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Clustering in dilute matter with medium effects

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Summary. — The formation and dissolution of light and heavy clusters in warm and dilute strongly interacting matter is studied using a generalized relativistic density functional. This phenomenological theoretical description is an extension of a relativistic mean-field model with density dependent nucleons-meson couplings. It considers nuclei as explicit degrees of freedom in addition to nucleons. Nuclei and nucleons are treated as quasiparticles with medium dependent masses. For clusters, one contribution to the mass shift represents an effective way to take into account the Pauli exclusion principle for nucleons, whether free or bound in nuclei. This mechanism causes the dissolution of clusters at high densities. The consequences are explored for compact star matter as an example for the application of the model in astrophysics. General features and open questions of the approach are discussed.

1. – Introduction

Strongly interacting matter offers a rich variety of phenomena depending on the prevailing conditions of the system under investigation. Aggregates of a finite number of nucleons form atomic nuclei, from light to (super-)heavy, including stable and exotic species. They can be studied in laboratory experiments with different techniques and many theoretical models have been developed to calculate their properties. The thermodynamic limit of infinite particle number will lead to nuclear matter, an idealized system of baryons interacting under the rule of the strong force and neglecting the electromagnetic interaction. One major facet of such matter is the occurrence of phase transitions. They are often discussed with the aid of a phase diagram that is spanned by the baryon density, temperature and isospin asymmetry as the main axes. If electrons (and muons) are added to nuclear matter so that the condition of charge neutrality can be fulfilled, one arrives at compact star matter that is an adequate approximation to matter found, *e.g.*, in neutron stars, their mergers, and core-collapse supernovae. At high densities or temperatures a change of the effective degrees of freedom from hadrons to quarks is expected. In contrast to that, inhomogeneities and the formation of nuclei or clusters occur at subsaturation densities and not too high temperatures.

The properties of the system are embodied in equations of state (EoS) that relate thermodynamic quantities such as pressure, energy or entropy density to variables like temperature, baryon density and isospin asymmetry. The EoS are essential ingredients in astrophysical model calculations that control the static properties of compact stars and the dynamical evolution of core-collapse supernovae and neutron-star mergers. Global, multi-purpose EoS are required for such astrophysical applications. They have to cover very large ranges of the thermodynamic variables, see, *e.g.*, the review [1] for details. The use of EoS is only reasonable if the timescale of reactions is much smaller than that of the system evolution so that (thermal, chemical, ...) equilibrium conditions are reached.

It is a tremendous challenge for nuclear theory to develop models that can describe infinite matter in the whole phase diagram. There are many different approaches, *e.g.*, hadronic "*ab initio*" methods with realistic interactions using a variety of many-body techniques, QCD-based or inspired models, or descriptions employing effective field theories. But these methods are not always applicable in the relevant part of the phase diagram because of methodological or technical limitations. Therefore, phenomenological models are the predominant choice in most applications. They usually consider nucleons, nuclei, leptons and photons as basic constituents. The models are often combinations of different approaches using, *e.g.*, nuclear statistical equilibrium descriptions, the virial EoS, density functionals derived from mean-field models with non-relativistic Skyrme or Gogny interactions or relativistic meson-exchange approaches, or classical/quantum molecular dynamics. For many years, only a limited number of global EoS were available [2-5]. However, many more EoS were developed in recent years, see, *e.g.*, refs. [6-9], and the CompOSE database at `https://compose.obspm.fr`.

In this contribution the focus is on the chemical composition of warm, dilute compact-star matter as predicted by a generalized relativistic density functional with mass shifts driving the cluster dissolution and a variation of the density dependence of the symmetry energy. In sect. **2** the basic features of the theoretical model are summarized. The systematics of cluster formation and dissolution is studied in sect. **3** using the example of compact star matter in β equilibrium. Experimental approaches to support the model predictions are mentioned. Open issues that need attention in the development of improved models in the future are discussed in sect. **4**. A summary is given in sect. **5**.

2. – Theoretical model

The generalized relativistic density functional (GRDF) was developed with the objective to construct an improved EoS model for astrophysical applications with an extended set of constituents, *i.e.*, not only nucleons, electrons and muons but also a full set of nuclei with possible extensions including hyperons, mesons, etc. Since GRDF is a phenomenological approach, it depends on a number of parameters that are determined by fitting properties of finite nuclei. Correlations have to be considered more seriously than before, in particular the dissolution of composite particles (clusters) due to the action of the Pauli principle.

The basic form of the density functional is derived from a relativistic Lagrangian density with nucleons and mesons as degrees of freedom in the mean-field approximation. The interaction is modeled by an exchange of scalar and vector mesons that couple minimally to the nucleons. Many parametrisations have been developed for different purposes [10]. In the present model, density dependent nucleon-meson couplings, which depend on the so-called vector density, are introduced to model the medium dependent interaction. This is in contrast to models with non-linear meson self-couplings. The first realistic parametrisation of the relativistic density functional was obtained in ref. [11] by fitting energies of a selected set of finite nuclei. A particular form of the density dependence was introduced that was used in many refined parametrisation in the following years. In contrast to the non-linear models existing at that time, a second parameter for the isovector part of the effective interaction was introduced that lead to improved (smaller) values of the nuclear incompressibility, the symmetry energy and the symmetry energy slope parameter as compared to models with the non-linear TM1 [12] or NL3 [13] parametrisations. As a result, the correlation between the neutron skin thickness of nuclei with the slope of the neutron matter EoS was more similar to Skyrme Hartree-Fock descriptions of nuclear matter [14]. In the present GRDF, the parametrisation DD2 with very reasonable nuclear matter parameters [15] is used as basic parameter set. It is consistent with the neutron matter EoS obtained from chiral effective field theory calculations in the N^3LO approximation [16, 17] and the parameters of the nuclear symmetry energy respect the unitary gas constraint [18].

The relativistic mean-field description of the nucleonic part of the matter is extended by including light nuclei (^{2}H, ^{3}H, ^{3}He, ^{4}He) and heavy nuclei ($A > 4$) as additional degrees of freedom that interact strongly by coupling to mesons, however, with reduced strength for heavy nuclei. Ground-state energies are taken as experimental values from the 2012/2016 atomic mass evaluations [19, 20] extended to exotic nuclei with masses from the DZ10/DZ31 models [21]. Thus shell effects in the binding energies are taken into account. Excited states of nuclei are included by introducing temperature-dependent degeneracy factors with simple approximations for the densities of states. Strongly interacting particles are considered as quasiparticles with effective masses that change in the medium due to the coupling to the scalar σ meson. For composite particles, *i.e.*, nuclear clusters, additional mass shifts arise with two contributions. The first, giving a reduction of the binding energy, is an effective means to incorporate the action of the Pauli principle that leads to cluster dissolution at high densities, *i.e.*, the Mott effect. For light clusters a simplified version of the parametrisation by G. Röpke is used and simple heuristic formulas are assumed for heavy nuclei. This mechanism replaces the traditional excluded-volume mechanism based on the geometric concept of spatially extended nuclei. The second contribution is an electromagnetic mass shift that originates from the screening of the Coulomb field. It is treated in Wigner-Seitz approximation and leads to an increase of binding energies. Details of the GRDF model can be found in refs. [15, 22-26].

Besides the original DD2 parametrisation, variations of the density-dependent isovector coupling were introduced in ref. [27] in order to explore effects of a changing density dependence of the symmetry energy. The slope coefficient L of the DD2 model of 55 MeV was readjusted to 70 MeV in the DD2$^+$ and 40 MeV in the DD2$^-$ model, respectively. This variation is correlated with the neutron skin thickness in heavy nuclei, larger values of L correspond to larger neutron skins. A second modification of the GRDF model concerns the parametrisation of the mass shifts of heavy nuclei that affects their dissolution, see ref. [28] for details. With the modified parametrisations, new global, multipurpose EoS tables were generated that will become available on the CompOSE website at `https://compose.obspm.fr`. The change of only a single property of the model will allow to study its impact on the dynamical evolution of core-collapse supernovae by direct comparison.

3. – Systematics of cluster formation and dissolution

The abundances of nucleons and nuclei in compact star matter change systematically with a variation of baryon density, temperature and isospin asymmetry. In the following

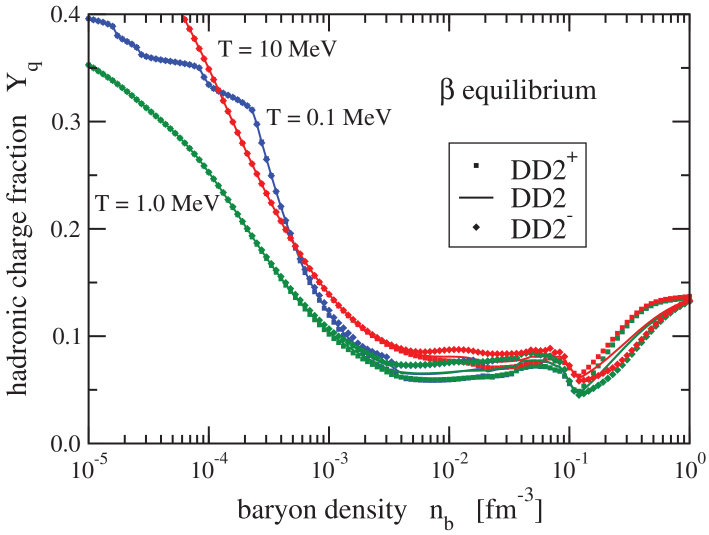

Fig. 1. – Density dependence of the hadronic charge fraction Y_q in compact star matter for three isotherms and parametrisations of the GRDF model.

only matter in β equilibrium is considered as it is expected to exist, *e.g.*, in neutron stars. This condition fixes the isospin asymmetry or, equivalently, the hadronic charge fraction that is identical to the electron fraction as long as muons do not appear. With increasing density a neutronisation of the system is observed with electron fractions below 10% at densities in the range from $0.002\,\text{fm}^{-3}$ to $0.2\,\text{fm}^{-3}$, see fig. 1. Lines of constant temperature are displayed for the three parametrisations DD2^{+} (squares), DD2 (full line), and DD2^{-} (diamonds). Major effects of a modification of the density dependence of the symmetry energy are only recognizable at densities above the nuclear saturation density $n_{\text{sat}} \approx 0.15\,\text{fm}^{-3}$ with a larger Y_q for a larger value of L.

The mass fractions of light nuclei evolve systematically with baryon density for given temperature with almost no difference when the calculations with the DD2^{+}, DD2, and DD2^{-} parametrisations are compared. In fig. 2 the results for deuterons and α particles are depicted as examples. A similar trend is observed for ^{3}H and ^{3}He clusters, not shown here.

The predictions for the cluster mass fractions in warm dilute matter can be tested by observing their yields in experiments with heavy-ion collisions producing compressed matter that expands and emits light nuclei from source regions that can be characterized by density and temperature, see, *e.g.*, refs. [29,30]. From the yields of clusters and nucleons the so-called chemical equilibrium constants can be calculated. They only depend on temperature in the case of an ideal gas mixture of nucleons and clusters without interaction. Experimental data show a definitely distinct behaviour from this simple description indicating the importance of medium effects. EoS models that take these modifications and interactions into account are compatible with experimental data, see ref. [24].

The formation of clusters in matter at subsaturation densities led to the conjecture that α particles should form at the surface of heavy nuclei where the density drops from values close to the saturation density in the nuclear bulk part to very small values [27]. The effective number of α particles was predicted to reduce substantially with increasing neutron number in the chain of Sn nuclei also modifying the neutron skin thickness. As an

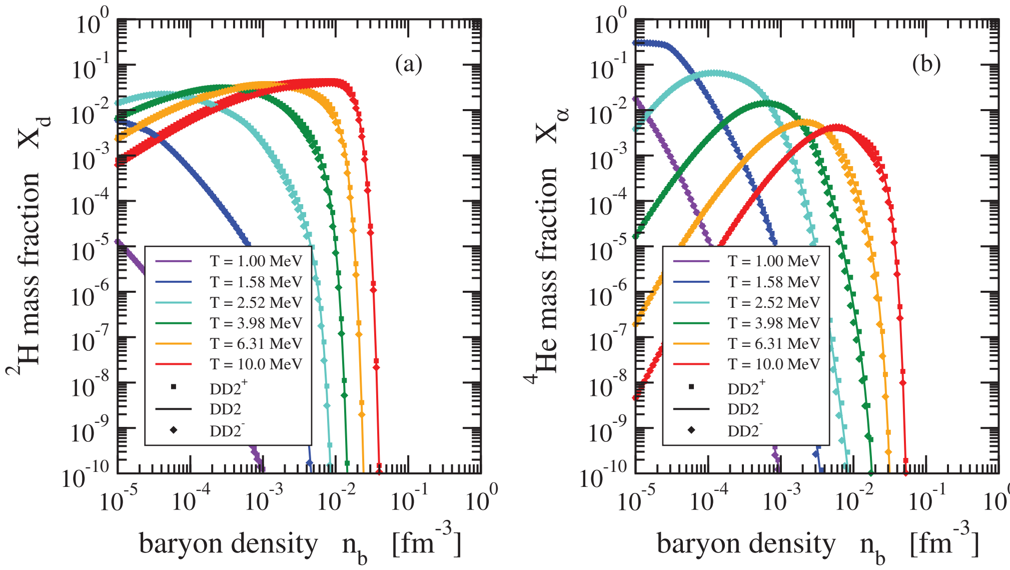

Fig. 2. – Density dependence of the mass fraction X_d of ^{2}H (a) and X_α of ^{4}He (b) in compact star matter for six isotherms and three parametrisations of the GRDF model.

experimental attempt to observe these α particles it was proposed to use quasifree (p,pα) knockout reaction on stable Sn isotopes with mass numbers $A = 112$, 116, 120, and 124 using a 400 MeV proton beam at RCNP, Osaka. The recent experiment in February 2018 successfully detected the knocked-out α particles with a cross section change consistent with the theoretical prediction [31]. The variation of the α particle abundances is also corroborated by the trend of α particle reduced widths in (d,^{6}Li) pickup reactions on Sn nuclei with a reduction when the neutron excess increases [32].

Besides light clusters, the predictions for heavy nuclei are of great interest. In fig. 3 the mass fraction of nuclei with $A > 4$ is depicted as a function of the baryon density for selected values of the temperatures in compact star matter in β equilibrium. At the lowest densities, heavy nuclei exist in bigger quantities only for the lowest temperatures. This is consistent with the expectation that a crust with heavy ions arranged in a crystal forms in the outer part of a cold neutron star. The mass fraction of heavy nuclei increases with density for higher temperatures until a density just below the nuclear saturation density is approached and the nuclei disappear. A variation of the model parametrisations from stiff to soft density dependencies of the symmetry energy has an effect for densities above approximately 0.001 fm^{-3} but the variation is not very strong. A larger impact has the choice of the dissolution mechanism [26] and the parametrisation of the mass shifts, *cf.* ref. [28].

The average mass number $\langle A\rangle$ of heavy nuclei also shows a characteristic change with baryon density along lines of constant temperature, see fig. 4. It does not exceed values of $\langle A\rangle \approx 90$ for temperatures above 1 MeV in the density range of fig. 4. The largest average mass numbers are found at densities below approximately 0.03 fm^{-3} for the lowest temperatures and the average mass number quickly drops with increasing temperature for constant baryon density. At densities above approximately 0.03 fm^{-3} a second region with large values of $\langle A\rangle$, almost independent of the temperature, can be noticed. This feature is an effect of the parametrisation of the mass shifts for heavy

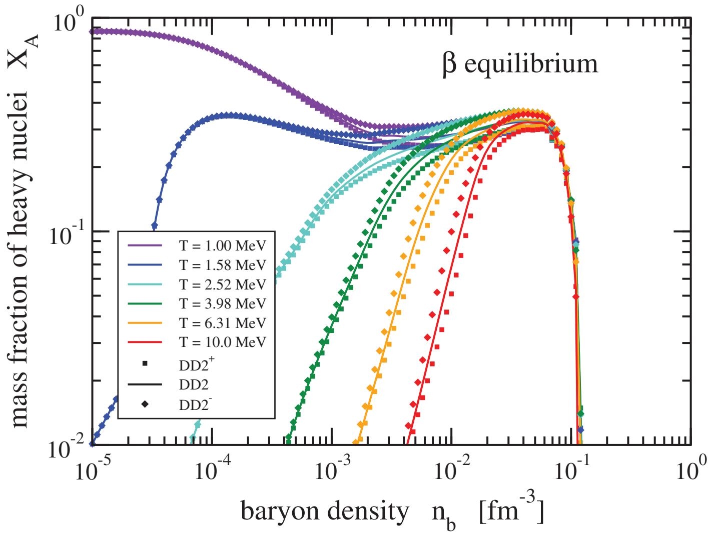

Fig. 3. – Density dependence of the mass fraction X_A of heavy nuclei with mass numbers $A > 4$ in compact star matter for six isotherms and three parametrisations of the GRDF model.

nuclei. The effective action of the Pauli principle leading to a reduced binding energy is partly compensated by the increased binding due to the coupling of the nucleons inside the nucleus to the meson fields. It is not very disturbing because the mass fraction of heavy nuclei quickly drops in this density range, cf. fig. 3. Furthermore, the appearance of phase transitions, which are neglected here, and in particular the formation of pasta structures at low temperatures will modify this picture.

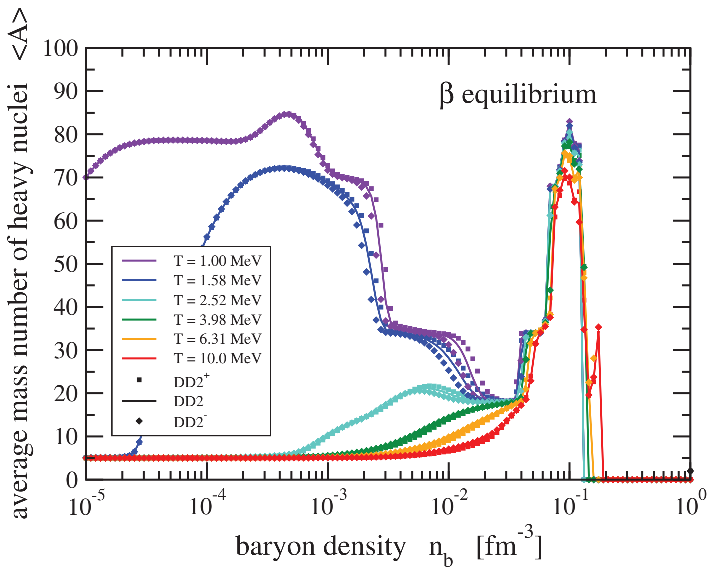

Fig. 4. – Density dependence of the average mass number of heavy nuclei in compact star matter for six isotherms and three parametrisations of the GRDF model.

4. – Open issues

Although the GRDF model with the parametrisation DD2 is consistent with many constraints and makes reasonable predictions for thermodynamic properties of compact star matter and its chemical composition, there are still open issues that require further improvements of the description.

The standard choice for nucleon-meson couplings is a dependence on the vector density. Other options, *e.g.*, couplings depending on the scalar density are also possible but less explored. In order to be thermodynamically consistent, rearrangement contributions appear in the vector or scalar self-energies of the nucleons when the couplings depend on vector or scalar densities, respectively. For a parametrisation like DD2 with a finite slope of the vector meson coupling as a function of the vector density at zero density, one finds that the condition of finite baryon density does not correspond to zero baryon chemical potential. In order to avoid such an effect, breaking the particle-antiparticle symmetry, new parametrisations have to be developed [33].

Another feature that is not yet incorporated into the model is the possible transition from hadronic to quark matter. At high densities or temperatures a change of the degrees of freedom is expected with the possible existence of a first-order phase transition. With a reinterpretation of a modified version of the traditional excluded-volume mechanism, a phenomenological description on the level of thermodynamic quantities can be formulated that mimics a hadron-quark phase transition [34].

The population of excited states of nuclei at finite temperatures also has to be revisited since the used level densities and the resulting temperature dependence of the degeneracy factors can lead to unphysical effects, *e.g.*, with respect to the temperature dependence of the entropy.

The GRDF model by construction suppresses the formation of clusters ≡ correlations at densities above saturation. Except for temperature effects there is no population of single-particle high-momentum states above the Fermi energy. However, it is well known that there are substantial nucleon-nucleon correlations at densities near saturation. Experiments with (e,e′pp) knockout reactions [35-37] clearly show the high-momentum tail due to short-range nucleon-nucleon correlations. It remains an open question how to realize such effects in an effective way in a phenomenological density functional approach to strongly interacting matter.

Extensive EoS tables with numerical data of thermodynamic properties of matter are usually generated for applications in astrophysical simulations. In general, it is expected that they are obtained from models that are thermodynamically consistent, *i.e.*, the standard relations for first-order and second-order derivatives of a thermodynamic potential, *e.g.*, the free energy, hold. However, this is only a local condition. To be fully consistent, the potential has to be a convex function of the corresponding thermodynamic variables. This is only guaranteed if phase transitions are correctly taken into account. In particular, a construction respecting the Gibbs conditions, *i.e.*, the equality of all intensive variables in the coexisting phases, is required. For more than one conserved quantity and related chemical potentials, this can be a rather complex endeavour. With a well chosen Legendre transformation to an appropriate thermodynamic potential with different variables, a transformation to a simple Maxwell construction is achieved, See, *e.g.*, ref. [38] with the example of the liquid-gas phase transition in nuclear matter, which shows a symmetry in isospin with respect to symmetric nuclear matter. The case of compact star matter with arbitrary electron fractions is more complicated due to the asymmetric contribution of electrons in pressure, energies and entropies.

Exploratory studies with existing EoS tables show the occurrence of multiple phase transitions.

5. – Summary

The formation and dissolution of clusters in warm dilute matter is an important feature that has to be considered in theoretical models attempting to describe such a system. Clusters change the chemical composition and thermodynamic properties of matter. They can be regarded as multi-nucleon correlations and their properties depend on the medium. An extension of a relativistic mean-field model that introduces clusters as explicit degrees of freedom in a phenomenological approach allows to explore how the clustering changes with density, temperature and isospin asymmetry of strongly interacting matter. The predictions of the model can be tested in laboratory experiments. An important application of the model is the generation of global, multi-purpose EoS tables for astrophysical simulations.

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