atomic nuclei heavier than iron through r-process or the rapid neutron-capture process [92]. In the hot and neutron rich environment of ejecta, the nuclei capture neutrons in succession and forms abundance peaks near mass numbers $A = 82$, 130 and 196. This process occurs in supernova explosions and also in neutron star

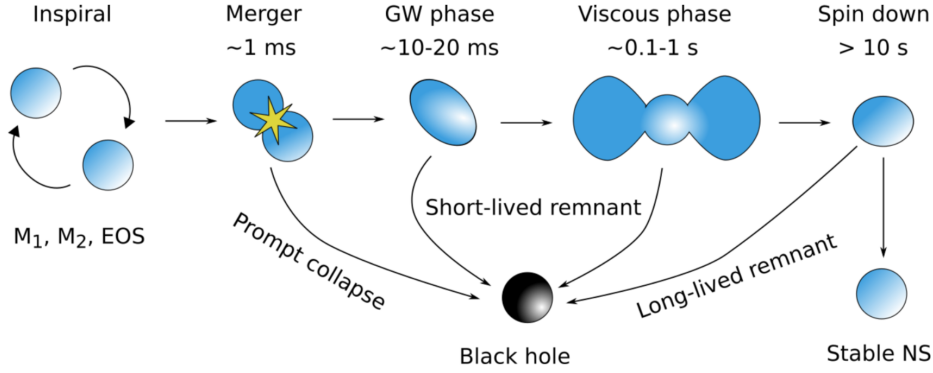


Figure 1.1: Overview of phases of neutron star mergers and the relative timescales from Ref. [65].

mergers and enriches our galaxy with heavy elements that are essential to human lives, for example, calcium, zinc and gold.

1.2 Neutron star mergers

Neutron star mergers recently show great promise to be the main sources of r-process elements. The detection of gravitational wave during the neutron star merger event GW170817 [53] and its counterpart in electromagnetic wave [1] opened up a new channel on constraining properties dense matter and also started the era of multi-messenger astrophysics. Long-standing questions like origin γ -ray bursts could be hopefully resolved with more data in the near future.

Fig. 1.1 shows an overview of phases of neutron star mergers and the relative timescales. In general, the phases could be divided into three parts, the inspiral, merger and postmerger evolution. During the inspiral, the stars rotate around each other for several minutes, or thousand of orbits. The eccentricity is radiated in the early evolution. Therefore, the motion could be well described by circular orbits when they are detected by the ground-based gravitational wave interferometers with frequency range $\sim 10 - 2048$ Hz. The quasi-adiabatic motion, namely the radiation timescale is longer than the orbital timescale, radiates gravitational wave with low frequency signal ($\lesssim 50$ Hz), which encodes the chirp mass that

could be measured. Subsequently, as the binary neutron stars merge close enough, the nuclear matter undergoes gravity-driven compression and centrifugally-driven expansion periodically. In the merger phase, while the cores of binary neutron stars rotate and fuse, the nuclear matter at the surface could be heated up to $70 - 110$ MeV, while the core remains cold ($T \lesssim 10$ MeV, entropy per baryon $\tilde{s} < 1 k_B$). A thick accretion disk forms out of materials expelled from the center with mass around $0.001 - 0.2 M_\odot$. The accretion disk eventually cools down after expansion from ~ 10 MeV (10^{-2} fm^{-3}) to ~ 0.1 MeV (10^{-11} fm^{-3}). The precess features a significant emission for the first $\sim 10 - 20$ ms after the merger called the gravitational wave dominated phase.

The outcome of binary neutron star mergers relies on the neutron star EOS and binary parameters, especially the total mass and the maximum mass for non-rotating neutron stars M_{max} . Sufficiently massive binary form black holes promptly during the merger phase. Otherwise, the remnant might go through transient phases ranging from $\sim 10 - 20$ ms to more than 10s. The differential rotation supports a higher maximum mass than non-rotating neutron stars. Thus some remnants might survive until they slow down and achieve uniform rotation due to viscosity, before they collapse to a black hole or form a stable neutron star.

It is like that neutron star mergers produce at least some r-process nuclei from the observation of GW170817 [17], even though it is not clear whether or not they produce all of them. The ejecta in poster merger phase synthesizes heavy elements and the radioactive decay of by-product of the r-process generates a thermal spectrum known as a kilonova, observed along with GW170817.

The observation of neutron star merger has now become a fundamental tool to study the dense nuclear matter. The gravitational wave signal during the inspiral phase could be used to constrain the nuclear EOS up to twice saturation density.

1.3 Neutron star structure

Neutron stars are remnants of supernova explosions, which contain the densest matter in the universe. Typical neutron has mass from 1.2 to $2.2 M_\odot$ and radius from 10 to 13 km. Stars more massive than $20 M_\odot$ are believed to collapse to black holes [82]. The nascent

proto-neutron star has temperature around 10^{11} K (8.62 MeV), but soon it cools down to 10^6 K (tens of KeV) after months of radiation. Even though the temperature is high in human terms, it is much smaller compared to the Fermi energy $p_{fc} = \hbar c (3\pi^2 \rho_0)^{1/3} \sim 330$ MeV, so $T \ll \mu$ and Fermi distribution $[\exp(E_k - \mu)/T + 1]^{-1} \sim 1$. Therefore it is considered cold and $T = 0$ is a good approximation.

The basic structure of cold neutron stars can be divided into four parts, outer crust, inner crust, outer core and inner core. The outer crust is comprised of a lattice of body-centered nuclei in iron region immersed in uniform electron background. As density increases inward, the neutron begins to drip out of nuclei as its chemical potential surpasses zero. In the inner crust, the nuclei coexist with neutron gas in so called nuclear statistical equilibrium, where nuclear abundances are determined by Saha equations. Between the inner crust and outer core, an exotic phase called “pasta phase” may represent lower energy level and appear before reaching saturation density 0.16 fm^{-3} ($3 \times 10^{14} \text{ g/cm}^3$), where a sequence of simplified shapes from cylindrical, slab, cylindrical hole and spherical hole may appear as the ground state [67, 33]. It is a result of competition between Coulomb energy and surface energy of the nuclear matter. However, sophisticated molecular simulations [70] or Hartree-Fock modeling [58] may show more complicated structures in this regime. The outer core has uniform nuclear matter begin with saturation density. The composition of the inner core is largely unknown but many postulate pion condensate, hyperons [54] or even quark deconfinement [2] that might appear beyond twice saturation density. In the last case, the neutron star has a quark core and a nuclear mantle. Fig. 1.2 shows a schematic plot of neutron stars, where several related properties are listed. Fig. 1.3 shows the phase diagram relevant for neutron stars.

Once given the microscopic description of the dense nucleonic matter $P(\epsilon)$, it is possible to find out the mass radius (M-R) relation of spherical non-rotating neutron stars by solving the Tolman-Oppenheimer-Volkoff (TOV) equations.

$$\begin{aligned} \frac{dP}{dr} &= -\frac{G[m(r) + 4\pi r^3 P/c^2][\epsilon + P/c^2]}{r[r - 2Gm(r)/c^2]} \\ \frac{dm}{dr} &= 4\pi \epsilon r^2 \end{aligned} \tag{1.1}$$

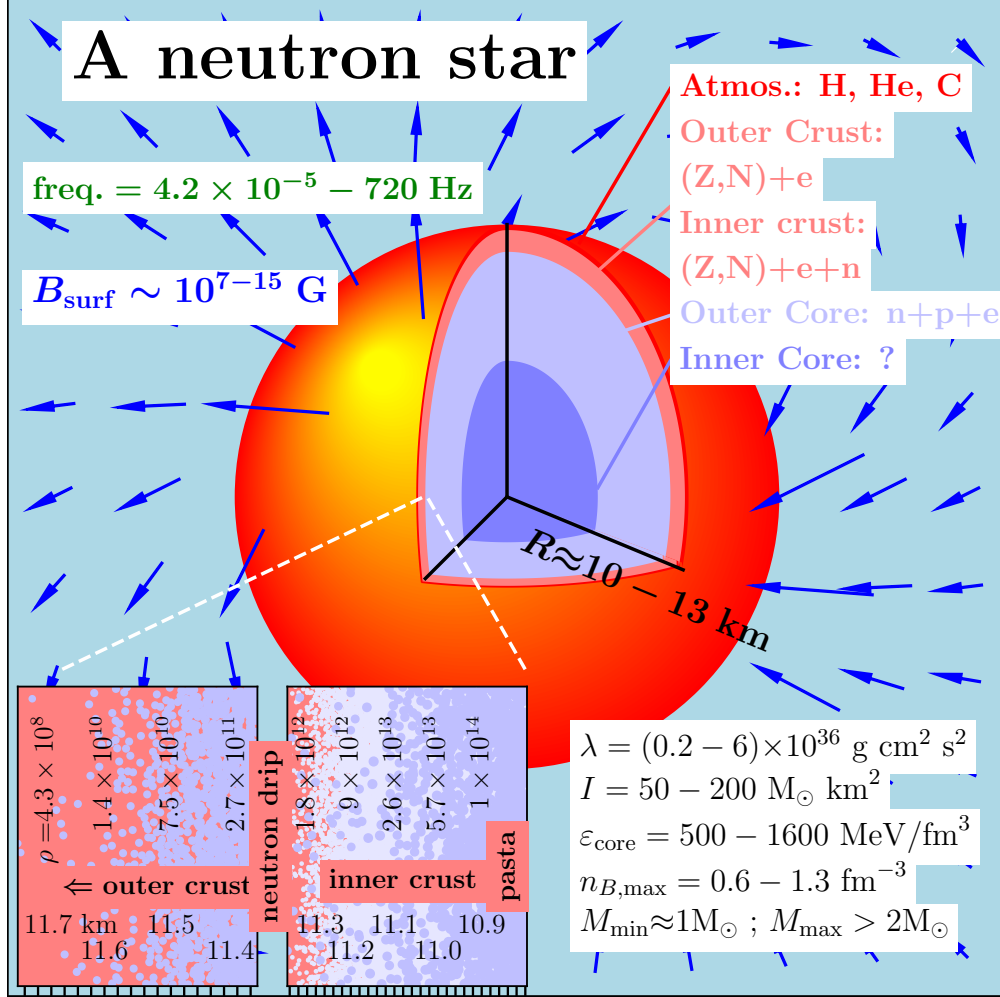


Figure 1.2: Structure of neutron stars with selected properties are given in Ref. [31]. The observational limit on the frequency [19, 39] and surface magnetic fields [91, 47] are given on the top left of the figure. The basic composition of each layer of the neutron star is given on the top right of the figure. A schematic plot of crust with radius is given on the bottom left of the figure. The red dots are nucleons and the blue dots are nuclei. Range of tidal deformability, moment of inertia, energy density, maximum baryon density and mass are given on the bottom right of the figure [77, 80].

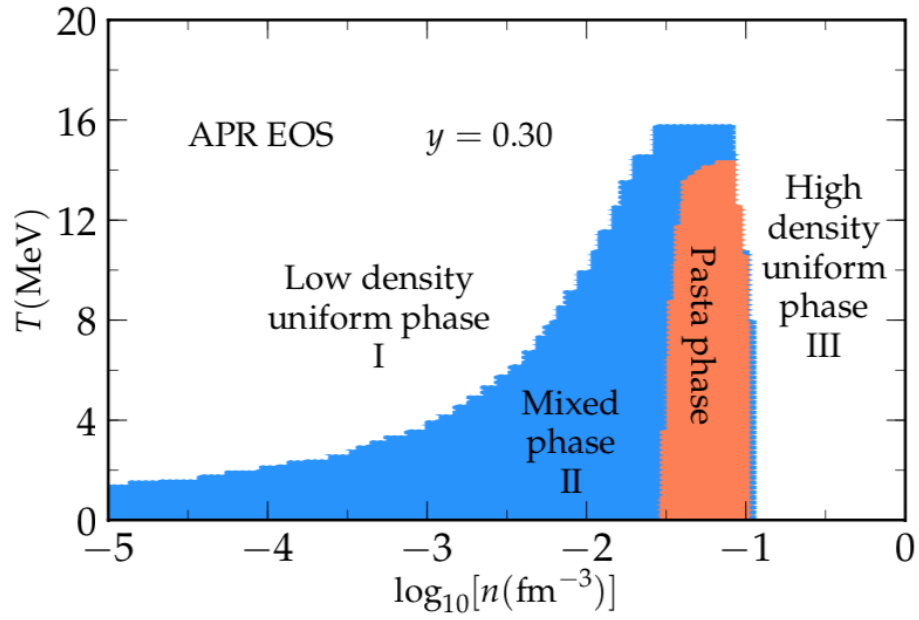


Figure 1.3: Phases in dense stellar matter from Ref. [49]. The cold neutron star matter (tens of KeV) corresponds to bottom region of the plot. From left to right, the matter passes through mixed phase, pasta phase and high density uniform phase.

where two boundary conditions are necessary: $m(r) = 0$ and $P(r = 0) = P_0$. Then, the solution of the equations will give a mass and pressure profile $m(r)$ with the pressure being zero at some point when $r = R$, giving the radius of the star. The equations also offer a one-to-one correspondence between the EOS and the M-R relation, thus providing a way to test the underlying nuclear physics through astronomical observations. There are a limited number of observations which lead to constraints on neutron star masses and radii. First, precise measurements of neutron star masses around 2 solar masses [20, 3, 18] set up a lower limit for maximum neutron star mass. Secondly, simultaneous datasets on neutron star mass and radius can be measured through either X-ray bursters with photospheric radius expansion or transient low-mass X-ray binaries [61, 79]. Lastly, recent detection of gravitational wave [53] and its electromagnetic counterpart [1] from binary neutron star merger, GW170817, put constraints on the tidal deformability

$$\tilde{\Lambda} = \frac{16}{3} \frac{(M_1 + 12M_2) M_1^4 \Lambda_1 + (M_2 + 12M_1) M_2^4 \Lambda_2}{(M_1 + M_2)^5} \quad (1.2)$$

where separately

$$\Lambda_{1,2} = \frac{2}{3} k_2 \left(\frac{R_{1,2} c^2}{GM_{1,2}} \right)^5 \quad (1.3)$$

The k_2 here is the Love number depending on the structure of the neutron star. Analysis of LIGO and Virgo results yield the chirp mass $\mathcal{M} = (M_1 M_2)^{3/5} / M^{1/5} = 1.188^{+0.004}_{-0.002} M_\odot$ and total mass $M = M_1 + M_2 = 2.74^{+0.04}_{-0.01} M_\odot$, where M_1 and M_2 are the companion masses. Therefore, the way is two-folded. On the one hand, we confirm the results of our calculation by checking with astrophysical data. We also use the astrophysical input to understand the theory of nuclear matter.

1.4 The Equation of State of Hot and Dense Matter

The equation of state (EOS) relates pressure or free energy density to baryon densities (n_B), proton fraction (Y_e), and temperature (T). In the following, we first express free energy density as function of n_B , Y_e and T as $f(n_B, Y_e, T)$ and then compute energy density, pressure, entropy and chemical potentials using thermodynamical relations. The reason is that the

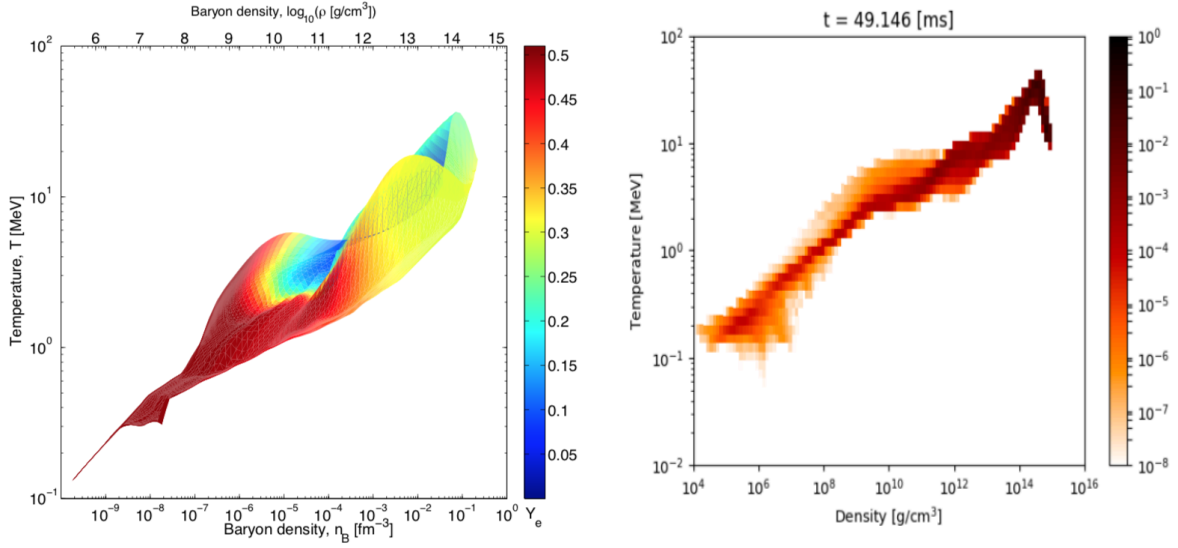


Figure 1.4: Temperatures and density profile (left panel) during a core-collapse supernova simulation at 1s post bounce. The color-coding shows the electron fraction from Ref. [26]. Histograms of the thermodynamics conditions (right panel) experienced by matter during a BNS merger from an equal mass merger simulation extending up to 40ms postmerger and employing the DD2 EOS from Ref. [65]. Note nuclear saturation density $n_0 = 0.16 \text{ fm}^{-3} = 2.7 \times 10^{14} \text{ g/cm}^3$.

function form is consistent with $df = \mu_n dn_n + \mu_p dn_p - sdT$. The weak equilibrium is not assumed since the reaction timescale of weak interaction is longer compared to the thermal equilibrium in the environment of simulations of core-collapse supernova and neutron star mergers. The (n_B, Y_e, T) forms a three-dimensional parameter space and has to covers the range explored by simulations. For supernova [25] and neutron star merger [50] simulations, profiles show T varies from 0 to 100 MeV, baryon density from 10^{-12} to 2.0 fm^{-3} and proton fraction from 0 to 0.6. Fig. 1.4 shows the temperature, density and proton fraction reached for a supernova simulation in 1s post bounce. In general, astrophysical simulations use EOS of dense matter as microscopic input in tabular form, which cover the range mentioned above.

There are several tabulated general purpose EOS available currently from CompOSE (CompStar Online Supernova Equations of State) database [86]. The first set of EOSs, developed by Lattimer and Swesty (LS) [52], was based on the liquid droplet model with single-nucleus approximation. The parameters of the liquid droplet model come from three different non-relativistic Skyrme interactions. Two of the three Skyrme interactions have nuclear incompressibilities (K) far outside of modern constraints [94, 75]. The third, with $K = 220 \text{ MeV}$, has a combination of symmetry energy (S) and slope of the symmetry energy (L) that are only slightly outside of current constraints ([24, 51, 41, 83]). The LS EOS with $K = 220 \text{ MeV}$ also produces a $2 M_\odot$ neutron star and is still important for simulations of core-collapse supernovae and neutron star mergers.

The second set of EOSs came from H. Shen et al. [74] (STOS) (also using the single-nucleus approximation) and was based on the NL3 relativistic mean-field Lagrangian. The values of K and L for NL3 are much larger than current neutron star observations (see the analysis in e.g., [79]) and nuclear theory [35] suggests.

While the single-nucleus approximation is sufficient to describe the bulk thermodynamics, it does not in general accurately describe the composition [10, 40, 7, 59, 4, 76] and the associated weak reaction rates. More modern EOS tables often include a more complete nuclear distribution as a result.

The third set from G. Shen et al. [73] (SHT) includes an EOS table based on a more modern relativistic mean-field model, “FSUGold” [84], and goes beyond the single nucleus

approximation to include a full distribution of nuclei in nuclear statistical equilibrium (NSE). This model has values of K , L and S that are within recent constraints from experiments and (in later versions) produce a neutron star maximum mass larger than $2 M_{\odot}$. These EOSs based on FSUGold include more modern nuclear physics input, including a proper treatment of nearly non-degenerate matter that matches the virial expansion.

The fourth set of EOS tables was based on the work of Hempel (HS) and others [36] that built upon several nucleon-nucleon interactions which produce reasonable values of K , S and L and generate $2 M_{\odot}$ neutron stars, including FSUGold, DD2 [87], IUFSU [23], SFHo [78] and SFHx [78]. The latter two interactions were designed to simultaneously match laboratory nuclei and give neutron star radii that match astronomical observations of neutron stars [79].

The fifth set is from Furusawa et al. [28] (FYSS) with a full distribution of nuclei in NSE. Phase transitions are considered by subtracting Coulomb terms out of nuclear masses from an empirical mass table and geometric functions are used for interpolation between nuclei phase and spherical hole phase. In a later paper [27], in-medium effects are taken into account phenomenologically.

In Chapter 4, we will compare our EOS with the other EOS mentioned above and examine the nuclear distributions at sub-nuclear densities.

Chapter 2

Homogeneous model for nuclear matter

2.1 Introduction

Over this large three-dimensional (n_B, Y_e, T) space, there are several different physical regimes each constrained by different observables and theoretical approaches. The first regime, zero temperature nuclear matter at nuclear saturation density, is closely connected to nuclear masses, charge radii, giant resonances, and other laboratory observables. Global fits to experimental data have been performed with Skyrme (e.g., Ref. [48]) and covariant mean-field models (e.g., Ref. [69]). The second regime, cold neutron matter below nuclear saturation density, is difficult to probe experimentally but is well-constrained by theoretical calculations based on semi-phenomenological nuclear forces or microscopic chiral effective field theory-based interactions [30, 34, 15]. The third regime, strongly-interacting high-temperature matter, is best described by interactions and many-body approaches similar to those applied to cold neutron matter near saturation density [57, 89, 13, 21]. The fourth regime, low-density and high-temperature matter that is nearly non-degenerate, is best described by the virial expansion. The equation of state in this regime is determined from nucleon-nucleon scattering phase shifts [45, 44]. Finally, neutron-rich matter at densities above twice saturation density is most strongly constrained by observations of neutron star masses and radii, particularly the observation of neutron stars with $M \simeq 2M_\odot$ [20, 3].

In this chapter, we construct a phenomenological free energy density that is consistent with observational and theoretical constraints in the five aforementioned physical regimes. This is in contrast to works that attempt to describe matter over the entire density and temperature range with a single detailed model of the nucleon-nucleon interaction. Many previous works proceed this way using a Skyrme-based or relativistic mean-field model to describe matter at all densities and temperatures. The principal problem is that these models are guaranteed to work well only for isospin-symmetric nuclear matter at zero temperature. Extrapolating these models to other density and temperature regimes may lead to inaccurate EOS results or may introduce unphysical correlations between the nature of matter across different regimes. For example, given a Skyrme model it is common to observe that the nuclear incompressibility is correlated with the maximum mass of neutron stars. Such a correlation has little physical meaning, however, since the neutron star maximum mass is determined by interactions in high-density matter that likely have little similarity to nucleons in the laboratory (see a similar argument in Ref. [64]). We avoid extrapolations where possible, but some extrapolation will still be required where experimental and theoretical guidance is lacking. Fig. 2.1 shows a schematic plot of the five different regimes we mentioned above and source of uncertainties associated with them.

Our second advance is in the treatment of uncertainties. The most relevant parameters which describe the uncertainties in different density and temperature regimes are not clearly related. The virial expansion provides a clear path forward for describing uncertainties at low-density and high-temperature, but higher-order virial terms are not necessarily useful for quantifying uncertainties at higher densities. In this chapter, through the construction of a phenomenological model one can vary uncertainties in different regimes independently, without spoiling agreement elsewhere.

2.1.1 Choice of parameters

The EOS table is constructed by combining an EOS for homogenous nucleonic matter consisting only of neutrons and protons. The EOS is written in the form of the Helmholtz free energy (including only the contribution from nucleons) $f_{\text{np}}(n_B, Y_e, T)$. In the discussion below, we remove the nucleon rest mass contributions from the free energy densities and

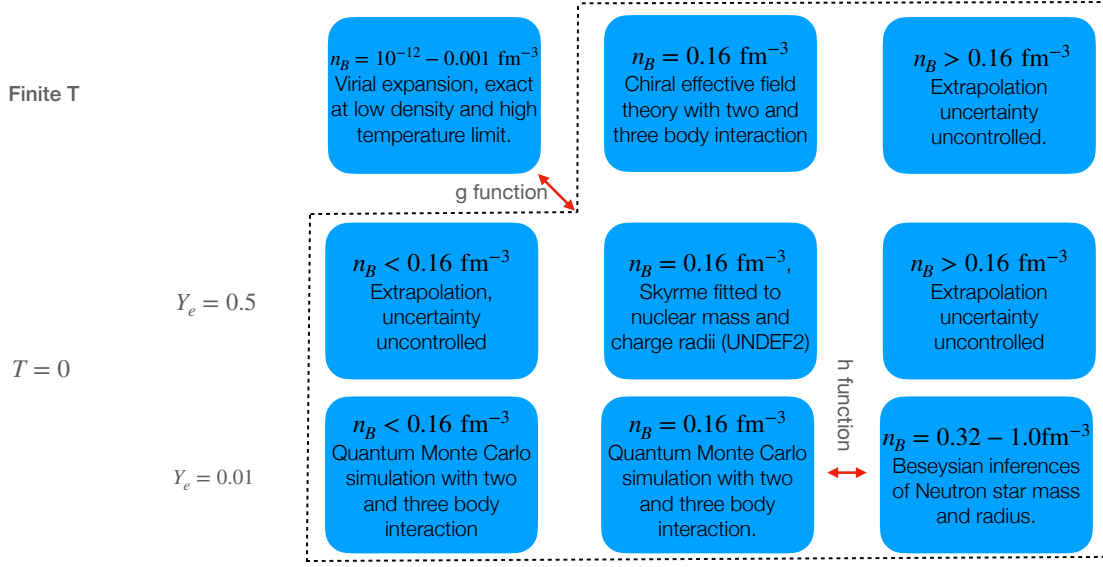


Figure 2.1: Schematic plot of uncertainty from five different regimes and uncertainties.

chemical potentials and use a tilde when these rest mass contributions are included, i.e.

$$\begin{aligned} \tilde{f}_{\text{np}}(n_B, Y_e, T) &\equiv f_{\text{np}}(n_B, Y_e, T) \\ &+ n_B [(1 - Y_e) m_n + Y_e m_p], \end{aligned} \quad (2.1)$$

where m_n and m_p are the neutron and proton masses. When electrons are included, their rest mass contribution to the free energy is also included. We ignore muons because they are rarely included in simulations [60]. We also ignore exotic particles at higher densities. Thus the proton fraction, x_p , is always equal to the electron fraction, Y_e .

2.2 Virial expansion for nuclear matter at high temperature

2.2.1 Thermodynamic quantities

The virial expansion is a model-independent way of describing systems of dilute gas. It in general treats both bound states and scattering resonances by including mixed terms among different constituents. [45, 44, 72]. With a system consists of protons and neutrons, the grand partition function Q can be expanded as a series of fugacities, which are defined by $z_i = \exp(\mu_i/T)$ $i = n, p$. The validity of the expansion is justified when $z_i \ll 1$. The thermodynamic pressure, which is related to the logarithm of the grand partition function is

$$\frac{P}{T} = \frac{\log Q}{V} = \frac{2}{\lambda^3} [z_n + z_p + (z_n^2 + z_p^2) b_n + 2z_p z_n b_{pn} + O(z_i^3)] \quad (2.2)$$

where λ is the thermal wavelength of nucleons $\lambda \equiv [4\pi / (m_n T + m_p T)]^{1/2}$. The difference caused by the mass of protons and neutrons is ignored for simplicity.

The number densities of nucleons are obtained by taking derivatives with respect to z_n and z_p , separately.

$$n_i = z_i \left(\frac{\partial}{\partial z_i} \frac{\log Q}{V} \right)_{V,T} \quad (2.3)$$

Therefore the system is described by the equations,

$$\begin{aligned} n_n &= 2\lambda^{-3} [z_n + 2z_n^2 b_n(T) + 2z_n z_p b_{pn}(T)] \\ n_p &= 2\lambda^{-3} [z_p + 2z_p^2 b_n(T) + 2z_n z_p b_{pn}(T)] \end{aligned} \quad (2.4)$$

Following from thermodynamics, the entropy, energy density and free energy density can be written as

$$\begin{aligned} s &= \frac{5P}{2T} - n_n \log z_n - n_p \log z_p + \frac{2T}{\lambda^3} [(z_n^2 + z_p^2) b'_n + 2z_p z_n b'_{pn}] \\ \epsilon &= Ts + \sum_{i=n,p} n_i \mu_i - P \\ &= \frac{3}{2}P + \frac{2T^2}{\lambda^3} [(z_n^2 + z_p^2) b'_n + 2z_p z_n b'_{pn}] \\ f &= \epsilon - Ts \end{aligned} \quad (2.5)$$

2.2.2 Virial coefficients

The second virial coefficients describing z^2 terms, $b_n \approx b_p$ and b_{pn} , can be computed by integrating over all partial waves of two-body elastic scattering phase shifts. The integrals are given by

$$b_n(T) = \frac{1}{2^{1/2}\pi T} \int_0^\infty dE e^{-E/2T} \delta_n^{\text{tot}}(E) - 2^{-5/2} \quad (2.6)$$

and

$$\begin{aligned} b_{pn}(T) &= b_{\text{nuc}}(T) - b_n(T) \\ b_{\text{nuc}}(T) &= \frac{1}{2^{3/2}\pi T} \int_0^\infty dE e^{-E/2T} \delta_{\text{nuc}}^{\text{tot}}(E) - 2^{-5/2} \end{aligned} \quad (2.7)$$

Here the term $-2^{-5/2}$ comes from contributions of the quantum effect of free Fermi gas. Different from Ref. [45], here the term $\frac{3}{2^{1/2}}(e^{E_d/T} - 1)$ is taken out since it represents the deuteron contribution. It will be added back when the full ensemble of nuclei are included through nuclear statistical equilibrium. The estimation of phase shifts has to include spin/isospin degeneracy factors of $2J + 1$ or $2T + 1$ for each separate state and are given by

$$\delta_n^{\text{tot}}(E) = \sum_{S,L,J} (2J + 1) \delta_{2S+1L_J}(E) \quad (2.8)$$

$$\delta_{\text{nuc}}^{\text{tot}}(E) = \sum_{S,L,J} (2J + 1)(2T + 1) \delta_{2S+1L_J}(E) \quad (2.9)$$

The third virial coefficients are related to nucleon-deuteron and three-nucleon interactions and are not well known. However, they correspond to higher order contributions and are relatively small.

Numerical results can be computed with NN or NP phase shifts from the Nijmegen partial wave analysis. In order to gain continuous expressions, we employ analytical fits similar to those in Ref. [46], but in order to their divergence behavior at $T \rightarrow 0$, we constrain the fit to match the finite-range expansion results for $T < 1$ MeV. The values of the virial coefficients at high temperature are not well-known, so we arbitrarily constrain the fits so that the virial coefficients give the value expected for noninteracting fermions at $T = 150$ MeV. For neutron

Table 2.1: Virial coefficient b_n obtained from partial wave analysis used for the virial EOS in this work.

parameter	value
b_0	0.28745
b_1	$2.2006 \times 10^{-3} \text{ MeV}^{-1}$
b_2	$-2.6210 \times 10^{-5} \text{ MeV}^{-2}$
b_3	$6.0617 \times 10^{-8} \text{ MeV}^{-3}$
b_4	1.0595×10^{-2}
b_5	$5.6734 \times 10^{-2} \text{ MeV}^{-2}$
b_6	3.4925 MeV
b_7	-2.7106×10^{-3}
b_8	3.1405 MeV^{-1}
b_9	1.2010 MeV

matter virial coefficient, three points were added at $T = 0.1, 0.5$ and 150 MeV , separately.

$$k \cot \delta = -\frac{1}{a} + \frac{1}{2} r_{\text{eff}} k^2 \quad (2.10)$$

For $T = 0.1$ and 0.5 MeV , only 1S_0 is significant. Scattering length $a = -18.9 \text{ fm}$ and effective range $r_{\text{eff}} = 2.75 \text{ fm}$ are determined from Ref. [32]. For $T = 150 \text{ MeV}$, non-interacting quantum result is used. The b_n is fitted to a 10-parameter functional form.

$$b_n(T) = b_0 + b_1 T + b_2 T^2 + b_3 T^3 + b_4 e^{-b_5(T-b_6)^2} + b_7 e^{-b_8(T-b_9)} \quad (2.11)$$

where the coefficients are showed in Table. 2.1.

The dominant contribution of phase shift comes from both 1S_0 and 3S_1 . Therefore the higher-order phase shift are ignored in finite-range expansion. We use the scattering length -23.74 fm and effective range 2.77 fm for 1S_0 channel[32] and the scattering length 5.418 fm and effective range 1.833 fm for the 3S_1 channel from Ref.[63]. The fit for b_{pn} is

$$b_{pn}(T) = c_0 e^{-c_1(T+c_2)^2} + c_3 e^{-c_4(T+c_5)} \quad (2.12)$$

where the coefficients are showed in Table. 2.2. The data and the fit are shown in Fig. 2.2.

Table 2.2: Virial coefficient b_{pn} obtained from partial wave analysis used for the virial EOS in this work.

parameter	value
c_0	1.5273
c_1	$1.7488 \times 10^{-4} \text{ MeV}^{-2}$
c_2	1.7550×10^1
c_3	0.45104
c_4	0.27513 MeV^{-1}
c_5	-1.1250 MeV

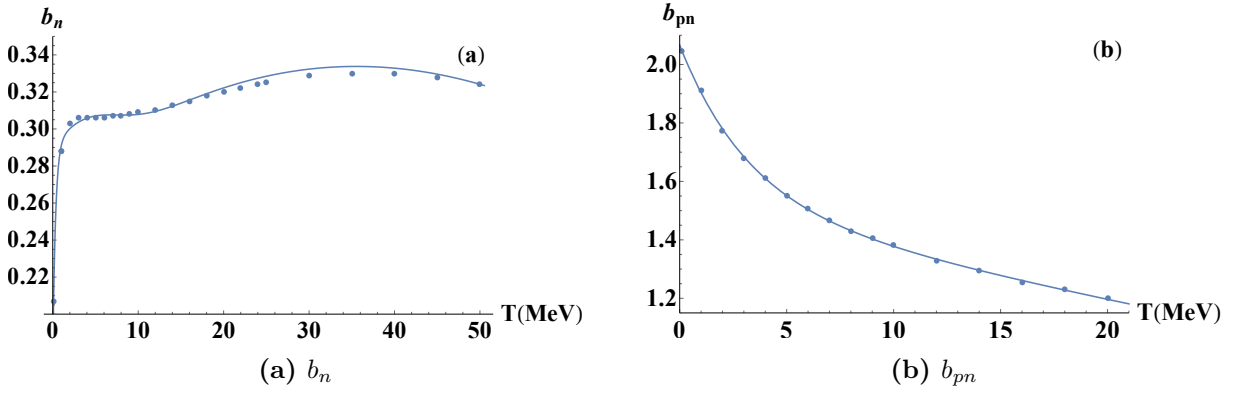


Figure 2.2: Fit of virial coefficients to data. The points at $T=0.1, 0.5$ MeV are computed through effective range expansion.

2.3 Symmetric matter at saturation density

For symmetric matter at saturation density, one of the most commonly used potential models is called the Skyrme model [88]. In this model, a three-body contact interaction is employed

$$v_{123}^{(3)} = t_3 \delta(\vec{r}_1 - \vec{r}_2) \delta(\vec{r}_2 - \vec{r}_3) . \quad (2.13)$$

The two-body interaction comes from a gaussian central force with exchange terms in coordinate space.

$$V_{12} = e^{-(r_{12}/\mu)^2} (W + BP_\sigma - HP_\tau - MP_\sigma P_\tau) \quad (2.14)$$

The P_τ , P_σ stand for isospin exchange and spin exchange operator defined as $P_\tau = \frac{1}{2}(1 + \hat{\tau} \cdot \hat{\tau}')$ and $P_\sigma = \frac{1}{2}(1 + \hat{\sigma} \cdot \hat{\sigma}')$, separately. The asymmetric requirement of fermion wave function also demands the spacial exchange operator $P_r P_\tau P_\sigma = -1$. Therefore, in fact $P_\tau P_\sigma = -P_r$. With the recognition of formula $(\hat{\tau} \cdot \hat{\tau}')^2 = 3 - 2\hat{\tau} \cdot \hat{\tau}'$ (similar for spin), the above four terms exhaust all possible terms one could come up with, which preserving usual invariance requirements.

In momentum space, this becomes

$$\begin{aligned} v_{12}^{(2)} = & t_0 (1 + x_0 P_\sigma) \delta(\vec{r}_1 - \vec{r}_2) \\ & + \frac{1}{2} t_1 [\delta(\vec{r}_1 - \vec{r}_2) k^2 + k^2 \delta(\vec{r}_1 - \vec{r}_2)] \\ & + t_2 \vec{k}' \cdot \delta(\vec{r}_1 - \vec{r}_2) \vec{k} + iW_0 (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k}' \times \delta(\vec{r}_1 - \vec{r}_2) \vec{k} . \end{aligned} \quad (2.15)$$

By applying time reversal invariance, the energy density is evaluated to be a functional form [81].

$$\mathcal{H} = \mathcal{H}_B + \mathcal{H}_G + \mathcal{H}_C + \mathcal{H}_J \quad (2.16)$$

The first term, $\mathcal{H}_B$, which represents the bulk term, is density dependent.

$$\begin{aligned}\mathcal{H}_B = & \frac{\hbar^2}{2m_n}\tau_n + \frac{\hbar^2}{2m_p}\tau_p + n(\tau_n + \tau_p) \left[\frac{t_1}{4} \left(1 + \frac{x_1}{2} \right) + \frac{t_2}{4} \left(1 + \frac{x_2}{2} \right) \right] \\ & + (\tau_n n_n + \tau_p n_p) \left[\frac{t_2}{4} \left(\frac{1}{2} + x_2 \right) - \frac{t_1}{4} \left(\frac{1}{2} + x_1 \right) \right] \\ & + \frac{t_0}{2} \left[\left(1 + \frac{x_0}{2} \right) n^2 - \left(\frac{1}{2} + x_0 \right) (n_n^2 + n_p^2) \right] \\ & + \frac{t_3}{12} \left[\left(1 + \frac{x_3}{2} \right) n^2 - \left(\frac{1}{2} + x_3 \right) (n_n^2 + n_p^2) \right] n^\epsilon\end{aligned}\quad (2.17)$$

$\mathcal{H}_G$ is associated with the gradient of nuclear density and surface tension of the nucleus

$$\mathcal{H}_G = \frac{1}{2} \left[Q_{nn} \left(\vec{\nabla} n_n \right)^2 + 2Q_{np} \vec{\nabla} n_n \cdot \vec{\nabla} n_p + Q_{pp} \left(\vec{\nabla} n_p \right)^2 \right] \quad (2.18)$$

where

$$\begin{aligned}Q_{nn} = Q_{pp} &= \frac{3}{16} [t_1 (1 - x_1) - t_2 (1 + x_2)] \\ Q_{np} = Q_{pn} &= \frac{1}{8} [3t_1 (1 + \frac{x_1}{2}) - t_2 (1 + \frac{x_2}{2})]\end{aligned}\quad (2.19)$$

$\mathcal{H}_C$ represents Coulomb interaction analogous to free electron gas. Since it is only related to proton density, this part is directly added to the sum. The second part is exchange Coulomb interaction.

$$\mathcal{H}_C(\vec{r}) = \frac{e^2 n_p(\vec{r})}{2} \int d^3 r' \frac{n_p(\vec{r}')}{|\vec{r} - \vec{r}'|} - \frac{3e^2}{4} \left(\frac{3}{\pi} \right)^{1/3} n_p(\vec{r})^{4/3} \quad (2.20)$$

$\mathcal{H}_J$ is spin-orbit interaction

$$\begin{aligned}\mathcal{H}_J = & -\frac{W_0}{2} \left(n_n \vec{\nabla} \cdot \vec{J}_n + n_p \vec{\nabla} \cdot \vec{J}_p + n \vec{\nabla} \cdot \vec{J} \right) \\ & + \frac{t_1}{16} \left(\vec{J}_n^2 + \vec{J}_p^2 - x_1 \vec{J}^2 \right) - \frac{t_2}{16} \left(\vec{J}_n^2 + \vec{J}_p^2 + x_2 \vec{J}^2 \right)\end{aligned}\quad (2.21)$$

The neutron spin-orbit density is defined as

$$\vec{J}_n = \sum_i^{neutron} \psi_i^\dagger \vec{\sigma} \times \vec{\nabla} \psi_i \quad (2.22)$$

and the total spin by

$$\vec{J} = \vec{J}_n + \vec{J}_p \quad (2.23)$$

Table 2.3: Parameters for Skyrme Hamiltonian $i_{\text{Skyrme}} = 738$ from ~ 1000 parametrization in Ref. [48], where i_{Skyrme} is the index.

t_0	t_1	t_2	t_3	x_0
-2719.7 MeV fm^3	417.64 MeV fm^5	-66.687 MeV fm^5	$15042 \text{ MeV fm}^{3(1+\alpha)}$	0.16154
x_1	x_2	x_3	α	
-0.047986	0.027170	0.13611	0.14416	

Since only homogeneous matter is considered, $\mathcal{H}_C$, $\mathcal{H}_J$ evaluates to be zero. The Skyrme model can be fit to nuclear masses, charge radii and pair energies with Bayesian inference. In this paper, a set of 1000 Skyrme parameterizations are selected from the posterior distribution [48]. Table 2.3 shows one typical parameter set for the Skyrme Hamiltonian.

There is little information for symmetric nuclear matter above saturation densities both in theory or experiment. For this reason, the Skyrme model is also extrapolated to higher densities and temperatures naively. It is not guaranteed the model still holds in the regime. The effective mass for nucleons could become negative for $n_B < 2 \text{ fm}^{-3}$ for some parameterizations. These models are removed for consistency.

$$m^*/m = (1 + \beta n_0)^{-1}, \quad \beta = \frac{M}{2\hbar^2} \left[\frac{1}{4} (3t_1 + 5t_2) + t_2 x_2 \right] \quad (2.24)$$

2.4 Pure neutron matter at/beyond saturation density

2.4.1 Quantum Monte Carlo method near saturation density

The Skyrme model is accurate in describing symmetric nuclear matter but it is not precise enough for neutron matter. With realistic two-nucleon and three-nucleon interactions, the non-perturbative many-body Hamiltonian of neutron matter can be solved with auxiliary field diffusion Monte Carlo techniques [29]. In this model, the Hamiltonian is,

$$H = -\frac{\nabla^2}{2m} + V_{2n} + V_{3n} \quad (2.25)$$

The 2n potential uses Argonne AV8' , which is a phenomenological interaction constructed to describe scattering data up to 600 MeV. The 3n potential includes s and p wave 2π exchange forces, an intermediate-range 3π loops force and a spin-independent short-range repulsive term. The ground state wave function and energy can be determined by evolving the many-body Schrödinger equation in imaginary time in which Hubbard-Stratonovich transformations are used to sample spin-isospin states. The method is first tested on light nuclei like ^{16}C and larger systems containing more than 100 nucleons are allowable later. The predictions of quantum Monte Carlo result (hereafter GCR) can be fitted with a four-parameter functional form.

$$\begin{aligned} \varepsilon_{\text{QMC}}(n_B) &= f_{\text{QMC}}(n_B) \\ &= n_B \left[a \left(\frac{n_B}{n_0} \right)^\alpha + b \left(\frac{n_B}{n_0} \right)^\beta \right] \end{aligned} \quad (2.26)$$

The range for the parameters $0.47 < a < 0.53$ and $12 \text{ MeV} < \alpha < 13 \text{ MeV}$ is chosen to include the limits caused by different combination of 2n and 3n potentials similar to [77].

The symmetry energy S and its slope L strongly constrains the relation of symmetric matter and pure neutron matter. The allowed region of S and L can be described by

$$(9.17S - 266 \text{ MeV}) < L < (14.3S - 379 \text{ MeV}) \quad (2.27)$$

where the limit of L is between 44 and 65 MeV and the limit of S is 29.5 and 36.1 MeV as [77]. The region is derived from various independent sources including heavy ion collision, giant dipole resonance, Sn neutron skin, ^{208}Pb dipole polarizability and neutron star observations. The Skyrme parametrization allowing computing S and L . some of them are certainly too large and failed to account for such corrections and also make correlating Skyrme results and quantum Monte Carlo results impossible. Those models are ignored for simplicity. The coefficient b and β are determined by

$$\begin{aligned} b &= S - a + (E/A)_{\text{sky}} \\ \beta &= \frac{1}{b} \left(\frac{L}{3} - \alpha a \right) \end{aligned} \quad (2.28)$$

where $(E/A)_{sky}$ is the binding energy per particle of nuclear matter from the Skyrme interaction. The results will be combined by assuming the symmetry energy is quadratic in x_p .

2.4.2 Pure neutron matter at high densities

For neutron matter above saturation density, the uncertainty from quantum Monte Carlo gradually accumulates, yet neutron star observations provide further constraints in that region. The EOS here [79] is determined by a dataset of six neutron stars including three type I X-ray bursters with photospheric radius expansion and three transient low-mass X-ray binaries. Several Markov chains were constructed randomly via using GCR and Model A (which models high-density matter using polytropes) based on the dataset mentioned above. The Markov chains are fit to the form below.

$$\begin{aligned} \varepsilon_{\text{NS}}(n_B) = f_{\text{NS}}(n_B) = & p_0 n_B \sqrt{n_B} + p_1 n_B^2 + p_2 n_B^2 \sqrt{n_B} \\ & + p_3 n_B^3 + p_4 n_B^4 \end{aligned} \quad (2.29)$$

A set of 1000 fits are selected from the posterior distribution. In order to combine the information from QMC near saturation density and information from neutron star observations, we used a function h

$$h = \frac{1}{1 + \exp[\gamma(n_B - \frac{3}{2}n_0)]} \quad (2.30)$$

where $\gamma = 20.0 \text{ fm}^{-3}$, to interpolate between the two regimes.

2.5 Forcing the neutron star EOS to be causal

Simple extrapolation to higher density regime beyond neutron star data ends up breaking causality. For zero temperature neutron matter, the speed of sound should be below 1.

$$c_s^2 = \left(\frac{dP}{d\epsilon} \right)_{n_B} < 1 \quad (2.31)$$

Below the largest density plausible be reached by astrophysical simulations $n_B = 2 \text{ fm}^{-3}$, we employ a simple prescription from Constantinou and Prakash(hereafter C&P)[14]. The EOS is determined by first choosing appropriate functions of c_s^2 between two end points, the largest density n_{Bf} in the Markov chain dataset and $n_B = 2 \text{ fm}^{-3}$. The function has to be integrable since c_s^2 is related second order thermodynamic quantities. An additional parameter ϕ , is added therefore $c_s^2(n_B = 2 \text{ fm}^{-3}) = \phi$.

If the speed of sound is larger at $n_B = n_{Bf}$, the c_s^2 is chosen to be a monotonic increasing function,

$$c_s^2 = 1 - a_1 + \frac{a_1 a_2 n_B^{a_1}}{1 + a_2 n_B^{a_1}} \quad (2.32)$$

the coefficient a_1 and a_2 is solved by matching $c_s^2(n_{Bf})$ and $c_s^2(n_B = 2 \text{ fm}^{-3})$ at both ends. The function has property of $c_s^2 \rightarrow 0$ for $n_B \rightarrow \infty$. Integrating twice results in

$$\varepsilon_{NS} = -m_n n_B + c_1 \left(\frac{1}{2} a_2 n_B^2 + \frac{n_B^{2-a_1}}{2-a_1} \right) + c_2 \quad (2.33)$$

where

$$\begin{aligned} c_1 &= \frac{\varepsilon_f + m_n n_{Bf} + P_f}{n_{Bf}^2 (a_2 + n_{Bf}^{-a_1})} \\ c_2 &= \frac{1}{2} \left[(\varepsilon_f + m_n n_{Bf} - P_f) + a_1 \frac{\varepsilon_f + m_n n_{Bf} + P_f}{(a_1 - 2) (1 + a_2 n_{Bf}^{a_1})} \right] \end{aligned} \quad (2.34)$$

If on the contrary, the speed of sound is smaller at $n_B = n_{Bf}$ than $n_B = 2 \text{ fm}^{-3}$, the c_s^2 is

$$c_s^2 = a_1 - \frac{a_1 a_2 n_B^{a_1}}{1 + a_2 n_B^{a_1}} \quad (2.35)$$

so when $n_B \rightarrow \infty$, $\beta \rightarrow 0$. The energy density is reconstructed to be

$$\varepsilon_{NS} = \frac{c_1 n_{B2} F_1 \left(1, -\frac{1}{a_1}, 1 - \frac{1}{a_1}, -\frac{n_B^{-a_1}}{a_2} \right)}{a_2} + c_2 - m_n n_B \quad (2.36)$$

where ${}_2F_1$ hyper-geometric function after Pfaff's transformation. The coefficients c_1 and c_2 are defined as

$$\begin{aligned} c_1 &= n_{B_f}^{-a_1-1} \left(a_2 n_{B_f}^{a_1} + 1 \right) (\varepsilon_f + m_n n_{B_f} + P_f) \\ c_2 &= n_{B_f}^{-a_1} \left[a_2 n_{B_f}^{a_1} (\varepsilon_f + m_n n_{B_f}) \right. \\ &\quad \left. - \left(a_2 n_{B_f}^{a_1} + 1 \right) {}_2F_1 \left(1, -\frac{1}{a_1}, 1 - \frac{1}{a_1}, -\frac{n_{B_f}^{-a_1}}{a_2} \right) \right. \\ &\quad \left. (\varepsilon_f + m_n n_{B_f} + P_f) \right] \frac{1}{a_2} \end{aligned} \quad (2.37)$$

When a rare case $c_s^2(n_{B_f}) = \phi = c_s^2(n_B = 2\text{fm}^{-3})$ happens, the c_s^2 is set to be a constant then. In such case,

$$\begin{aligned} \varepsilon_{NS} &= -m_n n_B + \frac{(\varepsilon_f + m_n n_{B_f} + P_f)}{(1 + C_{sf}^2)} \left(\frac{n_B}{n_{B_f}} \right)^{1+C_{sf}^2} \\ &\quad + \frac{C_{sf}^2 (\varepsilon_f + m_n n_{B_f}) - P_f}{1 + C_{sf}^2} \end{aligned} \quad (2.38)$$

The speed of sound is constrained to be no larger than the speed of light through the above procedure. In section 2.8, we will enforce causality similarly for the whole EOS for a finite temperature and multiple components system. It is equivalent to solving a partial differential equation in three-dimensional space subject to arbitrary boundary conditions. No analytical solution exists in that case, therefore numerical solutions are used instead.

2.6 Hot nuclear matter near saturation density

Nuclear two- and three-body forces based on chiral effective theory have shown great progress in computing the EOS of matter near nuclear saturation. In such case, the usual imaginary-time Matsubara sum based on the grand canonical ensemble does not apply since the system is unstable with phase mixing. The Kohn-Luttinger-Ward formalism is constructed through the canonical ensemble [90, 89]. The results is calculated separately for symmetric nuclear and pure neutron matter. It is fitted with the Skyrme interaction. Table 2.4 shows the coefficient of the interaction. In order to preserve the uncertainty at zero temperature, we fit only the finite-temperature correction from the chiral EOS. The finite temperature correction

Table 2.4: Skyrme parameters obtained from the chiral EOS used for the finite-temperature corrections in this work.

parameter	value
x_0	4.19756×10^1
x_1	-6.94792×10^{-2}
x_2	4.19202×10^{-1}
x_3	-2.87797×10^1
t_0	$9.99928 \times 10^5 \text{ MeV fm}^3$
t_1	$3.54185 \times 10^2 \text{ MeV fm}^5$
t_2	$-9.31632 \times 10^1 \text{ MeV fm}^5$
t_3	$-3.83996 \times 10^7 \text{ MeV fm}^{3(1+\alpha)}$
α	1.44165×10^{-1}

is therefore added on top of our EOS.

$$\Delta f_{\text{hot}}(n_B, x_p, T) \equiv f_{\text{hot}}(n_B, x_p, T) - f_{\text{hot}}(n_B, x_p, T = 0) \quad (2.39)$$

The results contain only two proton fraction, namely $x_p = 0$ and $x_p = 1/2$. We assume the correction is quadratic in isospin asymmetry, δ . As is showed in Ref. the quadratic approximation is a good approximation in most n_B and T regimes. Similar to the zero temperature case, the EOS of hot nuclear matter at saturation density is extrapolated to higher densities. This might lead to unphysical results in some regimes, as will be shown in Fig. 3.2, some of the high density and high temperature region, $ds/dT < 0$. Fortunately, this is fixed by the speed of sound correction there.

2.7 Full combined EOS

First, we combine the virial EOS for non-degenerate matter at subnuclear densities and the EOS for degenerate matter through

$$\begin{aligned} f_{\text{np}}(n_B, x_p, T) = & f_{\text{virial}}(n_B, x_p, T) g \\ & + f_{\text{deg}}(n_B, x_p, T) (1 - g) \end{aligned} \quad (2.40)$$

f_{virial} is the virial free energy density and f_{deg} stands for the free energy density when either neutrons or protons are sufficiently degenerate. The function g is defined by

$$g \equiv 1 / (1 + 10z_n^2 + 10z_p^2) \quad (2.41)$$

The interpolation ensures when virial expansion holds and $z_i \ll 1$, f_{deg} has leading terms in order of $O(z_i^6)$, since $f_{deg} \propto z_i^2$ and $1 - g \propto z_i^4$. The second term in consequence does not alter the virial results. The coefficient 10 enables a relatively fast transition so the entropy is positive in the entire region. The free energy density of degenerate matter can be divided into two parts, the zero temperature EOS and finite temperature correction from Chiral effective field theory.

$$\begin{aligned} f_{deg}(n_B, x_p, T) = & f_{\text{Skyrme}}(n_B, x_p = 1/2, T = 0) + \delta^2 \varepsilon_{\text{sym}}(n_B) + \\ & + \delta^2 \Delta f_{\text{hot}}(n_B, x_p = 0, T) + (1 - \delta^2) \Delta f_{\text{hot}}(n_B, x_p = 1/2, T) \end{aligned} \quad (2.42)$$

Previously, the EOS for zero temperature pure neutron matter is a combination of quantum Monte Carlo results at saturation density and neutron star EOS. This is included in the symmetric energy density to ensure the correlation relation between symmetry energy S and its slope L .

$$\begin{aligned} \varepsilon_{\text{sym}}(n_B) = & h(n_B) \varepsilon_{\text{QMC}}(n_B) + [1 - h(n_B)] \varepsilon_{\text{NS}}(n_B) \\ & - f_{\text{Skyrme}}(n_B, x_p = 1/2, T = 0) \end{aligned} \quad (2.43)$$

Using this formalism, the chemical potentials and entropy can be computed directly:

$$\begin{aligned}
\frac{\partial f_{\text{deg}}}{\partial n_n} = & \frac{1}{2} \mu_{n, \text{Skyrme}} (n_B, x_p = 1/2, T = 0) \\
& + \frac{1}{2} \mu_{p, \text{Skyrme}} (n_B, x_p = 1/2, T = 0) \\
& + \delta^2 \frac{\partial \varepsilon_{\text{sym}}}{\partial n_B} + \frac{2\delta(1-\delta)}{n_B} \varepsilon_{\text{sym}} \\
& + \frac{2\delta(1-\delta)}{n_B} \Delta f_{\text{hot}} (n_B, x_p = 0, T) \\
& + \delta^2 \Delta \mu_{n, \text{hot}} (n_B, x_p = 0, T) \\
& - \frac{2\delta(1-\delta)}{n_B} \Delta f_{\text{hot}} (n_B, x_p = 1/2, T) \\
& + (1-\delta^2) \Delta \mu_{n, \text{hot}} (n_B, x_p = 1/2, T)
\end{aligned} \tag{2.44}$$

$$\begin{aligned}
\frac{\partial f_{\text{deg}}}{\partial n_p} = & \frac{1}{2} \mu_{p, \text{Skyrme}} (n_B, x_p = 1/2, T = 0) \\
& + \frac{1}{2} \mu_{n, \text{Skyrme}} (n_B, x_p = 1/2, T = 0) \\
& + \delta^2 \frac{\partial \varepsilon_{\text{sym}}}{\partial n_B} - \frac{2\delta(1+\delta)}{n_B} \varepsilon_{\text{sym}} \\
& - \frac{2\delta(1+\delta)}{n_B} \Delta f_{\text{hot}} (n_B, x_p = 0, T) \\
& + \delta^2 \Delta \mu_{p, \text{hot}} (n_B, x_p = 0, T) \\
& + \frac{2\delta(1+\delta)}{n_B} \Delta f_{\text{hot}} (n_B, x_p = 1/2, T) \\
& + (1-\delta^2) \Delta \mu_{p, \text{hot}} (n_B, x_p = 1/2, T)
\end{aligned} \tag{2.45}$$

$$\begin{aligned}
s = \frac{\partial f_{\text{deg}}}{\partial T} = & -\delta^2 - s_{\text{hot}} (n_B, x_p = 0, T) - \\
& (1-\delta^2) s_{\text{hot}} (n_B, x_p = 1/2, T)
\end{aligned} \tag{2.46}$$

and

$$\begin{aligned}
\frac{\partial \varepsilon_{\text{sym}}}{\partial n_B} = & h' (n_B) \varepsilon_{\text{QMC}} (n_B) + h (n_B) \varepsilon'_{\text{QMC}} (n_B) \\
& - h' (n_B) \varepsilon_{\text{NS}} (n_B) + [1 - h (n_B)] \varepsilon'_{\text{NS}} (n_B) + \\
& - \frac{1}{2} [\mu_{n, \text{Skyrme}} (n_B, x_p = 1/2, T = 0) \\
& + \mu_{p, \text{Skyrme}} (n_B, x_p = 1/2, T = 0)]
\end{aligned} \tag{2.47}$$

2.8 Results of homogeneous matter

In sum, there are five parameters in total in this model. The a and α come from QMC functional form. Symmetry energy S and its slope L constrict the relation between symmetric nuclear matter and pure neutron matter. The quantity ϕ determines the form and asymptotic value of c_s^2 in C&P prescription. Besides, two indices are used to selected models from UNDEF2 parameterizations and Markov chains constructed on neutron star data.

2.8.1 Comparisons to limiting forms

Fig. 2.3 compare the result of EOS with its various limiting forms. One single parameter set is chosen randomly for the three cases. The left panel shows free energy per nucleon labeled as f_{total}/n_B compared to virial expansion at low density, high temperature in the non-degenerate limit. z_n and z_p are plot in the same panel. It is clear when both z_n and $z_p \rightarrow 0$, the full results smoothly match the virial EOS. The middle panel shows f_{total}/n_B compared to Quantum Monte Carlo results and neutron star EOS. The yellow curve corresponds to h function 2.30 mentioned before. Again f_{total}/n_B transits from f_{qmc}/n_B to f_{ns}/n_B as n_B increases. The right panel compares the full results at $T = 10\text{MeV}$ with zero temperature results only from Skyrme model. Small corrections due to finite temperature are presented which corresponds to the terms in the second line of Eq. 2.42.

2.8.2 Probability distributions from Monte Carlo simulations

Once the uncertainty of EOS is determined in each regime above, we can generate a distribution of EOSs by randomly selecting the 7 parameters α , a , S , L , index for Skyrme model and index for neutron star model. The Skyrme model is fitted to reproducing the charge radii and masses of various nuclei using Bayesian inference, but only the bulk matter terms are retained since we are only interested in the homogeneous matter. The neutron star model reproduces statistically allowed polytropic EOSs simultaneously matching data from photospheric radius expansion X-ray bursts and quiescent low-mass X-ray binaries.

Fig. 2.4 shows the variation of free energy per nucleon in the non-degenerate matter where the dominant contribution comes from virial expansion. The uncertainty is relatively

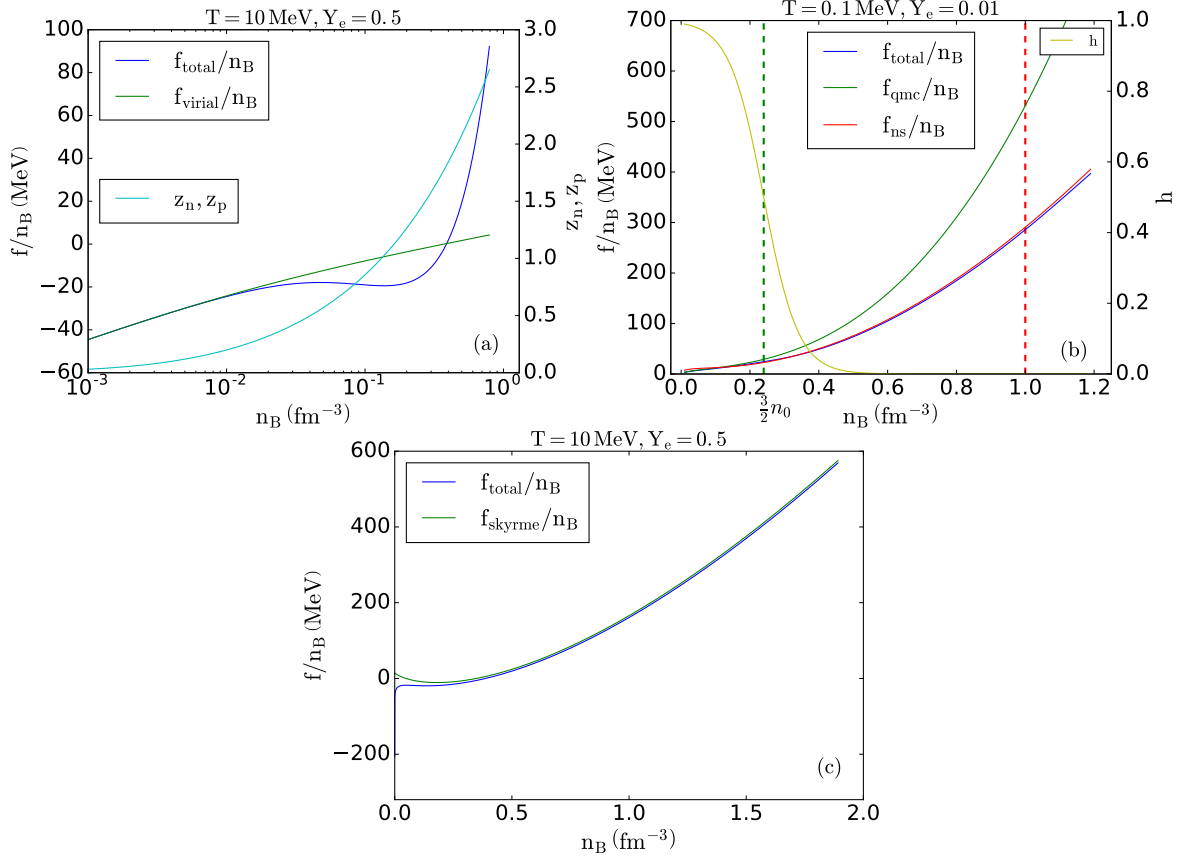


Figure 2.3: Three figures which show how the full EOS compares to the limiting forms. The left panel compares the full free energy to the result from the virial expansion and shows that they match at lower densities where the fugacities are much smaller than 1. The middle panel shows that the result for neutron matter matches the QMC free energy at low densities, the neutron star free energy at densities reached in the neutron star interiors, and is softened at high densities to ensure a speed of sound less than the speed of light. The right panel shows that free energy starts to deviate from the Skyrme interaction at higher temperatures as the corrections from the chiral EOS begin to contribute. These panels show the result from one of many EOSs generated in this work.

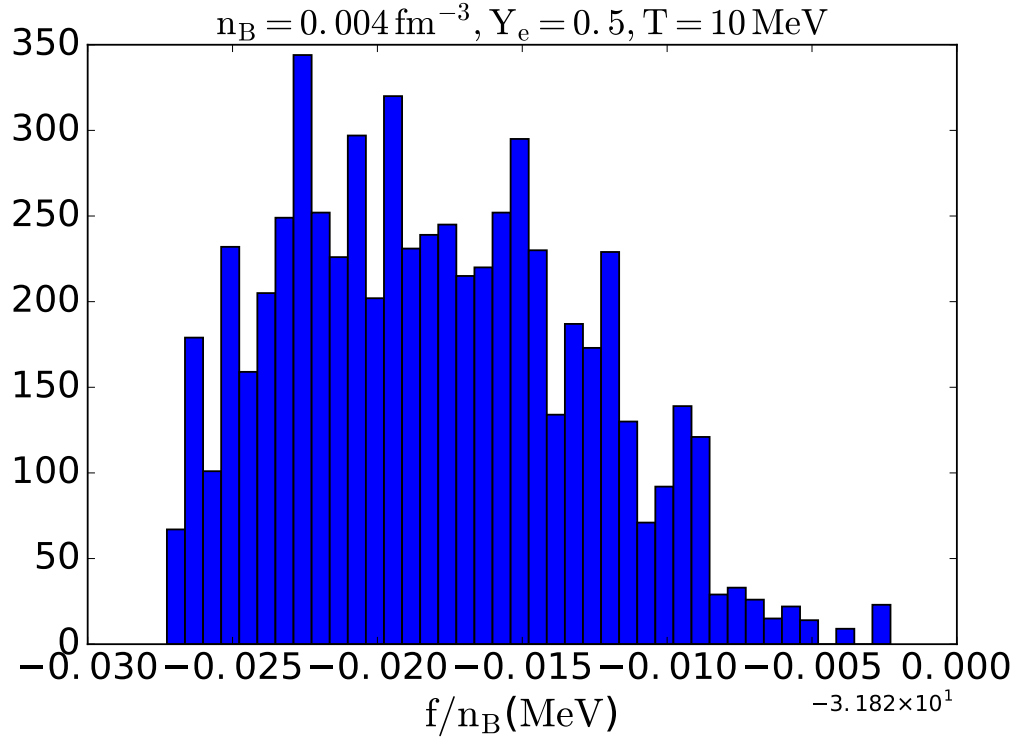


Figure 2.4: The probability distribution for the free energy per baryon at $n_B = 0.004 \text{ fm}^{-3}$, $Y_e = 0.5$, and $T = 10 \text{ MeV}$.

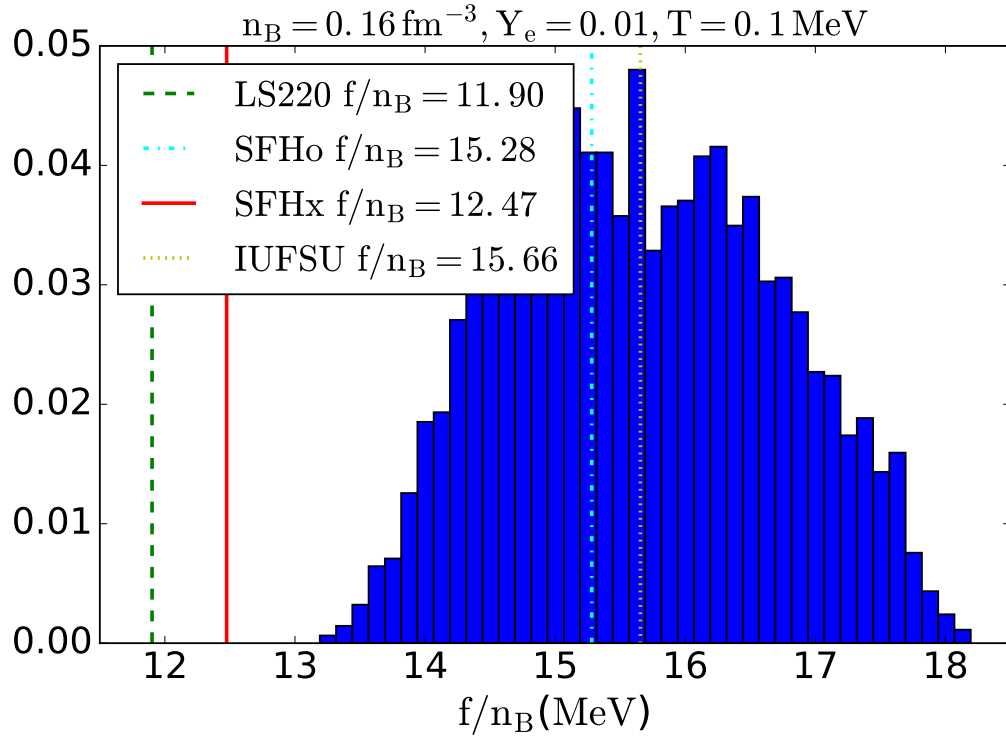


Figure 2.5: The probability distribution for the free energy per baryon at $n_B = 0.16 \text{ fm}^{-3}$, $Y_e = 0.01$, and $T = 0.1 \text{ MeV}$.

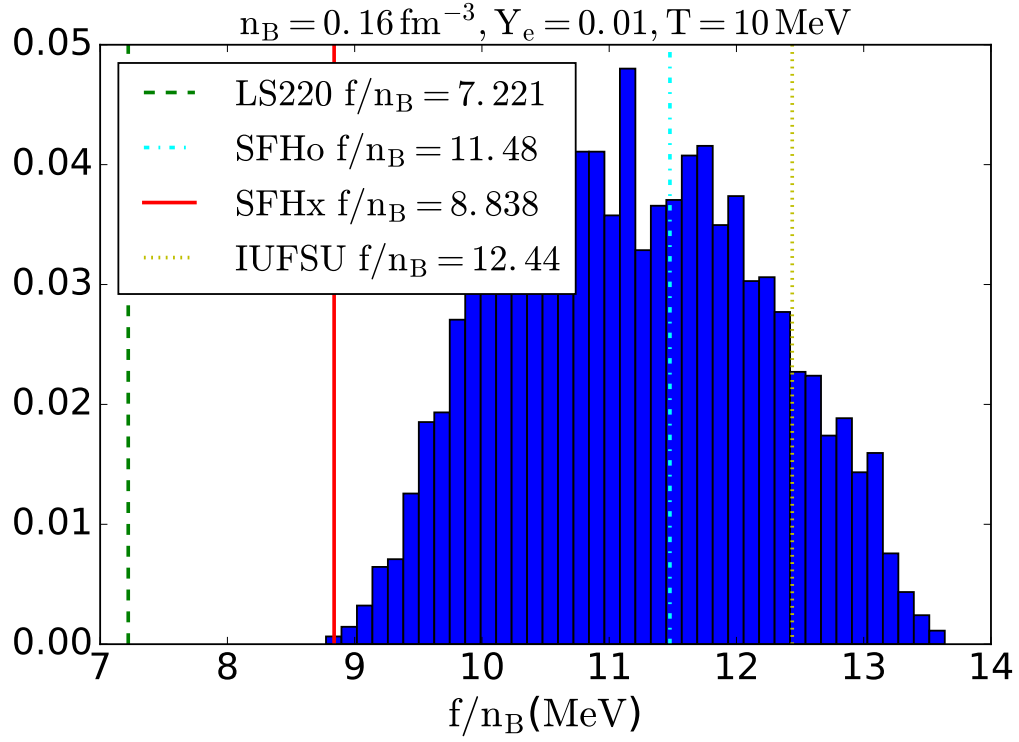


Figure 2.6: The probability distribution for the free energy per baryon at $n_B = 0.16 \text{ fm}^{-3}$, $Y_e = 0.01$, and $T = 10 \text{ MeV}$.

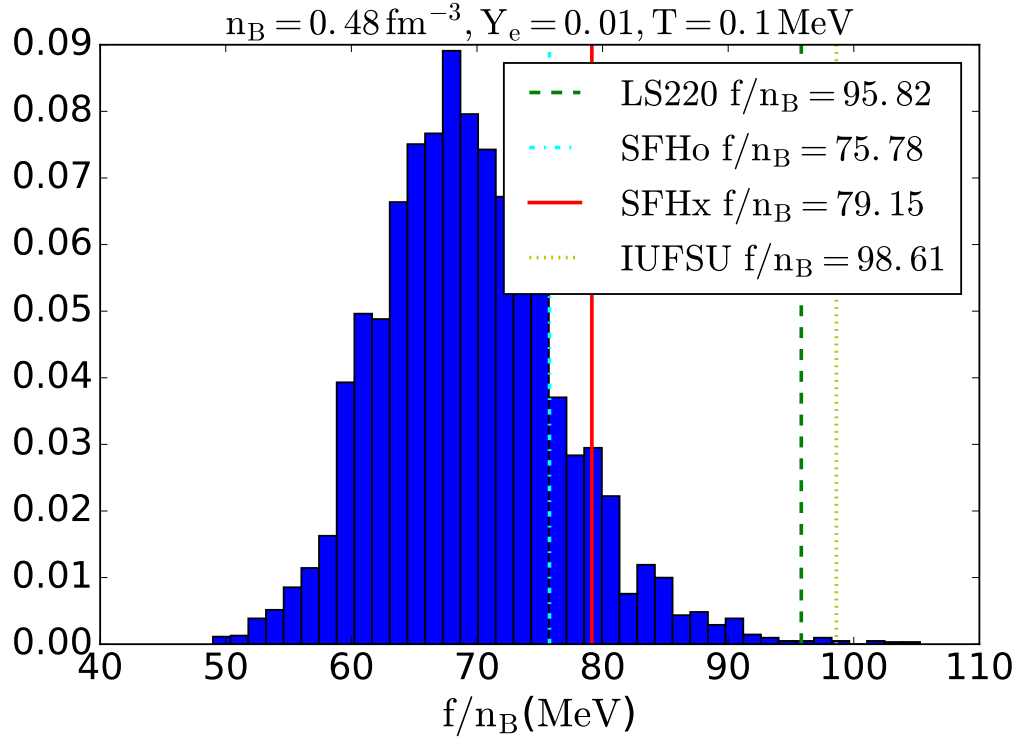


Figure 2.7: The probability distribution for the free energy per baryon at $n_B = 0.48 \text{ fm}^{-3}$, $Y_e = 0.10$, and $T = 0.1 \text{ MeV}$.

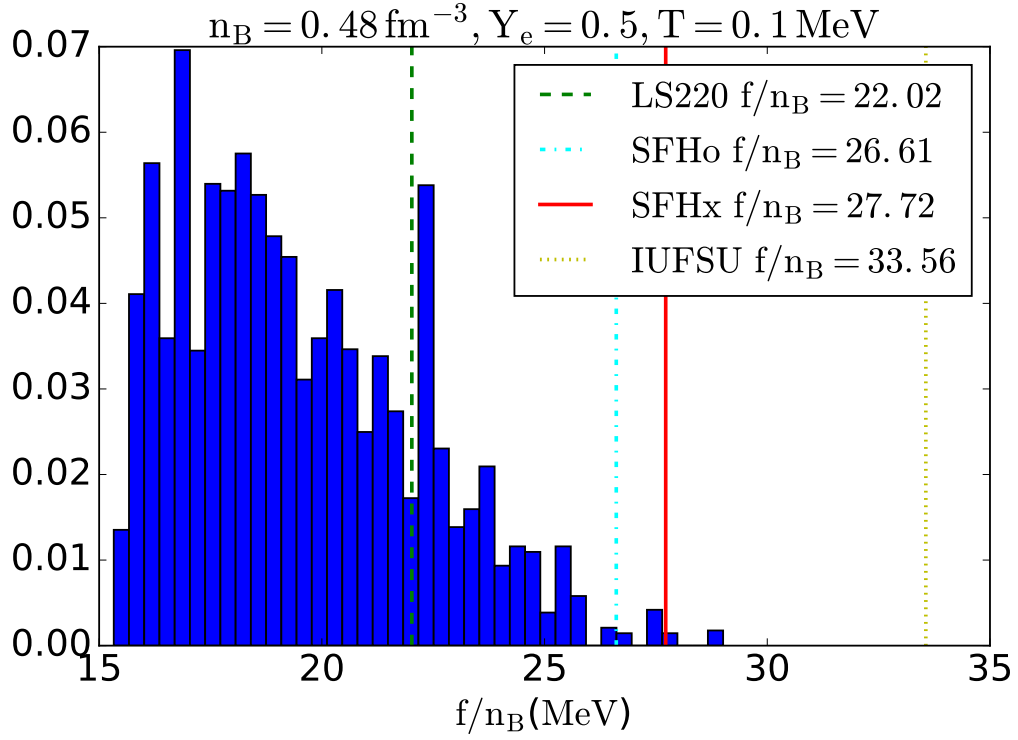


Figure 2.8: The probability distribution for the free energy per baryon at $n_B = 0.48 \text{ fm}^{-3}$, $Y_e = 0.5$, and $T = 0.1 \text{ MeV}$.

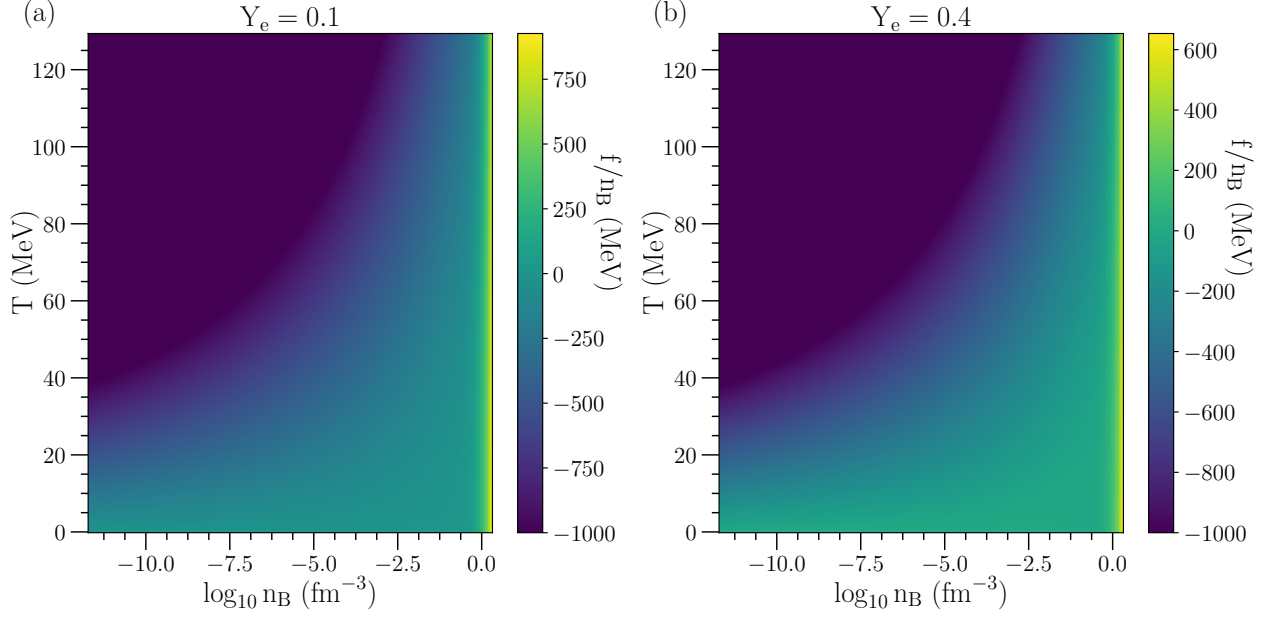


Figure 2.9: Density plots showing the free energy per baryon for matter at $Y_e = 0.1$ and $Y_e = 0.4$ over the full range of densities and temperatures considered in this work for one parameterization. Points with a free energy per baryon less than -1000 MeV are set equal to -1000 MeV to make the high-density behavior more clear. The main variation in the free energy per baryon from the lower-right region to the upper-left region in these plots is dominated by the virial contribution to the EOS. The degenerate part of the EOS is clear in the large increase in the free energy per baryon on the right-hand boundary (at large baryon densities).

small in this region. The distribution is not completely continuous on the right side, which originated from the limited sampling size of Skyrme fits.

Fig. 2.5 shows the variation for nearly pure neutron matter in the limit of zero temperature. The distribution is centered around 16 MeV, ranging from 13 to 18 MeV. The vertical lines showing results of other EOSs are plot also, including LS220, SFHo, SFHx and IUFSU. Those models less than 13 MeV are excluded by our model because they have symmetry energy less than 29.5 MeV.

Fig. 2.6 shows the distribution in the free energy per baryon at a slightly larger temperature, and the entropy contribution drops the free energy per baryon in each case. In comparison to the results from Fig. 2.5, the LS220 free energy per particle drops more than SFHo or SFHx because its effective mass (equal to the nucleon mass) is larger than that in SFHo/x (about 0.7 times the nucleon mass). The effective mass can be computed from the chiral interaction directly [43, 42], and close to the Fermi surface it is found to be nearly equal to the free-space nucleon mass. Second-order many-body perturbation theory contributions, however, produce a strong momentum dependence in this region, and averaging around $k = k_F$ the effective mass is about 0.85 times the free-space nucleon mass. The distribution in Fig. 2.6 is thus larger than LS220 because of the smaller symmetry energy ($S = 28.6$ MeV) and larger effective mass in the LS220 EOS.

Fig. 2.7 shows the probability distribution for the low-temperature neutron-rich matter free energy per baryon at higher densities. There is clearly a much larger spread in the free energy per baryon, corresponding to our larger ignorance regarding the nature of matter at higher density. While all models LS220, SFHo, SFHx and IUFSU are inside the region suggested by our parameterization, our distribution leans towards smaller values of the free energy because of the constraint from relatively small neutron star radii.

Fig. 2.8 shows low-temperature nuclear matter at higher densities. The non-smooth nature of the distribution is due to the small statistics afforded by the limited number of Skyrme models we have employed. IUFSU suggests a larger free energy here because it originates in a relativistic mean field model which tends to give larger pressures than the non-relativistic models like Skyrme. This region of parameter space is almost entirely unconstrained by experiment, since it is not possible to make cold isospin symmetric matter

at this density. However, dense isospin-symmetric matter is not as relevant for this work since simulations are typically neutron-rich at high density.

Fig. 2.9 shows the free energy per baryon for one of our parameterizations as a function of baryon density and temperature for two electron fractions. Using the formalism presented in this work, thousands of similar density plots can be generated with alternate parameterizations. The largest variation between parameterizations is in the free energy per particle at high density which changes with the “stiffness” of the EOS.

Chapter 3

Enforcing causality at high density

The speed of sound, c_s temperatures. When this condition is violated, we say that the EOS is “acausal”. When non-relativistic models are naively extrapolated to high density, most models are acausal by the time n_B exceeds $10 n_0$. Hydrodynamic simulations not only generate unphysical results but also could crash when the EOS is “acausal”. In the previous chapter, we applied a prescription for zero temperature pure neutron matter with C&P prescription [14], which contains only one variable n_B . This is equivalent to solving an ordinary differential equation. Integrate the equation twice gives Eq. 2.38, where the integral constants were chosen to match the boundary condition at $n_B = n_{Bf}$.

To generalize to a multi-component finite temperature system, an essential step is to ensure at each proton fraction and temperature, the speed of sound is less than the speed of light. Thus at each Y_e and T , a similar step has to be performed. However, the entropy and free energy density have not yet been recovered. Thermodynamic consistency must be preserved in Y_e and T direction so that μ_n , μ_p and S are continuous in those two directions. Solving the problem is equivalent to solving a partial differential equation with three variables n_B , Y_e and T subject to the boundary condition $c_s^2(n_B^*, Y_e, T) = 1.0$. An analytical solution does not exist in general, so we solve these equations numerically. The following section is taken from Ref. [22].

3.1 Numerical methods

We denote the baryon density as n_B^* , whenever the speed of sound is larger than the speed of light. To allow for finite precision errors in astrophysical simulations, a more conservative limit is applied, namely $c_s^2 < 0.9$. The simplest case in C&P prescription would be setting the c_s^2 to be a constant, equivalent to the case described in chapter 2.5.

We replace the EOS with such a casual EOS and the modified free energy density can be expressed as

$$\tilde{f}_{all} = \tilde{f}_{npe\gamma} \Theta(n_B^* - n_B) + \tilde{f}_{C\&P} \Theta(n_B - n_B^*) \quad (3.1)$$

where the electron and photon contribution is included along with neutrons and protons in $\tilde{f}_{npe\gamma}$ and the free energy density is added a tilde on top denoting we added the rest mass term. The Θ function guarantees that the old Helmholtz free energy density is replaced by C&P solutions after n_B^* . A couple of new symbols are introduced here to distinguish different thermodynamical quantities. We were using ϵ for energy density, ε is used when rest mass is included. S denotes for entropy, s for entropy density and $\tilde{s}$ for entropy per nucleon. The speed of sound is

$$c_s^2 = \left(\frac{dP}{d\varepsilon} \right)_{\tilde{s}, N_B, N_e} = \left(\frac{dP}{d\varepsilon} \right)_{\tilde{s}, N_B, Y_e} \quad (3.2)$$

where $\tilde{s} = S/N_B = s/n_B$, $Y_e = N_e/N_B$.

As is showed in the appendices, it can be computed by

$$\begin{aligned} c_s^2 = & \left[\sum_i \sum_k n_i n_k (f_{n_i n_k} - f_{n_k T} f_{n_i T} f_{TT}^{-1}) \right. \\ & \left. - 2 \sum_i s n_i f_{n_i T} f_{TT}^{-1} - s^2 f_{TT}^{-1} \right] \left(T s + \sum_i \mu_i n_i \right)^{-1}. \end{aligned} \quad (3.3)$$

where i sums over n, p, e, γ . The C&P derivation begins by noting that

$$P = -\varepsilon + n_B \left(\frac{\partial \varepsilon}{\partial n_B} \right)_{\tilde{s}, N_B, Y_e}. \quad (3.4)$$

To see this we can write

$$\begin{aligned} \left(\frac{\partial \varepsilon}{\partial n_B} \right)_{\tilde{s}, N_B, Y_e} &= \left[\frac{\partial(E/V)}{\partial V} \right]_{S, N_B, Y_e} \left[\frac{\partial(N_B/V)}{\partial V} \right]_{S, N_B, Y_e}^{-1} \\ &= \left(-\frac{P}{V} - \frac{E}{V^2} \right) \left(-\frac{N_B}{V^2} \right)^{-1} = \frac{(P + \varepsilon)}{n_B}. \end{aligned} \quad (3.5)$$

Taking the derivative of Eq. (3.4), we can also rewrite the pressure as a second derivative

$$\begin{aligned} \left(\frac{\partial P}{\partial n_B} \right)_{\tilde{s}, N_B, Y_e} &= - \left(\frac{\partial \varepsilon}{\partial n_B} \right)_{\tilde{s}, N_B, Y_e} + \left(\frac{\partial \varepsilon}{\partial n_B} \right)_{\tilde{s}, N_B, Y_e} \\ &\quad + n_B \left(\frac{\partial^2 \varepsilon}{\partial n_B^2} \right)_{\tilde{s}, N_B, Y_e} \end{aligned} \quad (3.6)$$

$$= n_B \left(\frac{\partial^2 \varepsilon}{\partial n_B^2} \right)_{\tilde{s}, N_B, Y_e}. \quad (3.7)$$

Thus we can proceed as C&P do,

$$\left(\frac{\partial^2 \varepsilon}{\partial n_B^2} \right)_{\tilde{s}, N_B, Y_e} - \frac{c_s^2}{n_B} \left(\frac{\partial \varepsilon}{\partial n_B} \right)_{\tilde{s}, N_B, Y_e} = 0. \quad (3.8)$$

Following the analytical continuation, at every value of $\tilde{s}$, N_B , and Y_e in the acausal region, we can use the C&P solution

$$\begin{aligned} \varepsilon_{C\&P}(\tilde{s}, n_B, N_B, Y_e) &= \left[\frac{\varepsilon^*(\tilde{s}, N_B, Y_e) + P^*(\tilde{s}, N_B, Y_e)}{\beta + 1} \right] \\ &\quad \times \left[\frac{n_B}{n_B^*(\tilde{s}, N_B, Y_e)} \right]^{\beta+1} \end{aligned} \quad (3.9)$$

$$+ \left[\frac{\beta \varepsilon^*(\tilde{s}, N_B, Y_e) - P^*(\tilde{s}, N_B, Y_e)}{\beta + 1} \right]. \quad (3.10)$$

If we assume that ε^* , P^* , and n_B^* are volume independent, then since they are determined at a fixed value of n_B , they cannot separately depend on N_B . Thus the full energy density

also does not depend on N_B . To show this explicitly, we start from

$$\begin{aligned}
E &= \mu_B N_B + \mu_L N_B Y_e + TS - PV, \\
dE &= (\mu_B + \mu_L Y_e + T\tilde{s}) dN_B + \mu_L N_B dY_e \\
&\quad + T N_B d\tilde{s} - P dV.
\end{aligned} \tag{3.11}$$

where $\mu_L \equiv \mu_p + \mu_e - \mu_n$. On the right hand side,

$$dV = \frac{1}{n_B} dN_B - \frac{N_B}{n_B^2} dn_B \tag{3.12}$$

and on the left hand side,

$$dE = d\left(\varepsilon \frac{N_B}{n_B}\right) = \frac{N_B}{n_B} d\varepsilon + \frac{\varepsilon}{n_B} dN_B - \frac{\varepsilon N_B}{n_B^2} dn_B. \tag{3.13}$$

Substituting the above two equations back into Eq. (3.11), we find

$$d\varepsilon = \mu_L n_B dY_e + T n_B d\tilde{s} + (\mu_B + \mu_L Y_e + T\tilde{s}) dn_B \tag{3.14}$$

and the N_B dependence disappears. Therefore $\varepsilon_{C\&P}(\tilde{s}, n_B, N_B, Y_e) = \varepsilon_{C\&P}(\tilde{s}, n_B, Y_e)$:

$$\begin{aligned}
\varepsilon_{C\&P}(\tilde{s}, n_B, Y_e) &= \left[\frac{\varepsilon^*(\tilde{s}, Y_e) + P^*(\tilde{s}, Y_e)}{\beta + 1} \right] \left[\frac{n_B}{n_B^*(\tilde{s}, Y_e)} \right]^{\beta+1} \\
&\quad + \left[\frac{\beta \varepsilon^*(\tilde{s}, Y_e) - P^*(\tilde{s}, Y_e)}{\beta + 1} \right].
\end{aligned} \tag{3.15}$$

We also find

$$\left(\frac{\partial \varepsilon_{C\&P}}{\partial Y_e} \right)_{\tilde{s}, n_B} = \mu_L n_B, \tag{3.16}$$

$$\left(\frac{\partial \varepsilon_{C\&P}}{\partial \tilde{s}} \right)_{n_B, Y_e} = T n_B, \tag{3.17}$$

$$\left(\frac{\partial \varepsilon_{C\&P}}{\partial n_B} \right)_{\tilde{s}, Y_e} = \mu_B + \mu_L Y_e + T\tilde{s}. \tag{3.18}$$

We choose to use this solution above the value of n_B , denoted $n_B^*(\tilde{s}, Y_e)$, for which $c_s^2 = \beta$. From Eq. (3.17) the temperature is

$$T = \frac{1}{n_B} \left(\frac{\partial \varepsilon_{C\&P}}{\partial \tilde{s}} \right)_{n_B, Y_e}. \quad (3.19)$$

We choose to use this solution above the value of n_B , denoted $n_B^*(\tilde{s}, Y_e)$, for which $c_s^2 = \beta$.

Thus computing the temperature using the method in Ref. [14] requires evaluating derivatives of the form $(\partial n_B^* / \partial \tilde{s})_{Y_e}$. These derivatives are computed along the surface for which the speed of sound is equal to its largest possible value (which we set to 0.9). Because the speed of sound requires two derivatives of the free energy, these derivatives (derivatives along a line of constant c_s^2) require third derivatives of the free energy. The chemical potentials require a similar calculation based on Eqs. (3.16) and (3.18) which we do not explicitly show here.

The numerical evaluation of third derivatives introduces quite a bit of noise. Our phenomenological formalism ensures that these derivatives can be computed analytically. We leave this calculation to future work. In the mean time, we can more easily compute the temperature by an indirect approach. Presuming we would like to compute the EOS at some fixed values of the baryon density $\widehat{n}_B$, electron fraction $\widehat{Y}_e$, and temperature $\widehat{T}$, one needs to solve the five equations

$$\begin{aligned} c_{s, \text{DS}}^2(n_{B1}^*, \widehat{Y}_e, T_1^*) &= \beta, \\ c_{s, \text{DS}}^2(n_{B2}^*, \widehat{Y}_e, T_2^*) &= \beta, \\ \tilde{s}_{\text{DS}}(n_{B1}^*, \widehat{Y}_e, T_1^*) &= \tilde{s}, \\ \tilde{s}_{\text{DS}}(n_{B2}^*, \widehat{Y}_e, T_2^*) &= \tilde{s} + \delta \tilde{s}, \\ \frac{1}{\widehat{n}_B} \frac{\epsilon_{\text{C\&P}}(\tilde{s} + \delta \tilde{s}, \widehat{Y}_e, n_B) - \epsilon_{\text{C\&P}}(\tilde{s}, \widehat{Y}_e, n_B)}{\delta \tilde{s}} &= \widehat{T} \end{aligned} \quad (3.20)$$

for the five values $n_{B1}^*, n_{B2}^*, T_1^*, T_2^*$, and $\tilde{s}$ given some small fixed stepsize in the entropy per baryon, $\delta \tilde{s}$. Here “DS” denotes our EOS while “C&P” denotes Eq. (3.9) from Ref. [14]. The required numerical derivatives to compute the temperature in the last equation of Eq. (3.20) can then be computed directly from finite differences. By solving the five equations above,

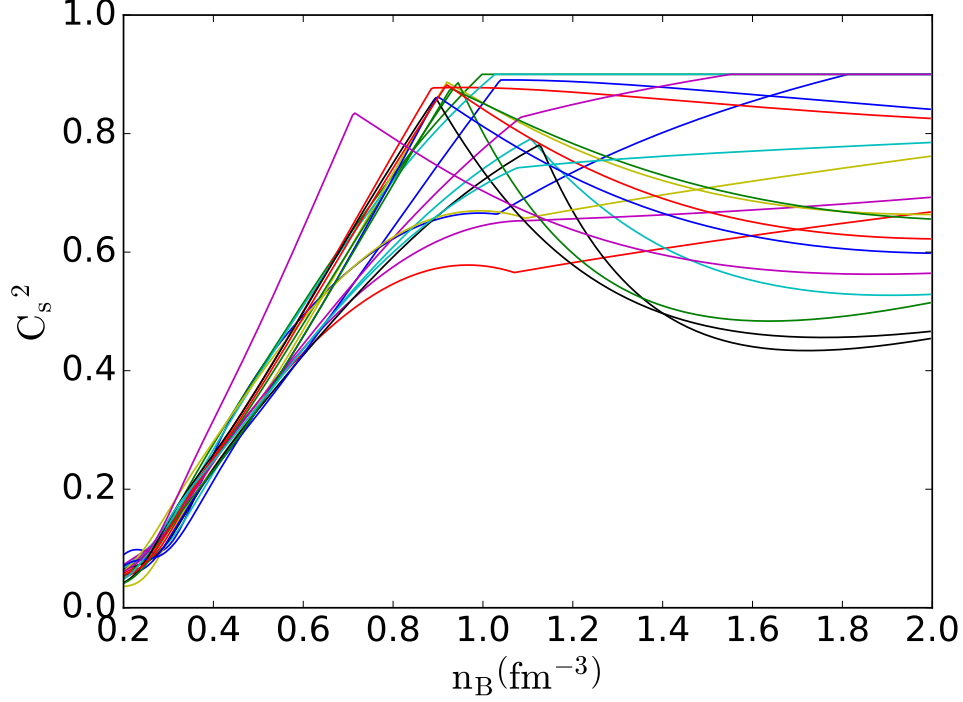


Figure 3.1: Values of n_B and c_s^2 explored by the EOS at $Y_e = 0.1$ and $\tilde{s}=0.5$, The different curves represent models which differ only by a different value of the parameter ϕ .

we get $\tilde{s}_{C\&P}(\widehat{n}_B, \widehat{Y}_e, \widehat{T})$, and then

$$\tilde{f}_{C\&P}(\widehat{n}_B, \widehat{Y}_e, \widehat{T}) = \varepsilon_{C\&P} - \widehat{T} \widehat{n}_B \tilde{s}_{C\&P}(\widehat{n}_B, \widehat{Y}_e, \widehat{T}). \quad (3.21)$$

3.2 Results

Since accurate neutron star radii have not yet been measured for large mass neutron stars, the speed of sound of matter at the highest densities probed in supernova and merger simulations is not constrained by experiment. We have parameterized this variation with ϕ . However, the speed of sound must increase at moderate densities in order to reproduce the observation of a two solar mass neutron star. Fig. 3.1 shows the behavior of the speed of sound in neutron-rich matter between $n_B = 0.1 \text{ fm}^{-3}$ and $n_B = 2 \text{ fm}^{-3}$ and demonstrates these two regimes. The speed of sound must increase quickly below 1 fm^{-3} to ensure that the neutron

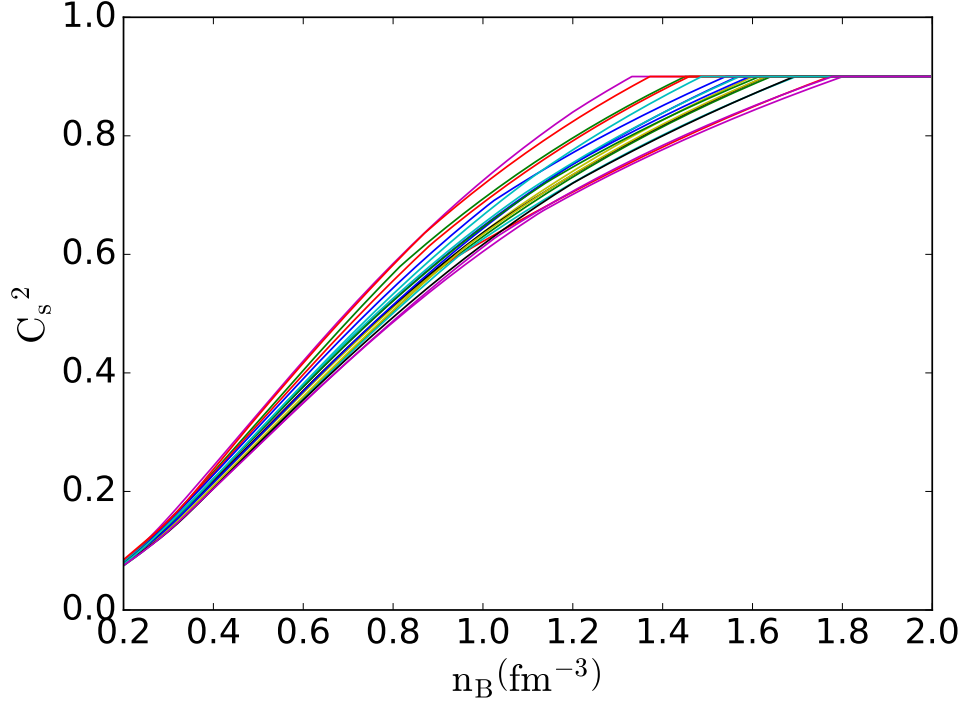


Figure 3.2: Values of n_B and c_s^2 explored by the EOS at $Y_e = 0.4$ and $\tilde{s}=0.5$. The different curves represent randomly selected models. Most of them have two kinks. The first one (often very slight) is the residual impact of fixing the speed of sound in neutron matter at high densities to ϕ as shown in Fig. 3.1. The second kink between $1.3 < n_B^* < 1.8 \text{ fm}^{-3}$ is due to the use of the C&P prescription to decrease the speed of sound above $n_B = n_B^*$.

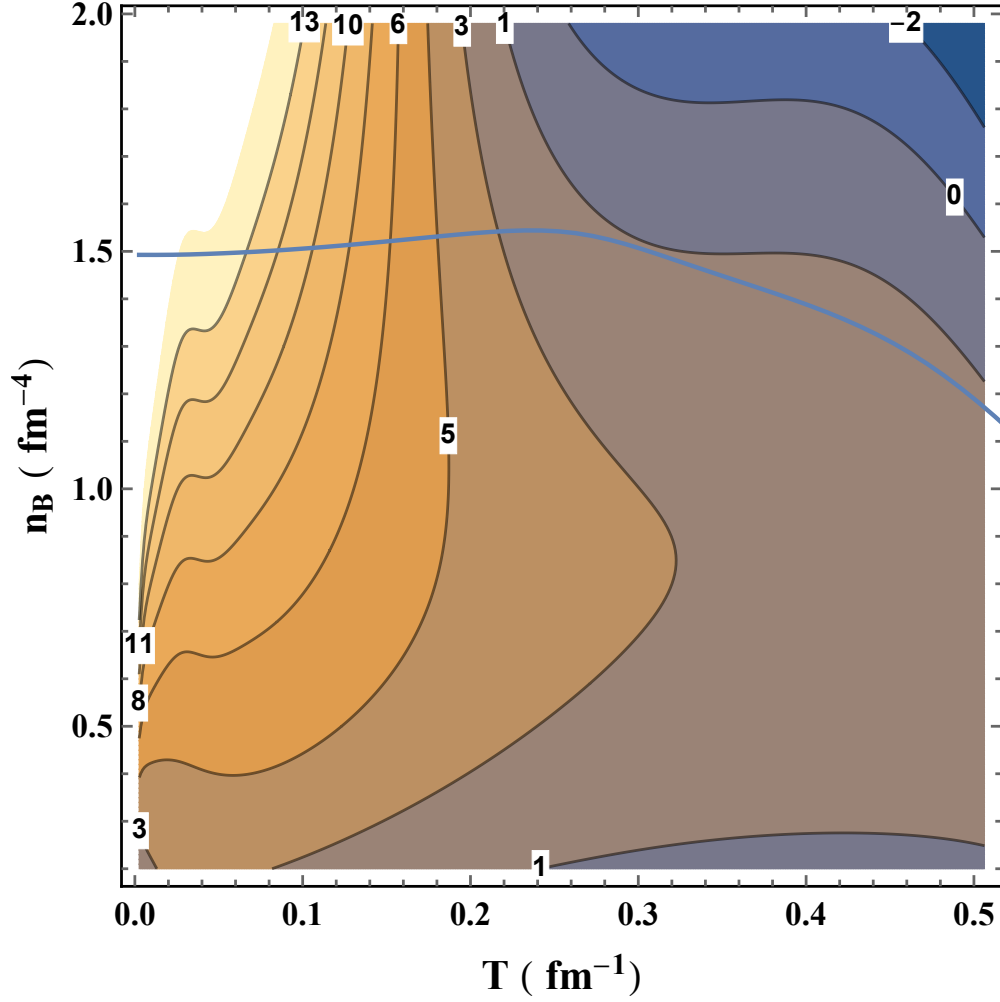


Figure 3.3: Contour plot of ds/dT as a function of n_B and T explored by the EOS for one of our EOS parameterizations. The speed of sound correction from the C&P prescription has not yet been applied. The blue line indicates the value $n_B = n_B^*$. The region above this line is replaced with the C&P EOS (including the region where $ds/dT < 0$).

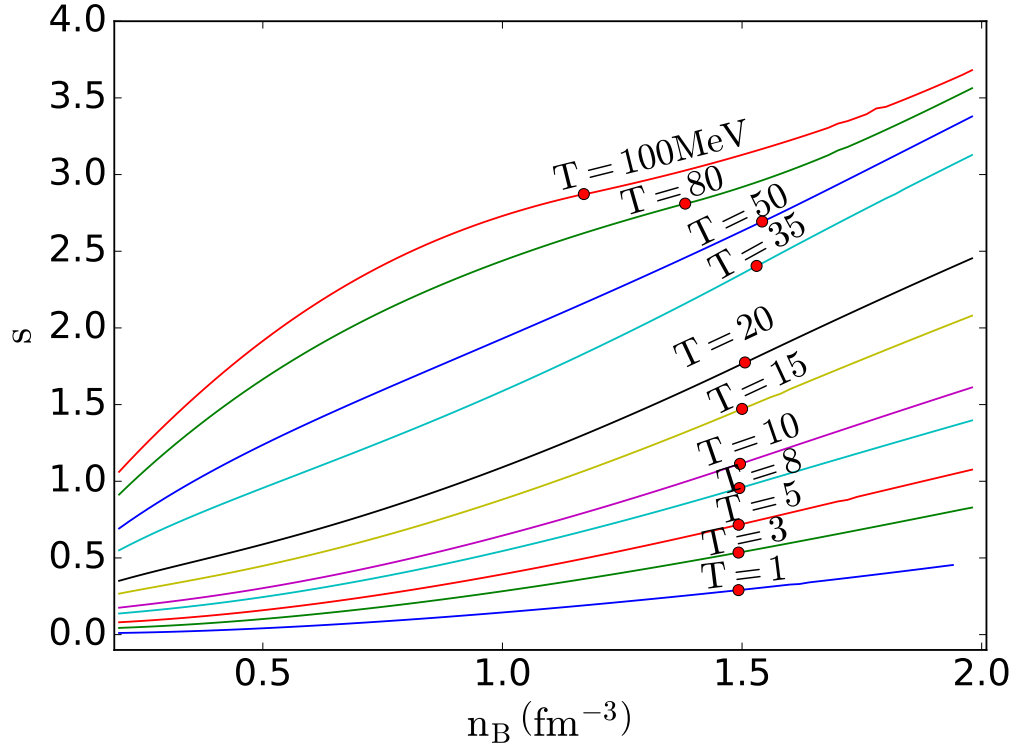


Figure 3.4: Values of n_B and s explored by the EOS. The dots represent boundaries where $c_s^2 = 0.9$ and C&P solution starts to take effect.

star maximum mass is sufficiently large [6], and the speed of sound at higher densities varies considerably depending on the value of ϕ . We restrict the speed of sound to be less than $c\sqrt{0.9}$ to ensure finite-precision errors in simulations do not create unphysical sound speeds.

In high-density isospin-symmetric matter, the speed of sound is dominated by the Skyrme model used for isospin-symmetric matter near the saturation density. This region is principally constrained to have a speed of sound less than $c\sqrt{0.9}$ by our implementation of the prescription from Ref. [14] as described in section 2.5. This is shown in Fig. 3.2. There is also a slight residual impact from the modification in the speed of sound from ϕ at values of Y_e which are nearly but not exactly equal to 1/2, so there are some slight kinks in the curves in Fig. 3.2 near $n_B = 1 \text{ fm}^{-3}$.

At sufficiently high density, the entropy from the chiral EOS begins decreasing with increasing temperature. Because of the presence of ds/dT in the speed of sound (see f_{TT} in the denominator of Eq. (13)), this unstable region implies a large speed of sound. Our use of the C&P prescription thus cures this instability in the extrapolated form of the finite-temperature corrections from the chiral EOS. This is demonstrated in Fig. 3.3, which shows contours of fixed ds/dT . This derivative becomes negative in the upper right region, but this is always at a density larger than n_B^* where the C&P EOS takes over.

As a final demonstration that our implementation of the C&P prescription generates a continuous EOS, we show the entropy as a function of density for several fixed temperatures in Fig. 3.4. Our EOS above is used for densities below n_B^* (indicated by the red dot) and the C&P EOS is used for densities above n_B^* . It appears in this plot that n_B^* is independent of temperature, but this is not exactly true as there is a weak temperature dependence as shown in Fig. 3.3. We have found that solving Eqs. (3.20) is numerically challenging because of the numerical derivatives involved in computing the speed of sound (we use exact expressions for the entropy and chemical potentials but numerical differentiation for the number susceptibilities and other second derivatives of the free energy). The combination of the numerical derivatives plus the numerical noise in the Newton-Raphson method used to solve Eqs. (3.20) leads to a bit of noise in the entropy at large densities. Future work will use exact expressions for second derivatives of the free energy and thus facilitate the correction to the speed of sound.

Chapter 4

EOS with nuclei

4.1 Introduction

Nuclear matter at subnuclear densities is unstable and tends to form clusters. Virial expansion describes the cluster formation through nucleonic interaction in terms of bound and resonance states in equal footing [45, 44]. However, this requires knowledge of computing higher order terms $O(z^6)$ poorly known at the moment [62], where three-body and even many-body terms start to play roles in the expansion. The cluster formation also can be introduced explicitly by adding a full ensemble of nuclei in the system with binding energies from either experimental measurements or theoretical calculations in dilute gas, when interactions among nucleons and nuclei can be safely ignored. In such case, nuclear statistical equilibrium (NSE) is reached thermodynamically in the system. NSE works as long as fugacities of nuclei are small enough $z_i \ll 1$, which approximately holds for $n_B < 0.001 \text{ fm}^{-3}$.

When baryon density gets larger, inter-particle spacing is comparable to the size of nuclei. The interaction among nuclei and the nucleonic gas is significant. One common solution is to simplify the interaction by only considering the size effect through the excluded volume approach. In the excluded volume approach, each Wigner-Seitz cell has one representative nuclei or a full ensemble of nuclei surrounded by dilute nucleonic gases. The gases outside could not explore the space occupied by the nuclei. The force in the model is similar to a repulsive force by hard spheres. However, counting states is simplified and it is not exactly equivalent to the case of hard sphere scattering scenario. The Wigner-Seitz cell

approximation claims the inter-cell interaction could be safely ignored where the size of the cell is determined by the sphere of electron gas presuming charge neutrality is reached individually in each cell. Experiments show such approximation works well for densities large enough when the neutrons and protons begin to drip out of nuclei.

At zero temperature, the inhomogeneous matter outside nuclei has lower neutron/proton chemical potential than neutron/proton separation energy, such that dripped out nucleons enable the system to stay in lower energy state. It is expected no nuclei outside neutron and proton dripline would exist in zero temperature in which case the chemical potential of neutrons and protons are positive then. For hot nuclear matter, unstable nuclei also exist in a small amount following from Fermi distribution. It is easy to see the excluded volume approach has the correct limit at zero temperature.

When nucleons get even closer right below saturation density, the nuclear matter could exist in an exotic phase known as pasta phase, when nuclear matter would turn itself inside out. Shapes from cylindrical, slab, cylindrical hole, spherical hole start to form in nuclear matter sequentially when finally saturation density is reached. In this method, we will not explore the possibilities of nuclear pasta while using a Maxwell construction for a transition from inhomogeneous to homogeneous matter. The pasta phase in the phase diagram is limited to a relatively small regime $n_B = 0.06 - 0.11 \text{ fm}^{-3}$ and $T = 0 - 12 \text{ MeV}$ therefore will not affect the behavior of astrophysics simulation greatly.

4.2 Basic formalism

We track light nuclei explicitly in addition to a full ensemble of heavy nuclei. The existence of light nuclei helps to shape the neutrino transportation and cooling rate in supernova and neutron star mergers. The nuclear matter at sub-nuclear density can be described by a gas consists of neutrons, protons, α particles, deuterons, tritons, ^4Li , ^3He and a full ensemble of heavy nuclei [38]. Our canonical partition function therefore can be written as

$$Z(n_n, n_p, \{n_i\}, T) = Z_n Z_p \prod_i Z_i Z_{\text{Coul}} Z_e \quad (4.1)$$

where i represents all light and heavy nuclei. The Coulomb contribution between the uniform electron background and the nuclei is temperature independent and can be decoupled from others as is showed above. The Helmholtz free energy density then is obtained by taking the logarithm.

$$f(n_n, n_p, \{n_i\}, T) = f_{np} + \sum_i f_i + f_{\text{Coul}} + f_e \quad (4.2)$$

In the following context, we will compute them separately and then take derivative with respect to the number density of each constituent.

Baryon number conservation and global charge neutrality implies two constraints, which we write as

$$\begin{aligned} n_B &= n_n + n_p + \sum_i n_i A_i \\ n_B Y_e &= n_e = n_p + \sum_i n_i Z_i \end{aligned} \quad (4.3)$$

The free energy density of nucleons outside the nuclei is given by our homogeneous model from the previous chapter which is denoted as DSH EOS. Due to the volume excluded effect(which is only turned on between nucleons and nuclei), the volume available to the nucleons is reduced by the nuclei. We denote the volume available to nucleons as $V' \equiv V - \sum_i N_i V_i$ where $N_i \equiv n_i V$ is the number of nuclei of type i in the Wigner-Seitz cell of volume v and $N_i = n_i V$ is the volume occupied by one nucleus of type i and n_0 is the saturation density, 0.16 fm^{-3} . The volume fraction which nucleons explore is $\xi = V'/V = 1 - \sum_i A_i n_i / n_0$. Thus, the free energy density of nucleonic gas is tuned by

$$f_{np} = \xi f'_{\text{DSH}}(n'_n, n'_p, T) \quad (4.4)$$

where the n'_n and n'_p are local densities and are defined by $n'_n \equiv N_n/V' = n_n/\xi$, $n'_p \equiv N_p/V' = n_p/\xi$ separately. Same as before, we ignore rest mass contribution here and put a tilde on top when it is added back.

The free energy density of the light nuclei and heavy nucleus are treated as classical Boltzmann particles.

$$f_i = -n_i T \left[\ln \left(\frac{\Omega_i \bar{V}}{N_i \lambda_i^3} \right) + 1 \right] \quad (4.5)$$

where λ_i is thermal wave length and given by,

$$\lambda_i = \left(\frac{2\pi}{m_i T} \right)^{1/2}, \quad (4.6)$$

Ω_i is the temperature-dependent partition function. The prescription we use follows from Fowler et al. and will be addressed in the next section. $\bar{V} \equiv \kappa V$ is the volume fraction explorable to the nucleus of type i , where $\kappa \equiv 1 - n_B/n_0$. Using these definitions

$$f_i = -n_i T \left[\ln \left(\frac{\Omega_i}{n_i \lambda_i^3} \right) + 1 \right] - n_i T \ln \kappa \quad (4.7)$$

The relation

$$\xi = \kappa + (n_n + n_p)/n_0 \quad (4.8)$$

is also useful below.

The Coulomb energy in the Wigner Seitz cell is following from Baym et. al.

$$E_i^{\text{Coul}} = -\frac{3}{5} \frac{Z_i^2 \alpha}{R_i} \left(\frac{3}{2} x_i - \frac{1}{2} x_i^3 \right) \quad (4.9)$$

where

$$x_i \equiv \left(\frac{n_B Y_e}{n_0} \frac{A_i}{Z_i} \right)^{1/3} = \frac{R_i}{R_{\text{WS},i}} \quad (4.10)$$

where $R_i^3 = (3A_i)/(4\pi n_0)$ is the nuclear radius, and the size of the Wigner-Seitz cell, R_{WS} is given by

$$Z_i = \frac{4\pi}{3} R_{\text{WS},i}^3 n_B Y_e. \quad (4.11)$$

The radius of nuclei is constrained by $R_i \leq R_{\text{ws},i}$ which limits $x_i \leq 1$.

We take into account all charged particles here except protons, the advantage is the Coulomb energy is merely a function of charge and atomic number given n_B and Y_e . After

applying charge neutrality, the total free energy density becomes

$$\begin{aligned}
f(n_n, n_p, \{n_i\}, T) = & \xi f_{\text{DSH}}(n'_n, n'_p, T) \\
& - \sum_i n_i T \left\{ \left[\ln \left(\frac{\Omega_i}{n_i \lambda_i^3} \right) + 1 \right] + \ln \kappa \right\} \\
& + \sum_i n_i E_i^{\text{Coul}} + f_e(n_B Y_e)
\end{aligned} \tag{4.12}$$

4.2.1 Homogeneous matter EOS

We slightly modify the DSH EOS to no longer enforce a quadratic expansion for the finite-temperature contributions. The free energy is separated into a contribution from the virial expansion and a contribution from degenerate matter

$$\begin{aligned}
f_{\text{DSH}}(n_B, x_p, T) = & f_{\text{virial}}(n_B, x_p, T)g \\
& + f_{\text{deg}}(n_B, x_p, T)(1 - g).
\end{aligned} \tag{4.13}$$

The free energy density for degenerate matter is

$$f_{\text{deg}}(n_B, x_p, T) = f_{\text{Skyrme}}(n_B, x_p = 1/2, T = 0) + \delta^2 \varepsilon_{\text{sym}}(n_B) + \Delta f_{\text{hot}}(n_B, x_p, T) \tag{4.14}$$

The derivatives of the degenerate free energy density are

$$\begin{aligned}
\frac{\partial f_{\text{deg}}}{\partial n_n} = & \frac{1}{2} \mu_{n, \text{Skyrme}}(n_B, x_p = 1/2, T = 0) \\
& + \frac{1}{2} \mu_{p, \text{Skyrme}}(n_B, x_p = 1/2, T = 0) \\
& + \delta^2 \frac{\partial \varepsilon_{\text{sym}}}{\partial n_B} + \frac{2\delta(1 - \delta)}{n_B} \varepsilon_{\text{sym}} \\
& + \Delta \mu_{n, \text{hot}}(n_B, x_p, T)
\end{aligned} \tag{4.15}$$

$$\begin{aligned}
\frac{\partial f_{\text{deg}}}{\partial n_p} &= \frac{1}{2} \mu_{p,\text{Skyrme}}(n_B, x_p = 1/2, T = 0) \\
&+ \frac{1}{2} \mu_{n,\text{Skyrme}}(n_B, x_p = 1/2, T = 0) \\
&+ \delta^2 \frac{\partial \varepsilon_{\text{sym}}}{\partial n_B} - \frac{2\delta(1+\delta)}{n_B} \varepsilon_{\text{sym}} \\
&+ \Delta \mu_{p,\text{hot}}(n_B, x_p, T)
\end{aligned} \tag{4.16}$$

and

$$\frac{\partial f_{\text{deg}}}{\partial T} = -s_{\text{hot}}(n_B, x_p, T) \tag{4.17}$$

where

$$\begin{aligned}
\frac{\partial \varepsilon_{\text{sym}}}{\partial n_B} &= h'(n_B) \varepsilon_{\text{QMC}}(n_B) + h(n_B) \varepsilon'_{\text{QMC}}(n_B) \\
&- h'(n_B) \varepsilon_{\text{NS}}(n_B) + [1 - h(n_B)] \varepsilon'_{\text{NS}}(n_B) + \\
&- \frac{1}{2} [\mu_{n,\text{Skyrme}}(n_B, x_p = 1/2, T = 0) \\
&+ \mu_{p,\text{Skyrme}}(n_B, x_p = 1/2, T = 0)] .
\end{aligned} \tag{4.18}$$

4.2.2 The Saha equations

In order to fix the densities of the nuclei, we solve the equations

$$\left(\frac{\partial f}{\partial n_i} \right)_{n_B, Y_e} = 0 . \tag{4.19}$$

Before we begin, it is useful to define

$$f_{i,\text{Cl}} = -n_i T \left[\ln \left(\frac{\Omega_i}{n_i \lambda_i^3} \right) + 1 \right] \tag{4.20}$$

as the classical part of the nuclear free energy.

We can rewrite the full free energy from Eq. 4.12 in terms of n_B and Y_e

$$f[n_n(n_B, Y_e, T), n_p(n_B, Y_e, T), \{n_i\}, T] , \tag{4.21}$$

to re-express the derivative (T is implicitly held constant)

$$\begin{aligned}
\left(\frac{\partial f}{\partial n_i}\right)_{n_B, Y_e} &= \left(\frac{\partial f}{\partial n_i}\right)_{n_p, n_n} + \left(\frac{\partial f}{\partial n_n}\right)_{n_p, \{n_i\}} \left(\frac{\partial n_n}{\partial n_i}\right)_{n_B, Y_e} \\
&\quad + \left(\frac{\partial f}{\partial n_p}\right)_{n_n, \{n_i\}} \left(\frac{\partial n_p}{\partial n_i}\right)_{n_B, Y_e} \\
&= \left(\frac{\partial f}{\partial n_i}\right)_{n_p, n_n} - \left(\frac{\partial f}{\partial n_n}\right)_{n_p, \{n_i\}} N_i \\
&\quad - \left(\frac{\partial f}{\partial n_p}\right)_{n_n, \{n_i\}} Z_i.
\end{aligned} \tag{4.22}$$

Thus, we obtain the Saha equations

$$\mu_i = \mu_n N_i + \mu_p Z_i, \tag{4.23}$$

with the chemical potentials defined by

$$\begin{aligned}
\mu_i &\equiv \left(\frac{\partial f}{\partial n_i}\right)_{n_p, n_n, T}, \quad \mu_n \equiv \left(\frac{\partial f}{\partial n_n}\right)_{n_p, \{n_i\}, T}, \quad \text{and} \\
\mu_p &\equiv \left(\frac{\partial f}{\partial n_p}\right)_{n_n, \{n_i\}, T}.
\end{aligned} \tag{4.24}$$

We also define $\mu_e \equiv (\partial f_e)/(\partial n_e)$. These chemical potentials can be written analytically. For the nuclei, we define

$$P_i^{\text{Coul}} \equiv -n_i \frac{3}{5} \frac{Z_i^2 \alpha}{R_i} \left(\frac{1}{2} x_i - \frac{1}{2} x_i^3 \right). \tag{4.25}$$

as in Ref. [38] and this definition implies

$$n_i \left(\frac{\partial E_i^{\text{Coul}}}{\partial n_i} \right)_{n_n, n_p} = \frac{P_i^{\text{Coul}} Z_i}{n_e} \tag{4.26}$$

For the nuclei, this definition gives

$$\begin{aligned}\mu_i = & -\left(\frac{A_i}{n_0}\right) f_{\text{DSH}} + \mu_{n,\text{DSH}} \left(\frac{A_i n_n}{\xi n_0}\right) + \mu_{p,\text{DSH}} \left(\frac{A_i n_p}{\xi n_0}\right) \\ & + \mu_{i,\text{cl}} - T \ln \kappa + \frac{T n_i A_i}{\kappa n_0} + E_i^{\text{Coul}} \\ & + \frac{Z_i P_i^{\text{Coul}}}{n_e} + Z_i \mu_e .\end{aligned}\tag{4.27}$$

where $\mu_{i,\text{cl}} \equiv (\partial f_{i,\text{cl}})/(\partial n_i)$. For the nucleons

$$\mu_n = \mu_{n,\text{DSH}} + \frac{T n_i}{\kappa n_0}\tag{4.28}$$

and

$$\mu_p = \mu_{p,\text{DSH}} + \frac{T n_i}{\kappa n_0} + \mu_e + \frac{P^{\text{Coul}}}{n_e}\tag{4.29}$$

where $\mu_{x,\text{DSH}} \equiv (\partial f_{\text{DSH}})/(\partial n_x)$ and $P^{\text{Coul}} \equiv \sum_i P_i^{\text{Coul}}$. Note that because we have not included electrons as separate degrees of freedom in Eq. 4.12, the electron chemical potential appears in 4.29. Thus, our chemical potentials above match those in Ref. [38]. Using the Saha equation, we find

$$\begin{aligned}\mu_{i,\text{cl}} = & \left(\frac{A_i}{n_0}\right) f_{\text{DSH}} + \mu_{n,\text{DSH}} \left[N_i - \left(\frac{A_i n_n}{\xi n_0}\right)\right] \\ & + \mu_{p,\text{DSH}} \left[Z_i - \left(\frac{A_i n_p}{\xi n_0}\right)\right] + T \ln \kappa - E_i^{\text{Coul}}\end{aligned}\tag{4.30}$$

which gives us a recipe for computing the free energy for each nucleus. Using $P_{\text{DSH}} \equiv -f_{\text{DSH}} + \mu_{n,\text{DSH}} n'_n + \mu_{p,\text{DSH}} n'_p$, we can rewrite this result slightly

$$\mu_{i,\text{cl}} = -V_i P_{\text{DSH}} + N_i \mu_{n,\text{DSH}} + Z_i \mu_{p,\text{DSH}} + T \ln \kappa - E_i^{\text{Coul}}.\tag{4.31}$$

The excluded volume effect reflected in the $T \ln \kappa$ and $-P_{\text{DSH}} V_i$ terms suppresses the number density of nuclei near saturation densities.

At a fixed grid point in (n_B, Y_e, T) space, given n_n and n_p , we can compute κ and ξ using their definitions above, compute the DSH EOS, and E_i^{Coul} and thus use Eq. 4.31 to compute

$\mu_{i,\text{cl}}$. This is then used to compute n_i and then we can solve Eqs. 4.3 to obtain the correct value of n_n and n_p .

4.2.3 First derivatives of thermodynamic quantities

After having solved the Saha equations for $n_i(n_n, n_p)$, it is useful to define new “effective” chemical potentials for the nucleons which include the nucleons both inside and outside nuclei

$$\nu_n \equiv \left(\frac{\partial f}{\partial n_n} \right)_{n_p, T} \quad \text{and} \quad \nu_p \equiv \left(\frac{\partial f}{\partial n_p} \right)_{n_n, T} \quad (4.32)$$

(note that these differ from Eq. 4.24 in that they no longer hold n_i constant) which gives a new thermodynamic identity

$$f(n_n, n_p, T) = -P(n_n, n_p, T) + \nu_n n_n + \nu_p n_p. \quad (4.33)$$

Rewriting the free energy again

$$f[n_n, n_p, \{n_i(n_n, n_p, T)\}, T], \quad (4.34)$$

which implies that the effective chemical potentials can be computed in terms of the definitions above

$$\nu_x = \mu_x + \sum_i \mu_i \left(\frac{\partial n_i}{\partial n_x} \right)_{n_{\hat{x}}} \quad (4.35)$$

for both $\{x, \hat{x}\} = \{n, p\}$ and $\{x, \hat{x}\} = \{p, n\}$. Defining

$$g_j \equiv \mu_j - \mu_n N_j - \mu_p Z_j \quad (4.36)$$

we can take advantage of the fact that all the g_j are constant to write

$$\left(\frac{\partial n_i}{\partial n_x} \right)_{n_{\hat{x}}, g_j} = - \left(\frac{\partial g_i}{\partial n_x} \right)_{n_i, n_{\hat{x}}, g_{j \neq i}} \left(\frac{\partial n_i}{\partial g_i} \right)_{n_x, n_{\hat{x}}, g_{j \neq i}} \quad (4.37)$$

The first derivative on the RHS can be obtained directly from Eqs. 4.27, 4.28, and 4.29. The second derivative is just an element along the diagonal of the inverse of the matrix

$$M_{ij} \equiv \left(\frac{\partial g_i}{\partial n_j} \right)_{n_x, n_{\hat{x}}, n_{k \neq j}}. \quad (4.38)$$

The numerical errors associated with inverting this large matrix decreases the benefit of the analytical formalism. Thus we compute ν_n and ν_p numerically for now. The entropy is easier to compute

$$s = - \left(\frac{\partial f}{\partial T} \right)_{n_n, n_p, \{n_i\}} = s_e + \sum_i s_i + \sum_i n_i \ln \kappa + \xi s_{\text{DSH}} \quad (4.39)$$

where $s_e = \partial f_e / \partial T$ and

$$s_i = n_i \left(\ln \frac{\Omega_i}{n_i \lambda_i^3} \right) + \frac{5}{2} + \frac{T}{\Omega_i} \frac{d\Omega_i}{dT}. \quad (4.40)$$

4.2.4 Nuclei

We use the nuclear masses from experiments [5] wherever they are available. The atomic mass tables usually include an empirical bounded electron contributions term $a_{el} Z^{2.39}$. They are subtracted from the binding energy since we only include bare nuclei. We use the theoretical masses from Ref. [56] for nuclei which do not have experimental mass measurements up to the neutron and proton drip lines. For nuclei beyond the drip lines, we use the spherical and macroscopic part of the mass formula from Ref. [56], refitting some of the parameters to match the predictions from Ref. [56]. This refit helps ensure that there are no spurious edge effects beyond the drip lines. In addition, we limit our nuclear distributions to $Z < 2.25N$ and $N < 2.25Z$ because our extrapolation of the model from Ref. [56] is unlikely to be accurate far from stability. This allows nuclei slightly outside neutron and proton drip line to existing in our EOS. Also, we limit maximum A to be 200.

4.2.5 Partition function

The partition function for light nuclei and the representative heavy nucleus we use follows from Ref. [73]. The continuum subtraction is ignored since it is only important above 10^{11} K. The nuclear partition function can be expressed as a sum of discrete states and an integral

of level density

$$\Omega_i = (2J + 1) + \int_{E_d}^{E_t} \rho(E) \exp(-E/T) , \quad (4.41)$$

where the level density $\rho(E)$ is the backshifted Fermi-gas formula given below. The limits on the integral in the partition function are determined from

$$E_d = \frac{1}{2} \min(S_n, S_p) \quad \text{and} \quad (4.42)$$

$$E_t = \min(S_n + E_R, S_p + E_R + \frac{1}{2}E_c) , \quad (4.43)$$

where S_n and S_p are the neutron and proton separation energies. The quantity $E_R \equiv 1/(2M_i R^2)$ is the zero-point energy and with the nuclear radius approximated by $R = 1.25(A - 1)^{1/3}$. The quantity $E_c \equiv (Z - 1)\alpha/R$ is the Coulomb barrier. When either S_n or S_p are negative, the contribution of the level density is neglected.

The expression for the level density begins by defining a backshift parameter δ for each nucleus. The prescription from Fowler et al. is

$$Z \leq 30 : \delta = \delta_p - 80/A \quad (4.44)$$

$$Z \geq 30 : \delta = \delta_p - 80/A - 0.5 \quad (4.45)$$

with $\delta_p = (11A^{-1/2} \text{ MeV})[1 + (1/2)(-1)^Z + 1/2(-1)^N]$. We will also need the level density, a , for which an approximate model is

$$Z \leq 30 : a = 0.052 \text{ MeV}^{-1} A^{1.2} \quad (4.46)$$

$$Z \geq 30 : a = 0.125 \text{ MeV}^{-1} A \quad (4.47)$$

Finally, different expressions are used for the level density depending on the relative size of δ and E_d . When δ is smaller E_d , the level density has the expression

$$\rho(E) = \frac{\pi}{12} \frac{\exp(2\sqrt{aU})}{a^{1/4} U^{5/4}} \quad (4.48)$$

where $U = E - \delta$.

When δ is larger than E_d , δ is set to E_d and the level density is ...

$$\rho(E) = \begin{cases} C \exp(U/T_c) & E_d < E < 2E_d \\ \frac{\pi}{12} \frac{\exp(2\sqrt{a}U)}{a^{1/4}U^{5/4}} & 2E_d < E < E_t \end{cases} \quad (4.49)$$

where the expressions for the parameters T_c and C are chosen to ensure that both the level density and the derivative (as given in Eq. 4.48 and Eq. 4.49) match at $\delta = E_d$. This requirement implies that

$$\begin{aligned} \frac{1}{T_c} &= \frac{5}{4} \frac{1}{U_c} + \frac{\sqrt{a}}{\sqrt{U_c}}, \text{ and} \\ C &= \frac{\sqrt{\pi}}{12} a^{-1/4} U_c^{-5/4} \exp\left(\frac{5}{4} + \sqrt{a}U_c\right). \end{aligned} \quad (4.50)$$

Additionally, since we took out the deuteron contribution from b_{pn} in the previous paper. It should be put back here. This makes $\Omega_{\text{deut}} = 3$ and the continuum part of partition is included equivalently in b_{pn} .

4.3 Results

In this section, we discuss various thermodynamic quantities and the composition of matter in the EOS. Thousands of EOSs can be computed by selecting random parameter sets which are mentioned in our previous paper. For the first two parameters, i_{Skyme} is the index for a set of ~ 1000 Skyrme parameterizations of posterior distributions from UNDEF2 collaboration [48]. i_{NS} is the index for a set of ~ 1000 polynomial EOS fitted to Markov chains based on neutron star mass and radius measurements [79, 77]. a and α are two parameters from quantum Monte Carlo functional form for pure neutron matter near saturation density [29]. S stands for symmetry energy and L is the slope of symmetry energy. The quantity ϕ is a random number between 0 and 1 generated for speed of sound squared for causality enforcement [14], when baryon density $n_B = 2.0 \text{ fm}^{-3}$ for pure neutron matter. In this paper, we computed six representative EOSs with each of them labeled by their special characteristics, i.e. large maximum mass, small radius or large S and L , etc. The parameters are listed in Table 4.1. The fiducial EOS is the one consistent with the most probable neutron star mass and radius

Table 4.1: Parameters for our fiducial EOS.

	i_{NS}	i_{Skyrme}	α	a	L (MeV)	S (MeV)	ϕ
P_{fiducial}	470	738	0.5	13.0	62.4	32.8	0.9
$P_{\text{large } M_{\text{max}}}$	783	738	0.5	13.0	62.4	32.8	0.9
$P_{\text{small } R}$	214	738	0.5	13.0	62.4	32.8	0.9
$P_{\text{smaller } R}$	256	738	0.5	13.0	62.4	32.8	0.9
$P_{\text{large } R}$	0	738	0.5	13.0	62.4	32.8	0.9
$P_{\text{small } SL}$	470	738	0.5	13.0	23.7	29.5	0.9
$P_{\text{large } SL}$	470	738	0.5	13.0	100.0	36.0	0.9

and has moderate S and L . The Skyrme parameters for our fiducial EOS are listed in Table 2.3. In the following, the figures are demonstrated for our fiducial EOS.

4.3.1 Mass fractions of nucleons and light nuclei

In Fig. 4.1, the mass fraction of free neutrons, protons, light nuclei and heavy nuclei are plotted as a function of baryon density for $Y_e = 0.1, 0.3$ and 0.5 , respectively. The system consists of only protons and neutrons at low densities. For $Y_e = 0.1$ and $T = 1.0$ MeV, as density increases, the fraction of light nuclei rises to around 0.2 for n_B between 10^{-7} and 10^{-6} fm^{-3} , in contrast the proton fraction drops to zero and neutron to around 0.7 due to excess of neutrons in the system. The NSE becomes important for the density range. In this range, α particles dominate over other light nuclei since they have larger binding energies. Above $n_B = 10^{-6} \text{ fm}^{-3}$, the light nuclei are gradually replaced by heavy nuclei. The transition density from light to heavy nuclei increases as temperature increases. For $Y_e = 0.3$, the protons and neutrons drop to almost zero right before the transition to homogeneous matter, since the formation of heavy nuclei is favored in order for the system to gain lower free energy density. It is also because the neutron and proton separation energy are smaller than their chemical potentials, respectively. The excluded volume effect dominates approaching saturation density, so the nuclei are expelled by the volume pressure and nucleon fractions get back to their original fractions in the system. For $Y_e = 0.5$, the protons and neutrons are almost zero from 10^{-6} to 10^{-1} fm^{-3} indicating an earlier formation of light and heavy nuclei for symmetric nuclear matter. The highest point for the peak of

α particles is almost one, which is easy to understand since all nucleons bind in terms of α s for symmetric nuclear matter. For higher temperatures, the rise of light nuclei is pushed to higher densities since the nucleons are more energetic and therefore are less inclined to form clusters. The light nuclei are soon replaced by heavy nuclei because they have larger binding energies. For all three proton fractions, the NSE will be replaced by homogeneous matter before reaching saturation density.

4.3.2 Average A and Z of heavy nuclei in non-uniform matter

Fig. 4.2 shows mass fractions X_n , X_p , X_α and X_d as a function of baryon density and temperature for $Y_e = 0.01, 0.1, 0.3, 0.5$, separately. For temperature below $1 \sim 2$ MeV, the system consists of entirely heavy nuclei at subnuclear densities. At high temperature and low density, the nuclear matter exists in forms of nucleonic gas. Either increasing density or decreasing temperature would favor forming clusters. The dark region for top panels shows when nuclei are abundant in the system. The light nuclei represented by α particles and deuterons are found at moderate temperatures. α s primarily exist in a narrow band above tens of MeV in temperature heavy nuclei are not yet able to appear. Deuterons with smaller binding energies appear in small amounts in higher temperatures around 100 MeV. As density increases further, the non-uniform clusters transform to uniform matter, where no nuclei could be found on the right. The transition density is observed to be above $1/3 n_B^0$ or 0.06 fm^{-3} . It is roughly independent of temperature and proton fraction Y_e . The critical temperature of the gas-liquid phase transition is around several to tens of MeV depending on the proton fraction.

Fig. 4.3 shows the average mass/proton number $\bar{A}/\bar{Z}$ as a function of baryon density and temperature. The maximum A for our EOS is limited to 200. The number 200 is set due to the limited computation power of CPUs. For symmetric nuclear matter, $\bar{A}$ reaches the upper limit we set upon reaching saturation density. Therefore, a larger maximum A in general would just allow the EOS to have heavier nuclei in this region. For comparison, Fig. 4.5 shows that STOS and FYSS have an average mass up to 1800 and 1400, respectively. FYSS set maximum A to be 3000. SRO is based on the same liquid droplet model with LS220 and they limited maximum A to be around 300. HS based on NSE also has a similar upper bound.

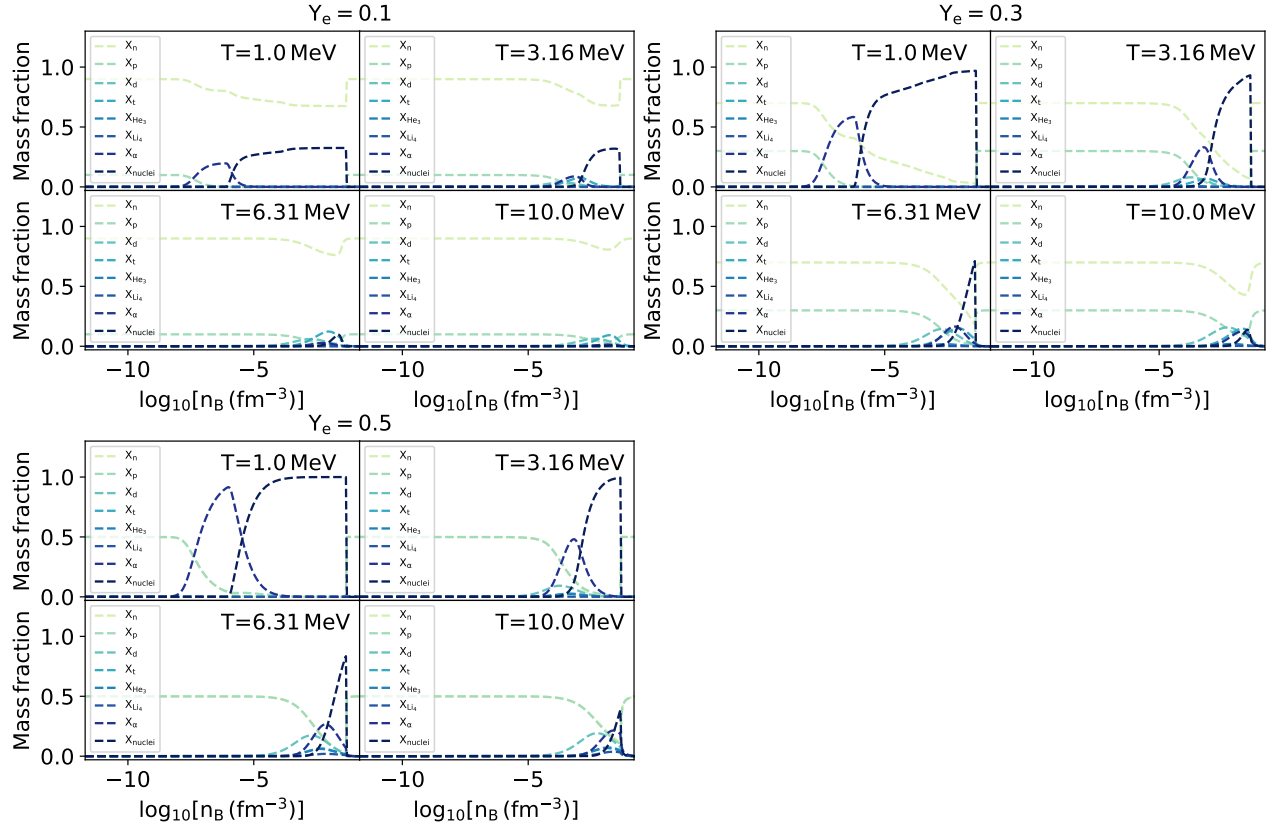


Figure 4.1: From top to bottom: $Y_e = 0.1, 0.3$ and 0.5 . Mass fractions of nucleons and light nuclei for $T=1.0, 3.16, 6.31, 10.0$ MeV, respectively. Baryon density n_B is in logarithmic scale. For $Y_e=0.1$ and $T=1.0$ MeV, nucleonic gas dominated below $n_B=10^{-8} \text{ fm}^{-3}$. Light nuclei appear as baryon density increases until 10^{-8} fm^{-5} , which are gradually replaced by heavy nuclei. When temperature increases, both mass fractions of light and heavy nuclei decreases until 10 MeV, indicating the critical temperature is reached. For $Y_e=0.3$ and $Y_e=0.5$, mass fractions of nuclei increases as stable nuclei are favorable for more symmetric matter.

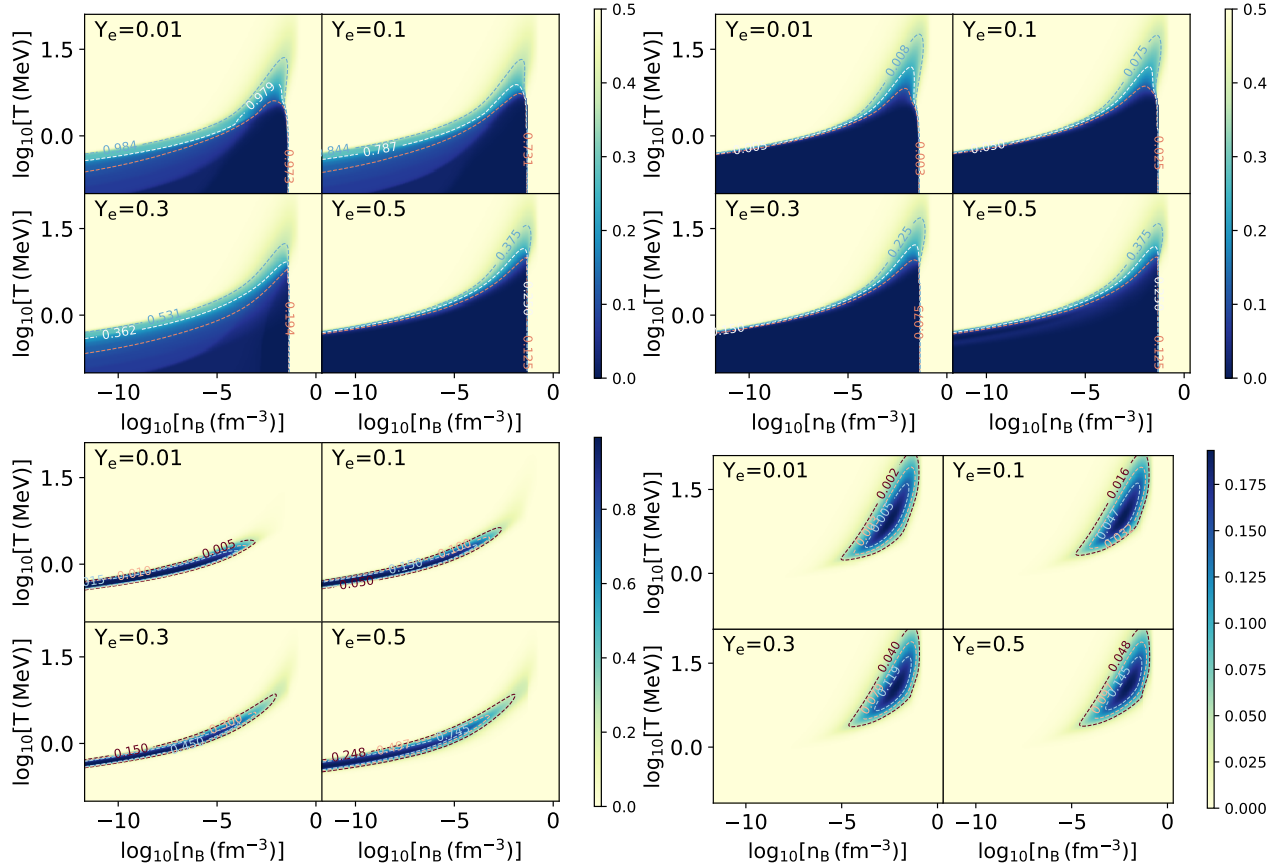


Figure 4.2: X_n (top left), X_p (top right), X_α (bottom left) and X_d (bottom right) as functions of baryon density and temperature for $Y_e=0.01, 0.1, 0.3, 0.5$, respectively. Baryon density n_B and temperature T are in logarithmic scale. The α particles and deuteron exist primarily at several to dozens of MeV. The region where α exists indicate they are dominant. The deuteron exist at slightly higher temperature with other light nuclei not shown in the figures.

SHT is based on a different model in different regions. For the nuclear matter at subnuclear densities, it adopts Hartree approximation and has the highest average A around 5000. Though different EOSs predict different mass numbers in the region, the thermodynamic quantities are not much affected [11]. For nearly pure neutron matter at $Y_e = 0.01$, the maximum $\bar{A}$ rises to ~ 40 . The shell structure of nuclei could be clearly distinguished in the figures, divided by different color coding of $\bar{A}$. As baryon density increases, $\bar{A}$ rises to several plateaus in sequence. It can be observed for symmetric matter, the plateaus have narrower width since the distribution favors sharp transition among doubly shell nuclei in the situation. The vertical line on the right indicates the transition to homogeneous matter, where the fraction of nuclei is identical to zero.

Fig. 4.4 shows the average mass/proton number $\bar{A}/\bar{Z}$ as a function of baryon density and proton fraction. The dark blue region indicates the “island” of heavy nuclei. For symmetric matter, heavy nuclei tend to form at higher densities due to shell effects, rendering a notch on the left around $Y_e = 0.5$. The asymmetric shape above and below $Y_e = 0.5$ is because of Coulomb symmetry breaking. The transition density from inhomogeneous matter to homogeneous matter also depends on proton fraction. For $Y_e < 0.2$, the transition density slightly decreases with proton fraction, while it is almost kept a constant above $Y_e = 0.2$. The exception between $Y_e = 0.3 \sim 0.4$ is due to the close values of free energy density between homogeneous matter and inhomogeneous matter. The system would favor the state with lower free energy density.

4.3.3 Comparison with other EOSs

Fig. 4.5 shows average mass number $\bar{A}$ as functions of baryon density and temperature for other EOSs used frequently in supernova simulations. Not surprisingly, significant differences can be found among these plots for the predictions of mass numbers in the inhomogeneous phase. The figures fall into two categories. STOS, SHT and FYSS allow nuclei with a maximum mass number around several thousand, while LS220, SRO and SFHo limit A below several hundred. For $Y_e < 0.5$, the first category features a decreasing transition density as proton fraction decreases, while for $Y_e > 0.5$, the transition density tends to be roughly invariant. However, all three EOSs included pasta phase before transiting to homogeneous

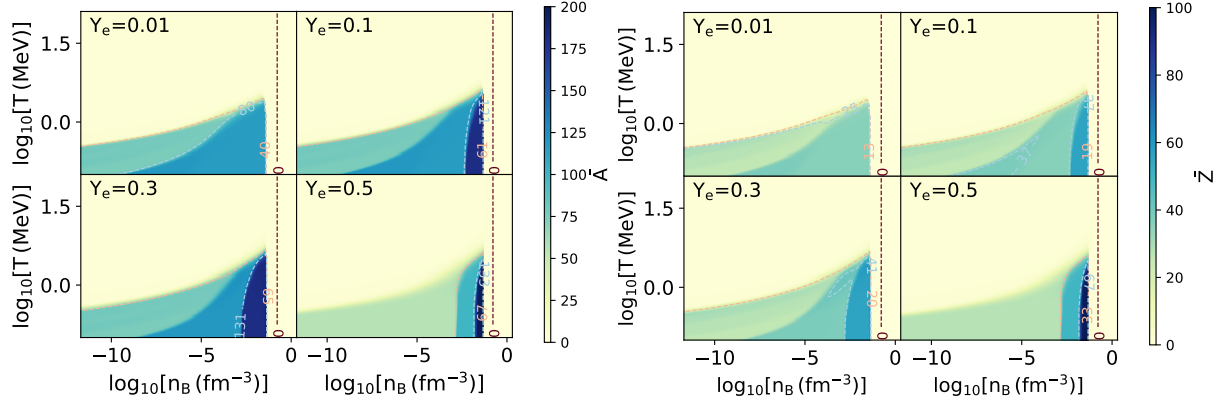


Figure 4.3: Average mass number (left), proton number (right) as functions of temperature and baryon density for $Y_e=0.01, 0.1, 0.3, 0.5$, respectively. Baryon density n_B and temperature T are in logarithmic scale. For symmetric nuclear matter, the average mass number reaches the upper limit of 200. For neutron rich matter the average mass number is smaller.

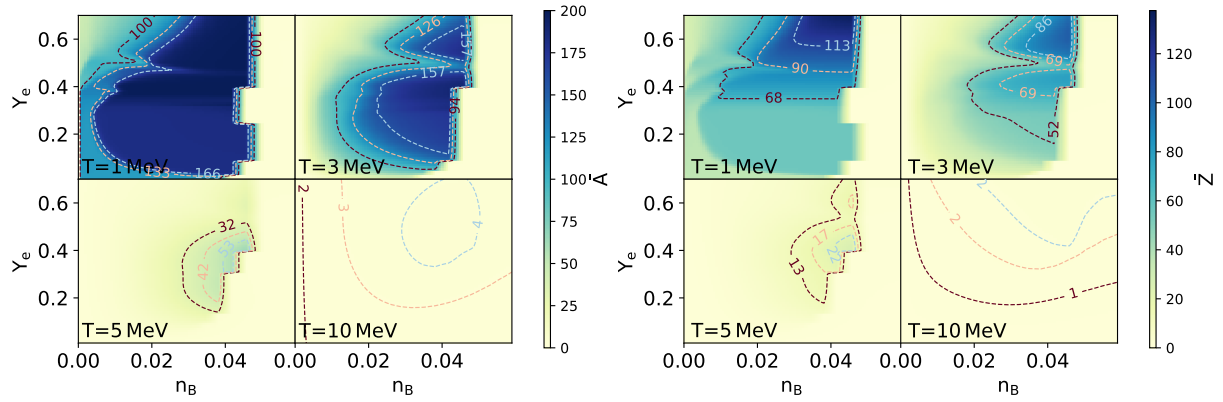


Figure 4.4: Average mass number (left) and proton number (right) number as functions of baryon density and proton fraction for $T=1.0, 3.0, 5.0, 10.0$, respectively. Baryon density n_B and temperature T are in logarithmic scale. The “island” of average mass number is not completely symmetric for $Y_e = 0.5$ due to Coulomb symmetry breaking. As temperature increases, the average mass number decreases since nucleons are favored more than nuclei. The transition density to homogeneous matter is roughly independent of proton fraction.

matter, which adds more complications. The inclusion of pasta phase in general decreases binding energy therefore favor a late transition to homogeneous matter. STOS and FYSS use the same nuclear EOS. Nuclei is added with Thomas-Fermi approximation for STOS, while FYSS adopted NSE with geometric interpolation to incorporate pasta phase. SHT uses Hartree approximation in this subregion and has highest average mass number. The second category, e.g. LS220, SFHo and SRO, also has decreasing transition density for small Y_e . But as Y_e increases above 0.5, the transition decreases drastically on the contrary. LS200 has a roughly constant transition density at high Y_e , but it is because it has a relatively smaller Y_e range 0.1 – 0.5, One notable feature is the EOSs in the first category have closed contour of mass number say 200 for around $Y_e = 0.5$, while the second doesn't. A possible explanation for the higher average mass number above $Y_e > 0.5$ in our EOS is we included a large ensemble of nuclei in the nuclei chart. The prescription $Z < 2.25N$ and $N < 2.25Z$ allows nuclei go beyond neutron and proton drip line modified by the Coulomb energy shift [66], while at high Y_e the nuclear distribution tends to lie across the border. This relaxes the constraints compared to some EOSs only including nuclei within drip lines. For the nuclear matter at zero temperature, this is not energetically favored. But at finite temperatures unbounded nuclei could exist in the ensemble without such limitations.

The primary uncertainty of mass number for different EOSs comes from the nuclear EOS it adopts, which symmetry energy S , its slope L and incompressibility K could differ greatly among different EOSs. The secondary source is whether it uses single nucleus approximation or full ensemble when nuclei are added. Obviously, without any limits, the mass number could go to a few thousand. Although the difference in mass number does not affect thermodynamic quantities as much [11].

4.3.4 Nuclear distribution

Fig. 4.6 shows the nuclear distribution for selected points in the EOS as in [73]. The behavior is similar. The top left panel shows $n_B = 0.0001 \text{ fm}^{-3}$, $T = 1 \text{ MeV}$ and $Y_e = 0.2$, the nuclei distribution is a gaussian peak around $N = 50$ and $Z = 35$. For the same density and temperature but $Y_e = 0.4$, a double peak showed around $N = 50$, $Z = 35$ and $N = 50$ and $Z = 45$, separately. At this density, the proton and neutron fugacities should be much

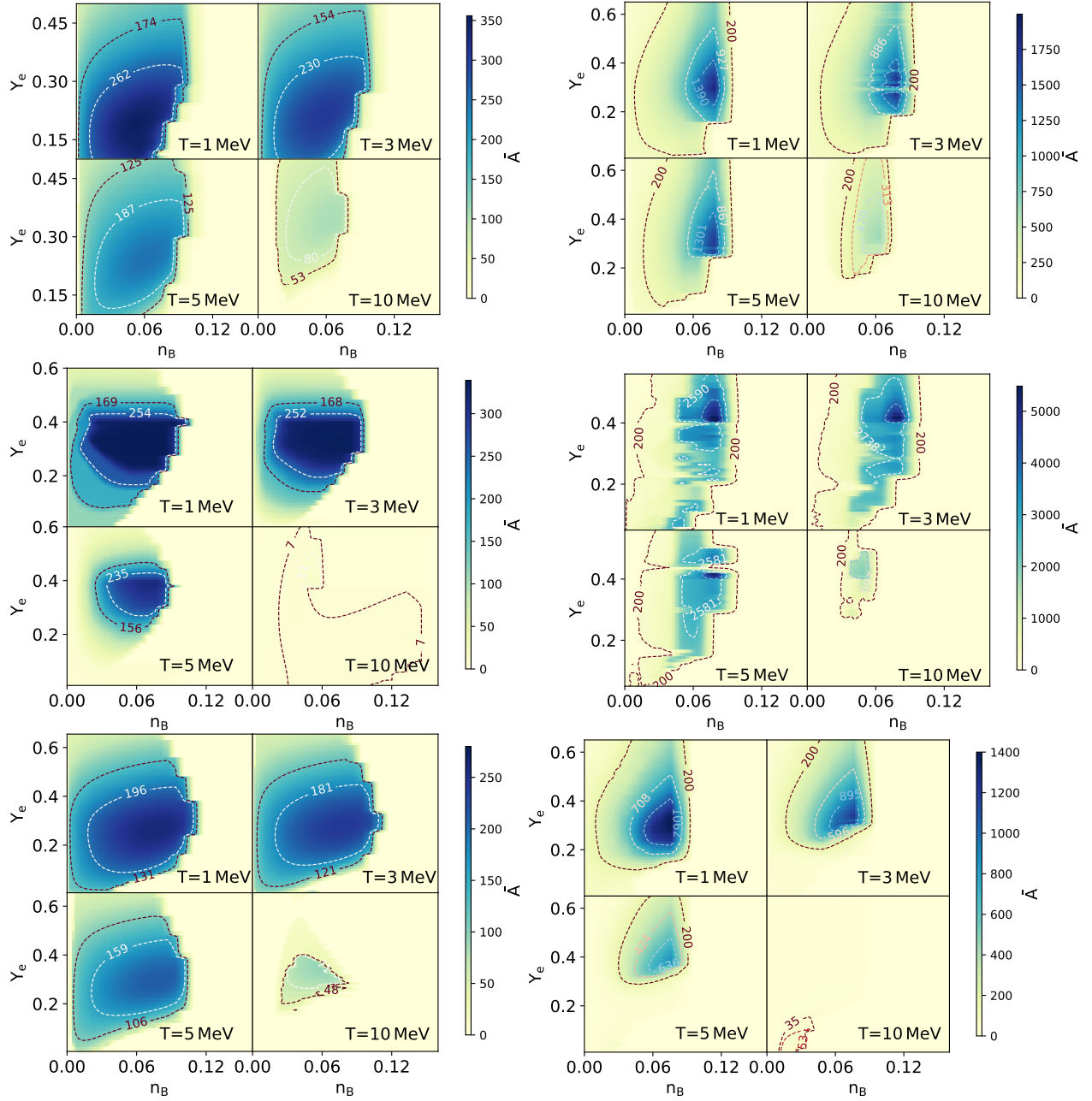


Figure 4.5: From left to right, top to bottom: LS220, STOS, SFHo, SHT, SRO, FYSS. Average mass number as functions of baryon density and proton fraction for $T=1.0, 3.0, 5.0, 10.0$, respectively. Baryon density n_B is in logarithmic scale. LS220, SFHo, and SRO have smaller upper limit of $\bar{A}$. The approximately symmetric behavior of average mass number is not observed for these models. STOS, SHT and FYSS have larger upper limit of $\bar{A}$.

smaller than one, so the dominant contribution comes from virial expansion and NSE. Fig. 4.7 showed the distribution by summing up all nuclei corresponding to the same proton number. The light green curve illustrates the case for $Y_e = 0.4$. The small peak appears on the lower left indicates the mass fraction of light nuclei is also significantly present in the region. There is a slight cut off on the left edge of the distribution due to the constraint we use to limit $N < 2.25Z$ and $Z < 2.25N$ but its influence on the results is negligible, since the nuclei not included have mass fraction less than 10^{-10} . Similarly, the bottom left panel shows results for a slightly larger density $n_B = 0.001 \text{ fm}^{-3}$ and $Y_e = 0.4$, but for two different temperature of 1.0 and 3.16 MeV, respectively. Both of them has a double peak of nuclei, reflecting that single nucleus approximation is not applicable in these regions. For $n_B = 0.001 \text{ fm}^{-3}$, $Y_e = 0.4$ and $T = 3.16 \text{ MeV}$, the two peaks are at $N = 20, Z = 15$ and $N = 30, Z = 25$, separately. For $n_B = 0.001 \text{ fm}^{-3}$, $Y_e = 0.4$ and $T = 1.0 \text{ MeV}$, the two peaks are at $N = 60, Z = 40$ and $N = 80, Z = 60$, separately.

4.3.5 Monte Carlo results

Fig. 4.8 shows four Monte Carlo figures of average mass number $\bar{A}$ for some selected points when the seven parameters in our EOS is randomly selected. Each figure is based on 10000 samples of Monte Carlo simulation. The variation gives an uncertainty of the full EOS in subnuclear density at relatively low temperatures. The plots show that the uncertainty of the EOS in these regions is relatively small. It demonstrates the uncertainty from DSH EOS actually has quite a minimal impact on the uncertainty of the ensemble of nuclei. The largest uncertainty is $\sim 1\%$ for low temperature, neutron rich matter at $n_B = 0.03 \text{ fm}^{-3}$, $Y_e = 0.1$ and $T = 3.0 \text{ MeV}$.

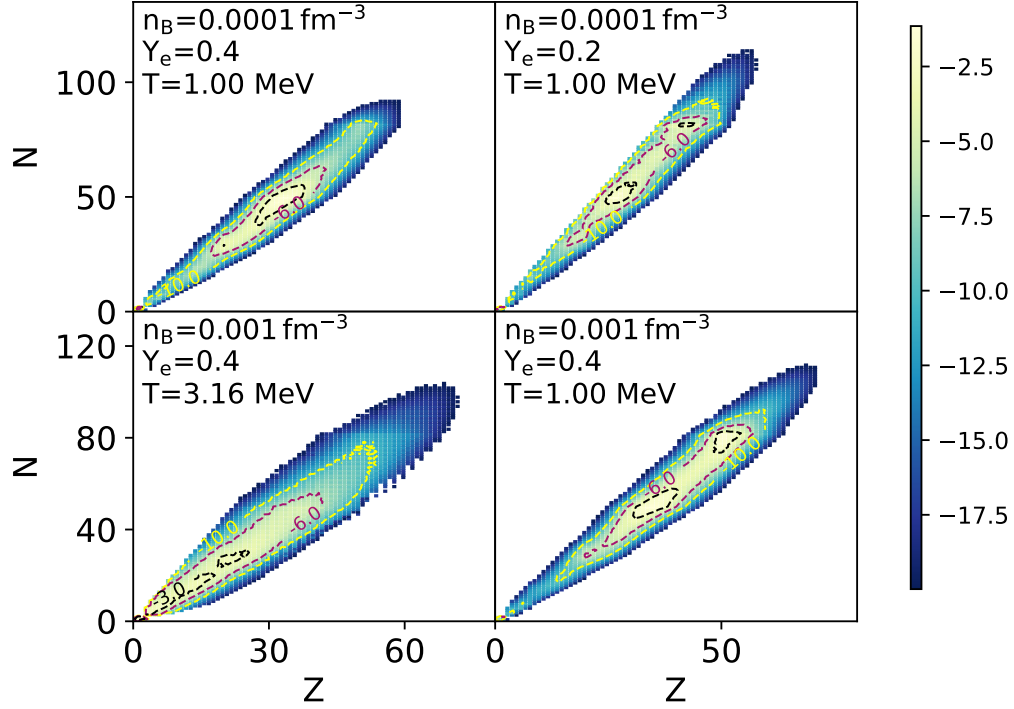


Figure 4.6: Mass fraction of nuclei in the nuclear chart for matter at several selected points of n_B , Y_e and T . The fraction of nuclei are coded with color in logarithmic scale. Contours of 10^{-3} , 10^{-6} , 10^{-10} are showed. For $n_B = 0.0001 \text{ fm}^{-3}$, $Y_e = 0.4$, $T = 1 \text{ MeV}$ at top left panel, a single peak appears around $N = 50$ and $Z = 35$. For the rest panels, all of them indicate double peaks. Slight cutoff shows for the point $n_B = 0.0001 \text{ fm}^{-3}$, $Y_e = 0.2$ and $T = 1.0 \text{ MeV}$ due to the limited nuclei that are included.

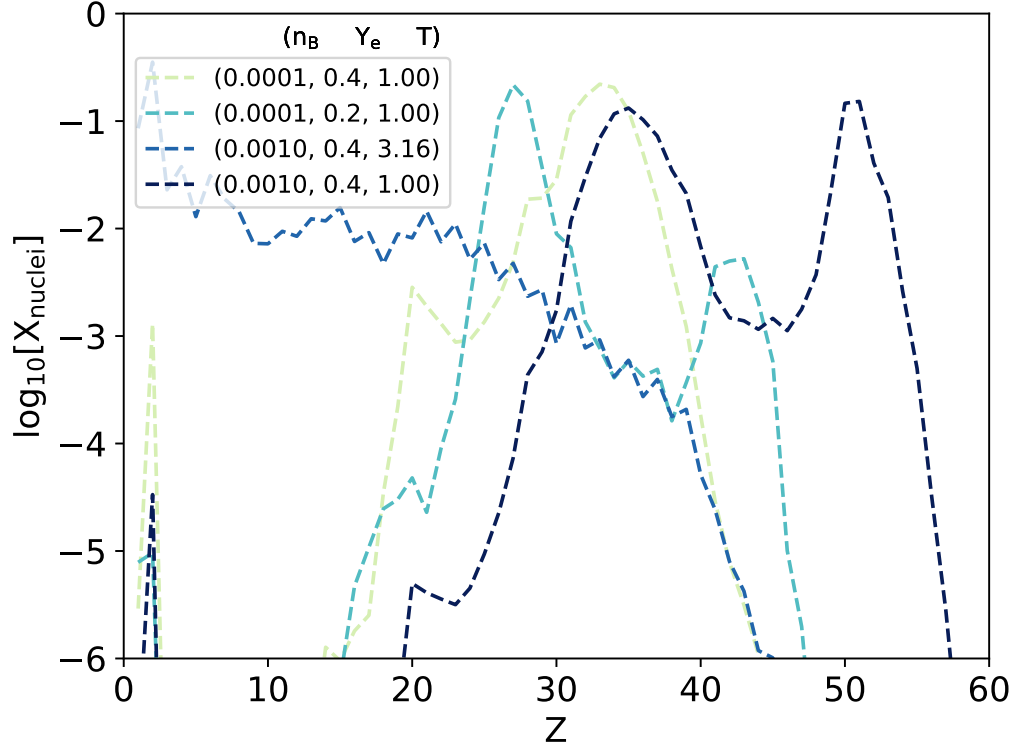


Figure 4.7: Mass fraction of nuclei as a function of fixed proton number Z for several selected points of n_B , Y_e and T . The mass fraction is in logarithmic scale. The peaks on the bottom left are light nuclei. A single peak is favored for $n_B = 0.0001 \text{ fm}^{-3}$, $Y_e = 0.4$, $T = 1.0 \text{ MeV}$. Double peaks are favored for $n_B = 0.0001 \text{ fm}^{-3}$, $Y_e = 0.2$, $T = 1.0 \text{ MeV}$ and $n_B = 0.001 \text{ fm}^{-3}$, $Y_e = 0.4$, $T = 1.0 \text{ MeV}$. Continuous distribution is favored for $n_B = 0.001 \text{ fm}^{-3}$, $Y_e = 0.4$, $T = 3.16 \text{ MeV}$.

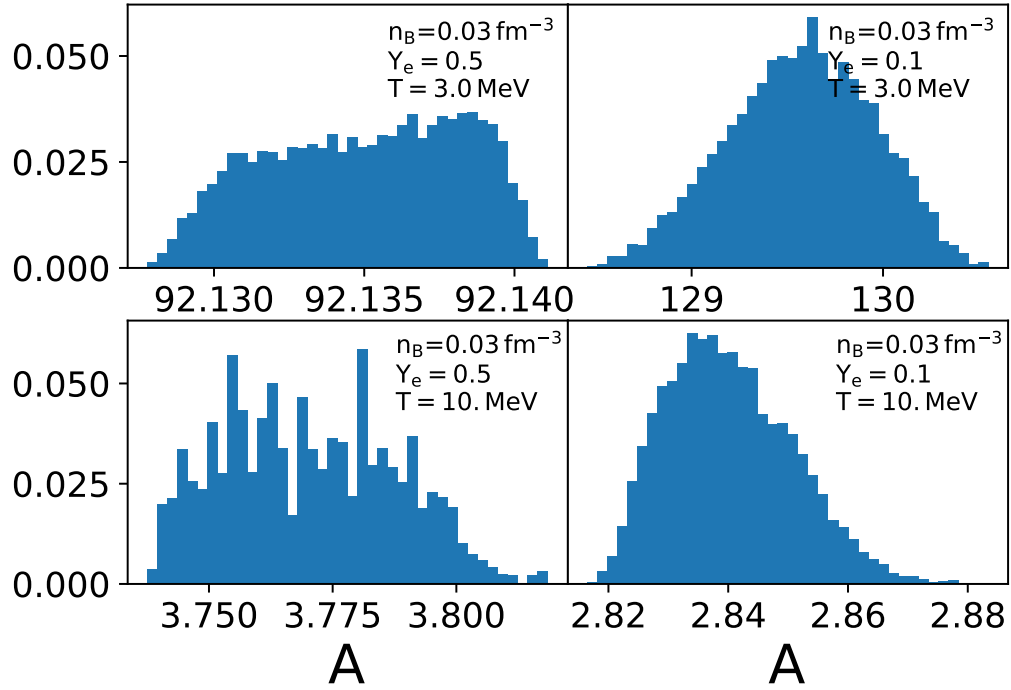


Figure 4.8: The probability distribution for several selected points of n_B , Y_e and T at subnuclear densities. The uncertainty are relative small on all selected points, reflecting a minimal impact from the uncertainty of homogeneous matter. The largest uncertainty is found for $n_B = 0.03 \text{ fm}^{-3}$, $Y_e = 0.1$, $T = 3.0 \text{ MeV}$.

Chapter 5

Conclusions

In this work, we have constructed a new class of phenomenological EOSs for astrophysical simulations. The nucleonic part of the EOS is built to simultaneously match five different regimes that are consistent with both experimental and observational constraints. The major advantage is one can vary uncertainties in different regimes independently, without spoiling agreement elsewhere. We added a full ensemble nuclei using the excluded volume approach and Wigner-Seitz cell approximation. It both has the correct limit at zero temperature and is thermodynamically consistent when baryon densities approach saturation density. The light nuclei are separately included in the table so it is possible to track neutrino dynamics on each component.

While we have attempted to explore the allowed EOS space as much as possible, there are several regions in which our parameterization is limited.

Compared to other EOSs, our EOS predicts lower transition density of 0.06 fm^{-3} . One way to increase the transition density is to perform Maxwell construction on top of the EOS table following Ref. [37]. The Maxwell construction also ensures the stability of the EOS, which requires $dP/dn \geq 0$. This involves solving for the equation

$$p^I = p^{II}, \quad (1 - Y_p) \mu_n^I + Y_p (\mu_p^I + \mu_e^I) = (1 - Y_p) \mu_n^{II} + Y_p (\mu_p^{II} + \mu_e^{II}) \quad (5.1)$$

where I and II represent low density and high density phase, separately. Equivalently, we could include pasta phase in our EOS following the prescription in Ref. [28]. The inclusion

of pasta phase also guarantees the stability of EOS. The exotic matter may appear above twice saturation density, for example, hyperons or quark matter. One of the advantages of our analytical form for the EOS is that our work can be easily generalized to an EOS which includes exotic matter at high densities if desired. The hyperon or quark EOS, once constructed, could be incorporated conveniently by matching to the old EOS using Maxwell or Gibbs construction.

Variations in the functions g and h could be explored, but modifications of these functions cannot be too large or they are likely to create small regions where the EOS has an acausal speed of sound. Better quantification of the uncertainties in the finite temperature part of the chiral EOS will be performed in future work. We have also naively extrapolated the Skyrme model used in isospin-symmetric matter at zero temperature near the saturation density to higher densities. There is some experimental constraint on matter in this region from heavy ion collisions [85], but the associated systematic uncertainties are not well-understood. In any case, dense and isospin-symmetric matter is not often explored in the neutron-rich matter encountered in neutron stars. Uncertainties in the EOS may be relevant for the timescale for core-collapse supernovae to explode after bounce [16] and also, for example, in determining the amount of r-process nucleosynthesis which occurs in the neutrino-driven wind [68]. EOS uncertainties are also relevant for neutron star mergers, as they dictate the lifetime of hypermassive neutron star remnants and also the amount of r-process material ejected [71].

Because we use the Markov chain from “Model A” in Ref. [77], our EOS specifically prefers more moderate phase transitions, which is appropriate to our assumption that matter consists only of nucleons and no exotic matter. Thus our uncertainties at high-density may be underestimated because strong phase transitions are disfavored.

Finally, the EOS uncertainties must be propagated through to the neutrino opacities. As this uncertainty quantification matures, the comparison of simulations with data points, such as GW170817 [53] and future nearby core-collapse supernovae will provide more insight into what models might be ruled out.

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Appendices

Using ε for energy density, S for entropy, s for entropy density, and $\tilde{s}$ for entropy per baryon, and assuming neutrinos are not trapped, the speed of sound is (all chemical potentials and energy densities below include the rest mass contribution even though not explicitly indicated)

$$c_s^2 = \left(\frac{\partial P}{\partial \varepsilon} \right)_{\tilde{s}, \{N_i\}}. \quad (2)$$

In infinite matter, it is useful to rewrite this derivative in terms of fixed volume rather than fixed number.

$$c_s^2 = \left(\frac{\partial P}{\partial \varepsilon} \right)_{S, \{N_i\}} = \left(\frac{\partial P}{\partial V} \right)_{S, \{N_i\}} \left(\frac{\partial \varepsilon}{\partial V} \right)_{S, \{N_i\}}^{-1}, \quad (3)$$

where the second derivative on the right-hand-side of this expression is

$$\begin{aligned} \left(\frac{\partial \varepsilon}{\partial V} \right)_{S, \{N_i\}} &= \left[\frac{\partial(E/V)}{\partial V} \right]_{S, \{N_i\}} = -\frac{1}{V}P - \frac{E}{V^2} \\ &= -\frac{P + \varepsilon}{V} = -\frac{Ts + \sum_i \mu_i n_i}{V} \end{aligned} \quad (4)$$

and the first derivative on the right-hand side is

$$\begin{aligned} \left(\frac{\partial P}{\partial V} \right)_{S, \{N_j\}} &= - \left(\frac{\partial \varepsilon}{\partial V} \right)_{S, \{N_j\}} + S \left[\frac{\partial(T/V)}{\partial V} \right]_{S, \{N_j\}} + \\ &\quad \sum_i N_i \left[\frac{\partial(\mu_i/V)}{\partial V} \right]_{S, \{N_j\}} \end{aligned} \quad (5)$$

$$\begin{aligned} &= - \left(\frac{\partial \varepsilon}{\partial V} \right)_{S, \{N_j\}} \\ &\quad + S \left[-\frac{T}{V^2} + \left(\frac{\partial T}{\partial V} \right)_{S, \{N_j\}} \right] \\ &\quad + \sum_i N_i \left[-\frac{\mu_i}{V^2} + \left(\frac{\partial \mu_i}{\partial V} \right)_{S, \{N_j\}} \right] \end{aligned} \quad (6)$$

$$\begin{aligned} &= \frac{P + \varepsilon}{V} + S \left[-\frac{T}{V^2} - \left(\frac{\partial P}{\partial S} \right)_{\{N_j\}, V} \right] \\ &\quad + \sum_i N_i \left[-\frac{\mu_i}{V^2} - \left(\frac{\partial P}{\partial N_i} \right)_{S, \{N_{j \neq i}\}, V} \right] \\ &= -S \left(\frac{\partial P}{\partial S} \right)_{\{n_j\}, V} - \sum_i N_i \left(\frac{\partial P}{\partial N_i} \right)_{S, \{n_{j \neq i}\}, V} \end{aligned} \quad (7)$$

Putting these two results together gives

$$c_s^2 = \frac{\left[s \left(\frac{\partial P}{\partial s} \right)_{\{n_j\}, V} + \sum_i n_i \left(\frac{\partial P}{\partial n_i} \right)_{s, \{n_{j \neq i}\}, V} \right]}{\left(Ts + \sum_i \mu_i n_i \right)^{-1}}. \quad (8)$$

To re-express this in terms of derivatives of the free energy,

$$c_s^2 = \left\{ s \left[\frac{\partial (\sum_i \mu_i n_i - f)}{\partial s} \right]_{\{n_j\}, V} + \sum_i n_i \left[\frac{\partial (\sum_k \mu_k n_k - f)}{\partial n_i} \right]_{s, \{n_{j \neq i}\}, V} \right\} \left(Ts + \sum_i \mu_i n_i \right)^{-1}. \quad (9)$$

For the sum over k , all densities are constant except for n_i , thus

$$\begin{aligned} & \sum_i n_i \frac{\partial}{\partial n_i} \left(\sum_k \mu_k n_k - f \right)_{s, \{n_{j \neq i}\}, V} \\ &= \sum_i n_i \frac{\partial}{\partial n_i} \left(\sum_{k \neq i} \mu_k n_k + \mu_i n_i - f \right)_{s, \{n_{j \neq i}\}, V} \\ &= \sum_i \left[\sum_k n_k \left(\frac{\partial \mu_k}{\partial n_i} \right)_{s, \{n_{j \neq i}\}, V} + \mu_i \right. \\ & \quad \left. - \left(\frac{\partial f}{\partial n_i} \right)_{s, \{n_{j \neq i}\}, V} \right]. \end{aligned} \quad (10)$$

To compute this we need

$$\begin{aligned}
\left(\frac{\partial f}{\partial n_i}\right)_{s,\{n_{j \neq i}\},V} &= \left(\frac{\partial f}{\partial n_i}\right)_{\{n_{j \neq i}\},T,V} \\
&\quad + \left(\frac{\partial f}{\partial T}\right)_{n_B,\{n_{j \neq i}\},V} \left(\frac{\partial T}{\partial n_i}\right)_{\{n_{j \neq i}\},s,V} \\
&= \mu_i - s \left(\frac{\partial T}{\partial n_i}\right)_{\{n_{j \neq i}\},s,V} \\
\left(\frac{\partial \mu_k}{\partial n_i}\right)_{s,\{n_{j \neq i}\},V} &= \left(\frac{\partial \mu_k}{\partial n_i}\right)_{\{n_{j \neq i}\},T,V} \\
&\quad + \left(\frac{\partial \mu_k}{\partial T}\right)_{n_i,\{n_{j \neq i}\},V} \left(\frac{\partial T}{\partial n_i}\right)_{\{n_{j \neq i}\},s,V} \\
&= f_{n_i n_k} + f_{n_k T} \left(\frac{\partial T}{\partial n_i}\right)_{\{n_{j \neq i}\},s,V}
\end{aligned} \tag{11}$$

which requires

$$\begin{aligned}
\left(\frac{\partial T}{\partial n_i}\right)_{\{n_{j \neq i}\},s,V} &= - \left(\frac{\partial s}{\partial n_i}\right)_{\{n_{j \neq i}\},T,V} \left(\frac{\partial s}{\partial T}\right)_{\{n\},V}^{-1} \\
&= -f_{n_i T} / f_{TT}
\end{aligned} \tag{12}$$

Finally, we get

$$\begin{aligned}
c_s^2 &= \left\{ - \left(\frac{s}{f_{TT}}\right) \left(\sum_i n_i f_{n_i T} + s\right) \right. \\
&\quad \left. + \sum_i n_i \left[\sum_k n_k (f_{n_i n_k} - f_{n_k T} f_{n_i T} f_{TT}^{-1}) - s f_{n_i T} f_{TT}^{-1} \right] \right\} \\
&\quad \left(Ts + \sum_i \mu_i n_i \right)^{-1} \\
&= \left[\sum_i \sum_k n_i n_k (f_{n_i n_k} - f_{n_k T} f_{n_i T} f_{TT}^{-1}) \right. \\
&\quad \left. - 2 \sum_i s n_i f_{n_i T} f_{TT}^{-1} - s^2 f_{TT}^{-1} \right] \left(Ts + \sum_i \mu_i n_i \right)^{-1}.
\end{aligned} \tag{13}$$

Vita

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