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Comparison of EoS models with different cluster suppression mechanisms

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Summary. — The dissolution of clusters in strongly interacting matter with increasing density and temperature can be modeled with different approaches, in particular a geometric excluded-volume mechanism or a more microscopic model with medium dependent mass shift. The predictions of the chemical composition and of thermodynamic properties are compared for two such equation-of-state models that realize these approaches but use the same model for the interaction of nucleons, *i.e.*, a relativistic mean-field model with density-dependent nucleon-meson couplings. The main differences are found for heavy nuclei in the chemical composition of neutron star matter, but the thermodynamic properties of the two models are quite similar.

1. – Introduction

Many astrophysical simulations require the equation of state (EoS) of strongly interacting matter as an essential ingredient. The EoS determines the static properties of neutron stars [1-5], the dynamical evolution of core-collapse supernovae [6-9] and of neutron star mergers [10-12] and it sets the conditions for nucleosynthesis processes. In a general sense, the EoS provides not only information on the energetics of matter but also on the chemical composition. An EoS can only be applied in dynamical simulations if the time scales of the relevant reactions are much shorter than the timescales of the system evolution, so that thermal, mechanical and chemical equilibrium can be assumed. Otherwise, a time-dependent description with a full network of reactions has to be followed. Since wide ranges of the thermodynamic variables temperature, density and isospin asymmetry have to be covered, global multi-purpose EoS are required in the application to astrophysics.

An important aspect of matter at astrophysical conditions is the appearance of inhomogeneous phases and, in particular, of nuclear clusters at baryon densities n_b below the nuclear saturation density $n_{\mathrm{sat}} \approx 0.16\,\mathrm{fm}^{-3}$ and not too high temperatures $T \lesssim 15\,\mathrm{MeV}$.

A simple description in terms of a nuclear statistical equilibrium (NSE) is not sufficient to model the transition from clustered matter to homogeneous matter. There are different approaches to model the dissolution of clusters. A simple geometric picture utilizing the finite size of nuclei leads to the excluded-volume (EV) mechanism producing only a density-dependent effect. A more microscopic approach takes a modification of cluster properties inside the medium into account in which the Pauli principle is the main effect. This can be implemented in the model as a mass shift (MS) of the clusters. It is expected that the chosen theoretical model will affect the predictions of the chemical composition and of the thermodynamic properties of the matter.

In the present contribution, two different approaches to describe the dissolution of clusters will be compared. Both use the same model for the nuclear interaction so that differences in the results can be attributed to the employed mechanism for cluster suppression. The statistical model of Hempel and Schaffner-Bielich (HS) [13-16] uses the EV mechanism whereas the generalized relativistic density functional (gRDF) [17-20] utilizes the MS approach. Here only the main characteristics of the models and the most important differences in the results will be presented. More details and figures can be found in ref. [21].

2. – Theoretical models

Both the HS and the gRDF model describe the interaction between nucleons in a relativistic mean-field (RMF) approach with density dependent meson-nucleon couplings using the parametrization DD2 [17], which is a refit of the earlier DD parameter set [22] with experimental nucleon masses. This DD2 interaction has very reasonable nuclear matter parameters (saturation density $n_{\mathrm{sat}} = 0.149\,\mathrm{fm}^{-3}$, binding energy per nucleon at saturation $a_V = 16.02\,\mathrm{MeV}$, incompressibility $K = 242.7\,\mathrm{MeV}$, symmetry energy $J = 31.67\,\mathrm{MeV}$ and symmetry energy slope parameter $L = 55.04\,\mathrm{MeV}$) consistent with most empirical constraints and the predicted neutron matter EoS lies within the limits given by chiral EFT(N^{3}LO) calculations [23, 24].

There are differences in the choice of the constituent particles for the full EoS table. The HS statistical model takes nucleons (n, p), electrons (e), photons (γ), light clusters (^{2}H, ^{3}H, ^{3}He, ^{4}He) and heavy nuclei into account. The binding energies of nuclei are taken from the AME2003 mass table [25] and the FRDM mass table [26] for nuclei with experimentally unknown masses. Excited states of nuclei are considered by using temperature dependent degeneracy factors with densities of states from [27] and a cutoff of the integrals at the nuclear binding energies. The gRDF model also includes muons (μ) and two-nucleon scattering states ($np_{^3S_1}$, $np_{^1S_0}$, $nn_{^1S_0}$, $pp_{^1S_0}$) in order to reproduce the empirical virial EoS at low densities [18]. It uses the AME2012 mass tables [28] extended with masses from the DZ10 mass model [29]. Temperature dependent degeneracy factors are calculated with a density-of-states model from [30] using an integral cutoff at the minimum of the nucleon separation energies, a pairing correction and a further temperature cutoff.

The EV mechanism can be formulated in various ways. In general, the full system volume V is reduced to the available volume $V_{\mathrm{avail}} = V - V_{\mathrm{ex}} = \Phi V$ with the available volume fraction $\Phi = 1 - V_{\mathrm{ex}}/V$. In the so-called "model I", see, *e.g.*, [31], the excluded volume $V_{\mathrm{ex}} = \frac{1}{\varepsilon_0}\sum_i E_i$ is proportional to the particle energies E_i with an energy ε_0 as parameter. This leads to a limiting energy density but there are issues with the theoretical formulation. In the HS approach, "model II" is used with an excluded volume $V_{\mathrm{ex}} = \sum_i v_i n_i$ that is given by a sum of particle number densities n_i with particle

volumes v_i as parameters proportional the mass numbers A_i of the nuclei. Here, a limiting density results beyond which no nuclei occur in dense matter. A generalization of the EV mechanism with an individual treatment of particles with different available volume fractions of general functional form can be found in ref. [32]. There, classical and quantum statistical descriptions are treated. The quasi-particle picture is used to derive the general form of the rearrangement terms to achieve thermodynamic consistency.

The mass shifts of light nuclei in the gRDF model are derived from parametrizations provided by Röpke in ref. [17]. They are simplified with modifications at high densities and temperatures. The mass shifts of the two-nucleon scattering states are adopted from those of the deuteron and for heavy nuclei a simpler parametrization is employed. The mass shift of a nucleus i can be written as

$$\Delta m_i^{(\mathrm{strong})} = f_i(n_i^{(\mathrm{eff}}, T, A_i) B_i^{(0)} \tag{1}$$

with the binding energy $B_i^{(0)}$ of the nucleus in vacuum and a function f_i. It depends on the temperature T, mass number A_i, charge number Z_i, neutron number $N_i = A_i - Z_i$ and an effective density

$$n_i^{(\mathrm{eff})} = 2\frac{Z_i Y_q + N_i(1-Y_q)}{Z_i + N_i} n_b, \tag{2}$$

that introduces a dependence on the isospin asymmetry of the medium through the hadronic charge fraction Y_q. Explicit expressions for f_i are given in ref. [21].

The HS statistical model is formulated with the help of the free energy density

$$\begin{aligned} f = &\sum_{(A,Z)} \left[f_{A,Z}(T, n_{A,Z}) + n_{A,Z} E_{A,Z}^{\mathrm{Coul}} \right] - T \sum_{(A,Z)} n_{A,Z} \ln(\kappa) \\ &+ \xi f_{\mathrm{nuc}}^0(T, \frac{n_n}{\xi}, \frac{n_p}{\xi}) + f_e(T, n_e) + f_\gamma(T), \end{aligned} \tag{3}$$

that contains contributions of individual nuclei $f_{A,Z}^0$ (in Maxwell-Boltzmann approximation), nucleons f_{nuc}^0 (including mesons), electrons f_e and photons f_γ. $E_{A,Z}^{\mathrm{Coul}}$ is the Coulomb energy in Wigner-Seitz approximation and the term with

$$\kappa = 1 - \frac{n_b}{n_{\mathrm{sat}}} \tag{4}$$

(corresponding to Φ) implements the EV mechanism for nuclei. The available volume fraction of nucleons is chosen differently from that of nuclei as

$$\xi = 1 - \sum_{(A,Z)} A \frac{n_{A,Z}}{n_{\mathrm{sat}}}, \tag{5}$$

considering only the volume occupied by nuclei. Since nucleons are assumed not to penetrate into nuclei in the HS approach, the neutron and proton densities of the system have to be rescaled with ξ in the nucleon contribution as well as f_{nuc}^0 itself.

In the gRDF model, the starting point is a grand-canonical potential density

$$\omega(T, \{\mu_i\}) + \sum_i \omega_i + \omega_{\mathrm{meson}} - \omega^{(r)} \tag{6}$$

with contributions ω_i of the particles i, ω_{meson} of the mesons and a rearrangement term $\omega^{(r)}$ that is required for thermodynamic consistency. All strongly interacting particles, *i.e.* nucleons and, contrary to the HS model, light and heavy clusters, are considered as quasi-particles with scalar potentials S_i and vector potentials V_i due to the coupling to the meson fields. The effective mass of all composite particles, *i.e.* nuclei, is given by

$$m_i^* = m_i - S_i + \Delta m_i \tag{7}$$

with the mass shift

$$\Delta m_i = \Delta m_i^{(\mathrm{Coul})} + \Delta m_i^{(\mathrm{strong})}, \tag{8}$$

that includes the Coulomb shift $\Delta m_i^{(\mathrm{Coul})} = E_{A,Z}^{\mathrm{Coul}}$ in Wigner-Seitz approximation as in the HS model and the strong shift $\Delta m_i^{(\mathrm{strong})}$ due to the action of the Pauli principle, see ref. [21] for details.

From the free energy density (3) and the grand-canonical potential density (6) all thermodynamic properties can be derived consistently. Chemical equilibrium connects the chemical potentials μ_i of all particles. The condition of local charge neutrality ensures that the temperature T, the baryon density n_b and the hadronic charge fraction Y_q are sufficient to define the state of the system uniquely.

3. – Results

Predictions of the two EoS models for the thermodynamic properties and the chemical composition are available as EoS tables in the CompOSE format [33]. They cover baryon densities n_b in the range $10^{-10}\,\mathrm{fm}^{-3} \leq n_b \leq 1\,\mathrm{fm}^{-3}$, temperatures T in the range $0.1\,\mathrm{MeV} \leq T \leq 100\,\mathrm{MeV}$ and hadronic charge fractions Y_q in the range $0.0 \leq Y_q \leq 0.6$. From these global EoS tables, the properties of matter in β-equilibrium were extracted by interpolation using the condition of vanishing lepton chemical potential that determines Y_q uniquely for given T and n_b. See ref. [21] for the figures.

At first glance, the HS and the gRDF model show a very similar evolution of the hadronic charge fraction Y_q at β-equilibrium with T and n_b. The lowest values of Y_q are reached in a density range from 10^{-2} to $10^{-1}\,\mathrm{fm}^{-3}$ almost independent of temperature up to $T \approx 10\,\mathrm{MeV}$. The largest differences are at the highest densities because muons are considered in the gRDF model but not the HS model. The mass fractions of the light clusters evolve very similar with T and n_b in both models with two major exceptions. The total deuteron fraction vanishes above about 20 MeV temperature at densities below $10^{-2}\,\mathrm{fm}^{-3}$ in the gRDF model since the bound state contribution is canceled by the continuum contribution at higher temperatures. In the HS model the light particle fractions are set to zero artificially above $T = 50\,\mathrm{MeV}$.

At the lowest temperatures, the chemical composition of neutron star matter is dominated by heavy nuclei. The gRDF model predicts a complete dissolution of heavy nuclei for temperatures above $\approx$10 MeV due to the specific temperature dependence of the effective degeneracy factors in that model. Heavy nuclei survive at even higher temperatures in the HS model, however, above 50 MeV their appearance is suppressed artificially as for light nuclei. For temperatures below about 2 MeV, heavy nuclei dissolve earlier with increasing density in the HS model (at $\approx 4 \cdot 10^{-2}\,\mathrm{fm}^{-3}$) than in the gRDF model (at $\approx 10^{-1}\,\mathrm{fm}^{-3}$). The main differences between the models are observed for the average

mass, charge and neutron numbers of the heavy nuclei. In the gRDF model, $\langle A \rangle$, $\langle Z \rangle$, and $\langle N \rangle$ reduce smoothly with density above $\approx 10^{-3}\,\mathrm{fm}^{-3}$ whereas there is a more abrupt dissolution of the heavy nuclei with almost the largest size in the HS model. At the lowest temperatures, the average mass, charge and neutron numbers are driven strongly by shell effects. Their influence disappears gradually with increasing temperature.

Despite the differences for the chemical composition of neutron-star matter, the HS and gRDF models exhibit rather similar predictions for thermodynamic quantities, such as pressure and entropy per nucleon. They smoothly change with temperature and baryon density. As expected, the highest pressures are found for the higher densities increasing with temperature. In contrast, the entropy per nucleon is largest for low densities and high temperatures. Variations from the gradual decline with T and n_b are only observed for conditions where the chemical composition changes rapidly from heavy to light clusters. There are no signs of a phase transition in neutron star matter at finite temperatures in these hadronic EoS models.

4. – Conclusions

Clustering in dilute matter is an important feature that has to be considered in the preparation of global, multi-purpose EoS tables for astrophysical applications. It is a consequence of correlations in a many-body system with short-range nuclear and long-range Coulomb interactions. There are different approaches to describe the formation and dissolution of clusters in EoS models. Here two methods were compared: the excluded-volume mechanism and an approach with in-medium mass shifts. They are realized in the HS model and the gRDF model, respectively, which are extensions of RMF models with density-dependent meson-nucleon couplings. Since both models use the same parametrization of the nuclear interaction, differences in the predictions can be attributed to the cluster description.

The choice of the cluster suppression mechanism affects mainly the chemical composition of neutron star matter, in particular the average mass, charge and neutron numbers of heavy nuclei. In contrast, the thermodynamic properties of both models are very similar. Consequences of the differences on the dynamical evolution of, *e.g.*, core-collapse supernovae should be studied in numerical simulations in the future. Although developed for astrophysical applications, the HS and gRDF models can be adapted to describe isotopic abundances of nuclei observed in heavy-ion collisions. This will provide another possibility to check the reliability of the predictions.

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