Cluster correlations in dilute matter and equation of state

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Abstract. Cluster correlations are an important feature in strongly interacting matter at subsaturation densities. They modify the chemical composition of the system and the thermodynamic properties, which are encoded in the equation of state. The formation and dissolution of clusters can be described in a generalized relativistic density functional approach. Clusters are included as explicit degrees of freedom with medium-dependent properties. They are considered as quasiparticles with scalar and vector self-energies that represent the effective in-medium interaction. Essential ingredients in the self-energies are rearrangement contributions, which guarantee the thermodynamic consistency of the model, and mass shifts of composite particles, which take into account the effects of the Pauli exclusion principle. They cause the dissolution of clusters at high densities. The occurrence of $\alpha$-particle clusters on the surface of heavy nuclei can be considered by adapting the generalized relativistic density functional approach to nuclear structure calculations. A systematic variation of the $\alpha$-particle abundance and neutron skin thickness with the neutron excess of the nucleus and the strength of the isovector contribution to the effective interaction is observed. The surface $\alpha$-clustering affects the correlation of the neutron skin thickness of heavy nuclei with the density dependence of the symmetry energy, which is relevant for calculations of neutron star structure.

1. Introduction
Dilute matter, i.e. matter with densities smaller than nuclear saturation density $n_{\text{sat}} \approx 0.15 \text{ fm}^{-3}$, can be found at various places in nature, e.g. in astrophysical environments such as the crust of neutron stars or expanding matter in core-collapse supernovae. It can be studied experimentally in the laboratory in heavy-ion collisions or surface-dominated reactions of atomic nuclei.

All the above mentioned systems are very different. They cover microscopic to macroscopic length scales under cold to hot thermal conditions in static equilibrium or dynamical evolution. Nevertheless, they are all interacting many-body systems where correlations are essential. Assuming equilibrium conditions, their thermodynamic properties and chemical composition can be described with appropriate equations of state (EoS). One important aspect is the occurrence of clustering at low densities due to the action of competing attractive and repulsive interactions between the constituents. Low-density matter is found on the surface of heavy nuclei where the nucleon densities drop steeply with increasing distance from the center. Four-nucleon correlations, in particular, can appear as $\alpha$ particles, which have to be preformed in order to facilitate the radioactive decay of unstable heavy nuclei.

Two specific systems have to be distinguished in the discussion. On the one hand, only strongly interacting particles are considered in nuclear matter, where the electromagnetic
interaction is not taken into account. In isospin asymmetric systems with baryon number densities \( n_b \), below \( n_{sat} \) at not too high temperatures \( T \), a ‘non-congruent’ liquid-gas phase transition is observed with the coexistence of a more isospin asymmetric low-density phase and a more isospin symmetric high-density phase [1]. On the other hand, both the strong and electromagnetic interactions have to be considered in stellar matter with hadrons and leptons as constituent particles under the specific condition of charge neutrality. Under these circumstances, new particle species (nuclei) or ‘pasta’ phases are formed, e.g. in the crust of neutron stars. Coulomb correlations are responsible for the occurrence of lattice structures and the gas-solid phase transition at low temperatures.

Information on correlations in interacting many-body systems is contained in spectral functions, which show a complicated structure in general. The description is simplified by using a quasiparticle approximation with self-energies that take into account a part of the correlations by an in-medium change of the particle properties. With this approach the strength of residual correlations is reduced. The quasiparticle concept is very successful in nuclear physics. E.g. phenomenological mean-field models of Skyrme, Gogny or relativistic type [2] use nucleonic quasiparticles. Pairing correlations are efficiently treated by introducing quasiparticles with the help of a Bogoliubov transformation. In the extreme limit, an exact diagonalisation of a interacting many-body Hamiltonian leads to a system of independent quasiparticles, which are many-body states in this case, without residual correlations. In dilute matter at densities much below \( n_{sat} \) clusters/nuclei appear as new degrees of freedom and the properties of the system are described by the model-independent virial equation of state (V\( EoS \)) [3], which can be used as a benchmark for model calculations. The considerations above initiated the development of a generalized relativistic density functional (gRDF) for nuclear and stellar matter with the correct limits and explicit cluster of freedom [4, 5, 6].

2. Generalized relativistic density functional

A thermodynamic consistent formulation of the gRDF with an extended set of constituents is most simply obtained by using a grand canonical approach. The grand canonical potential \( A \) is most simply obtained by using a grand canonical approach. The grand canonical potential \( A \) is thermodynamic consistent formulation of the gRDF with an extended set of constituents.

The list of constituent particles in the full gRDF model comprises baryons (nucleons and hyperons at densities above \( n_{sat} \)), four light nuclei (\( ^2H, ^3H, ^3He, ^4He \)) and 16745 heavy nuclei \( A_iZ_i \) with mass numbers \( A_i > 4 \), neutron numbers \( N_i \leq 184 \) and proton numbers \( Z_i \leq 184 \). Experimental binding energies of the nuclei are taken from the 2012 Atomic mass evaluation [8] when available. For all other nuclei between the neutron and protons driplines (determined without the Coulomb contribution to the energy) the predictions of the DZ10 model [9] are used. Nucleon-nucleon scattering correlations are represented by effective resonances in the continuum [5]. In stellar matter, leptons and photons are added without any problems. The dispersion relation of all interacting quasiparticles \( i \) depends on scalar potentials \( S_i \) and vector
potentials $V_i$ that represent the effective in-medium interaction. For pure nucleonic matter they can be parametrized by suitable functions [10]. In general, scalar and vector potentials receive contributions from Lorentz scalar mesons ($\sigma$, $\delta$, $\sigma^*$, ...) and Lorentz vector mesons ($\omega$, $\rho$, $\phi$, ...), respectively. These are treated as classical fields in the model. The coupled field equations are derived in the standard way by variation. They have to be solved self-consistently for given temperature, baryon number density and baryonic charge fraction. The parametrization DD2 [4] is used for the density dependence of the nucleon-meson couplings. This effective interaction is characterized by very reasonable nuclear matter parameters (saturation density $n_{\text{sat}} = 0.149 \text{ fm}^{-3}$, energy per nucleon at saturation $E/A|_{\text{sat}} = -16.02 \text{ MeV}$, incompressibility $K = 242.7 \text{ MeV}$, symmetry energy $J = 31.67 \text{ MeV}$, symmetry energy slope parameter $L = 55.04 \text{ MeV}$), which are compatible with most of current constraints. The neutron matter EoS lies nicely inside the error bounds given by ab-initio N$^3$LO calculations in chiral effective field theory ($\chi$EFT) [11, 12], see figure 1. Note that effects of clustering or phase transitions on the symmetric matter EoS [6] are not taken into account in the figure.

In addition to the standard mesonic terms, the vector potential $V_i$ contains “rearrangement” contributions and an effective electromagnetic contribution that represents Coulomb correlations, which even appear in uniform systems. The scalar potential $S_i$ includes the medium dependent mass shifts $\Delta m_i$ of composite particles. It allows to describe their formation and dissolution with changing density and temperature. There are two contributions to the mass shift $\Delta m_i$. The strong shift originates mainly from the Pauli exclusion principle. It blocks states in the medium that can no longer participate in the formation of cluster correlations. Thus the binding energies are reduced and the Mott effect, i.e. the dissolution of clusters, is observed with increasing density. This microscopic mechanism replaces the traditional geometric excluded-volume mechanism in order to suppress the cluster formation at high densities. The electromagnetic contribution to the mass shift appears only in stellar matter. It increases the binding energies of clusters because the almost uniformly distributed electrons lead to a screening of the Coulomb field. The mass shifts of light clusters can be calculated by solving in-medium few-body Schrödinger-like equations with realistic nucleon-nucleon potentials. A simple parametrization of the extracted mass shift is used in the gRDF calculations [4]. For heavy nuclei fully self-consistent spherical Wigner-Seitz cell calculations with the gRDF for nucleons and electrons are performed in an extended Thomas-Fermi approximation [13]. From a comparison with calculations of uniform matter, the increase of the binding energy due to cluster formation.
can be determined. Presently, only a simplified parametrization of the thus determined mass shifts is employed. The description will be improved with more systematic calculations in the future covering the whole chart of nuclei for various temperatures and densities of the medium.

The modification of the in-medium properties of composite particles has important consequences for the chemical composition of matter. These effects can be explored by studying the mass number fractions \( X_i = A_i n_i / n_b \) with \( n_b = \sum_i A_i n_i \). For given temperature \( T \) and proton fraction \( Y_p \), only two-body correlations are relevant at low \( n_b \) and the chemical composition is dominated by nucleons and a few deuteron-like correlations. With increasing density the fraction \( X_d \) increases and three-, four- and many-nucleon cluster become more and more significant. Close to the saturation density \( n_{\text{sat}} \), the clusters dissolve and nucleonic matter remains at higher densities, see, e.g., the right panel of figure 10 in reference [13]. In figure 2, the mass fractions of nucleons, light and heavy clusters, and electrons are depicted as a function of the temperature \( T \) at given baryon number density \( n_b = 0.001 \text{ fm}^{-3} \) and total proton fraction \( Y_p \), from a preliminary calculation in the gRDF approach. At high temperatures the matter is mainly composed of nucleons, electrons and very few deuterons. The abundances of light clusters increase when the system is cooled down. At temperatures below approx. 3 MeV, light clusters disappear and heavy clusters dominate the chemical composition. The corresponding evolution of the average mass and charge numbers of the heavy clusters is shown in figure 3. Their strong increase with decreasing temperature is obvious. At very low temperatures, a phase transition from the gas to the solid crystal phase is expected. According to Monte Carlo simulations in the so-called one-component plasma (OCP) model this transition occurs at a plasma parameter \( \Gamma_{\text{heavy}} = \langle Z \rangle_{\text{heavy}}^{5/3} e^2 / (a_e T) \approx 175 \) containing the characteristic length scale \( a_e = [(3/(4\pi n_e))]^{1/3} \) that depends on the electron density \( n_e \), see e.g. reference [14]. The vertical dashed line in figure 3 indicates the corresponding temperature for solidification or melting. All the effects of cluster formation and phase transitions have to be implemented in EoS models to provide a reliable input to astrophysical simulations.

**Figure 2.** Temperature dependence of the mass fractions \( X_i \) for nucleons (n,p), light and heavy clusters (A) and electrons (e) in stellar matter at baryon number density \( n_b = 0.001 \text{ fm}^{-3} \) and proton fraction \( Y_p = 0.4 \).

**Figure 3.** Temperature dependence of the average mass and charge number of heavy clusters and of the plasma parameter \( \Gamma_{\text{heavy}} \) in stellar matter at baryon number density \( n_b = 0.001 \text{ fm}^{-3} \) and proton fraction \( Y_p = 0.4 \).
3. Symmetry energy and neutron skins

The energy of nuclear matter at given baryon density \( n_b \) depends strongly on the isospin asymmetry of the system, i.e. the proton-to-neutron ratio. This effect can be quantified with the help of the density dependent symmetry energy \( E_{\text{sym}}(n_b) \) of nuclear matter. It measures the difference of the energy per baryon in pure neutron matter and symmetric nuclear matter. There is a well-known correlation between the neutron skin thickness of heavy nuclei, i.e. the difference between the neutron and proton root-mean-square radii, and the stiffness of the neutron matter EoS [15, 16] or, equivalently, the slope parameter \( L = 3n_{\text{sat}} \frac{dE_{\text{sym}}(n_b)}{dn_b} |_{n_b=n_{\text{sat}}} \) of the symmetry energy [17], see, e.g., figure 2 in reference [18]. There have been many attempts in recent years to determine experimentally the symmetry energy at saturation \( J = E_{\text{sym}}(n_{\text{sat}}) \) and the slope parameter \( L \), see, e.g., references [18, 19]. One approach, PREX@JLab [20], uses parity violating electron scattering on \( ^{208}\text{Pb} \) that is mainly sensitive to the neutron distribution in nuclei. Combining the results with charge distribution measurements in ordinary electron scattering, the neutron skin thickness \( r_{\text{skin}} \) can be determined. The \( r_{\text{skin}} \leftrightarrow L \) correlation can then be used to extract the slope coefficient \( L \) of the symmetry energy. However, this correlation is based only on relativistic and non-relativistic mean-field calculations of nuclei that do not take into account the effect of clustering beyond pairing correlations. Thus the question arises how strongly will the \( r_{\text{skin}} \leftrightarrow L \) correlation be affected by clustering in the neutron skin of nuclei.

Finite temperature gRDF calculations in spherical Wigner-Seitz cells using an extended relativistic Thomas-Fermi (RTF) approximation can describe the formation of heavy nuclei inside dilute stellar matter [13]. They show an increased probability of finding light clusters on the surface of nuclei when these additional degrees of freedom are considered, see figure 11 in reference [13]. In order to apply the gRDF approach to nuclei at zero temperature in the vacuum, the model has to be adapted to this particular situation. When \( T \) approaches zero, only \( \alpha \) particles remain as relevant clusters. Since they are bosons, a Thomas-Fermi approximation cannot be used for them but their density distribution has to be obtained from a ground-state wave function, which is calculated in the WKB approximation self-consistently with the nucleon distributions. The original DD2 parametrization [4] had to be modified slightly in the Thomas-Fermi calculation in order to improve the description of heavy nuclei because the parameter set was determined by fits to properties of nuclei in the relativistic Hartree (RH) approximation but not in TF approximation. This was achieved by rescaling the \( \sigma \) meson mass and coupling without affecting nuclear matter parameters.

The neutron skin thickness of Sn nuclei with mass numbers from \( A = 107 \) to \( A = 133 \) is depicted in figure 4. Without \( \alpha \)-particle correlations on the surface there is an almost linear increase of \( r_{\text{skin}} \) with the mass number \( A \). Taking \( \alpha \)-cluster formation into account modifies the mass number dependence of \( r_{\text{skin}} \) clearly. The largest effect is observed at intermediate mass numbers where the occurrence of \( \alpha \) particles reduces the neutron skin thickness considerably since the asymmetry of the density distributions of neutrons and protons is reduced. For very neutron-rich nuclei, almost no \( \alpha \) clusters can form in the highly neutron-rich low-density matter on the surface and the reduction of the neutron skin thickness is insignificant. For nuclei with more or less equal numbers of protons and neutrons, no neutron skin develops even if \( \alpha \) particles can form abundantly on the nuclear surface. The density distribution of \( \alpha \) particles always peaks close to the nuclear matter radius, see figure 1 in reference [21], since \( \alpha \) clusters cannot penetrate into the bulk nucleon distributions. The absolute effective number of \( \alpha \) particles is always less than one half in the present gRDF model calculations as depicted in figure 4 of reference [21].

In order to study the change of the neutron skin thickness of \( ^{208}\text{Pb} \) with the slope parameter \( L \) including surface \( \alpha \)-particle clustering, the isovector part of the effective interaction, which is represented by the \( \rho \) meson exchange, was systematically varied. The density dependent \( \rho \) meson coupling \( \Gamma_\rho(n_b) = \Gamma_\rho(n_{\text{ref}}) \exp[-a_\rho(n_b/n_{\text{ref}} - 1)] \) depends on two parameters: \( \Gamma_\rho(n_{\text{ref}}) \) at the reference density \( n_{\text{ref}} = n_{\text{sat}} \) and \( a_\rho \). These two parameters were determined by fits to
properties of finite nuclei as for the original DD2 parametrization, however demanding specific values of the slope parameter $L$ between 25 MeV and 100 MeV. Actual values for $\Gamma_{\rho(n_{\text{ref}})}$, $a_{\rho}$ and the symmetry energy $J$ at saturation are given in table 1 of reference [21]. The correlation of the neutron skin thickness of $^{208}\text{Pb}$ with $L$ is shown in figure 5 for three different calculations. The full blue line with circles represents the results of the original relativistic Hartree calculation without $\alpha$-particle correlations for different parametrizations of the isovector interaction. When $L$ rises from 25 MeV to 100 MeV, the neutron skin thickness increases from about 0.10 fm to approx. 0.27 fm. The increase is not linear as in the usual representations of the $r_{\text{skin}} \leftrightarrow L$ correlation because only the parameters of the $\rho$-meson coupling were adjusted in the fit and not all coupling parameters. Changing from the RH to the RTF calculations causes an overall reduction of the neutron skin thickness, however the trend is very similar as in the RH calculation. When $\alpha$-particle correlations on the surface are included, a further reduction of $r_{\text{skin}}$ in the order of 0.02 fm is found. This is a sizeable fraction of the neutron skin thickness if the slope parameter $L$ and correspondingly $r_{\text{skin}}$ is already small. The $\alpha$-clustering effect leads a shift of the $r_{\text{skin}} \leftrightarrow L$ correlation that should be taken into account at least as a systematic error when $L$ is determined from experimentally measured neutron-skin thicknesses of heavy nuclei.

4. Conclusions
Thermodynamic properties and the chemical composition of nuclear and stellar matter can be described properly only if many-body correlations are taken into account with suitable methods. In a generalized relativistic density functional approach cluster correlations are included as explicit degrees of freedom. All constituents in dense matter are considered as quasiparticles with medium-dependent properties, which are represented by scalar and vector self-energies. The effective in-medium interaction is modeled by the exchange of mesons with density-dependent couplings, which are well constrained by properties of finite nuclei. Composite particles receive additional contributions to their self-energies from explicit mass shifts. They incorporate the Pauli exclusion principle and lead to the dissolution of clusters at high densities. In order to reproduce the correct low-density limit, which is given by the virial equation of state, nucleon-
nucleon scattering correlation have to be included in the model. A proper treatment of Coulomb correlations is required to describe the phase transition to a crystal at low temperatures. The thermodynamic consistency of the approach is ensured through the appearance of rearrangement contributions.

The gRDF approach can be applied to the construction of equation of state tables for astrophysical simulations such as core-collapse supernovae or for the description of static properties of neutron stars. A substantial variation of the chemical composition is observed, in particular in dilute matter at subsaturation densities, as a function of temperature, baryon density and isospin asymmetry.

With appropriate adjustments, the gRDF can also be used to describe the properties of atomic nuclei in vacuum at zero temperature. Since atomic nuclei are surrounded by very dilute nucleonic matter it is expected that cluster correlations can affect their surface properties. In first calculations employing simple approximations, it is found that α-particle correlations appear on the surface of heavy nuclei. The actual amount of α clusters depends strongly on the neutron excess of the nucleus. It modifies the neutron thickness as compared to conventional mean-field calculations without explicit four-nucleon correlations. This effect pertains also to the correlation between the neutron skin thickness of heavy nuclei and the slope coefficient of the nuclear symmetry energy, which in turn is related to the stiffness of the neutron matter equation of state.

The prediction of α-cluster correlations on the surface of heavy nuclei can be tested experimentally with quasifree (p, pα) reactions. Such investigations are planned for the future at RCNP Osaka [22].

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