# Nuclear matter equation of state including two-, three-, and four-nucleon correlations

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Light clusters (mass number  $A \le 4$ ) in nuclear matter at subsaturation densities are described using a quantum statistical approach to calculate the quasiparticle properties and abundances of light elements. I review the formalism and approximations used and extend it with respect to the treatment of continuum correlations. Virial coefficients are derived from continuum contributions to the partial densities which depend on temperature, densities, and total momentum. The Pauli blocking is modified taking correlations in the medium into account. Both effects of continuum correlations lead to an enhancement of cluster abundances in nuclear matter at higher densities. Based on calculations for A = 2, estimates for the contributions with A = 3,4 are given. The properties of light clusters and continuum correlations in dense matter are of interest for nuclear structure calculations, heavy-ion collisions, and astrophysical applications such as the formation of neutron stars in core-collapse supernovae.

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## I. INTRODUCTION

Nuclear matter is a strongly interacting quantum system, and the determination of the physical properties is a challenging issue in many-body theory. In this work, nuclear matter in thermodynamic equilibrium is investigated, confined in the volume  $\Omega$  at temperature T, and consisting of  $N_n$ neutrons (total neutron density  $n_n^{\text{tot}} = N_n / \Omega$ ) and  $N_p$  protons (total proton density  $n_p^{\text{tot}} = N_n / \Omega$ ). In the thermodynamic limit, the state is given by the parameter set  $\{T, n_n^{\text{tot}}, n_n^{\text{tot}}\}$ ; the dependence on  $\Omega$  is trivial. The subsaturation region will be considered where the baryon density  $n_B = n_n^{\text{tot}} + n_p^{\text{tot}} \leq n_{\text{sat}}$ (with the saturation density  $n_{\rm sat} \approx 0.16 \, {\rm fm}^{-3}$ ), the temperature  $T \leq 20$  MeV, and the proton fraction  $Y_p = n_p^{\text{tot}}/n_B$  between 0 and 1. This region of warm dense matter is of interest not only for nuclear structure calculations and heavy-ion collisions explored in laboratory experiments [1], but also in astrophysical applications. For instance, core-collapse supernovae at postbounce stage evolve in this region of the phase space [2], and different processes such as neutrino emission and absorption, which strongly depend on the composition of warm dense matter, influence the mechanism of core-collapse supernovae.

Recently, standard versions [3,4] of the nuclear-matter equation of state (EOS) for astrophysical simulations have been improved, see Refs. [5–23]. Here I do not discuss different approaches but rather contribute to a special question, the treatment of light clusters which is a long-standing problem [24]. A simple chemical equilibrium of free nuclei is not applicable up to saturation density because medium modifications by self-energy shifts and Pauli blocking become relevant. Concepts such as the heuristic excluded-volume approach or in-medium nuclear cluster energies within the extended Thomas-Fermi approach may be applied to heavier clusters but are not satisfactory to describe light clusters that require a more fundamental quantum statistical approach. For the strongly interacting nuclear matter considered here, in particular warm dense matter in the low-density region, correlations are important, and a simple mean-field description is clearly insufficient. A signature of strong correlations is the formation of bound states. In the low-density limit, one can consider the many-nucleon system as an ideal mixture of nucleons and bound clusters (nuclei) where the interaction is reduced to accidental, reacting collisions, leading to chemical equilibrium as given by the mass-action law. This so-called nuclear statistical equilibrium (NSE) (see Ref. [10]) has several shortcomings, such as the exclusion of excited states, in particular continuum correlations, and the failure to account for the interaction between the different components (single nucleons as well as nuclei), which is indispensable when approaching saturation density.

Both problems are solved within a quantum statistical (QS) approach [29,30] which is able to cover the entire region from the low-density limit up to saturation density. The many-particle aspects are treated in a systematic way, using the methods of thermodynamic Green's functions, diagram techniques, or path-integral methods. Motivated by

To treat the many-nucleon system (nuclei and nuclear matter) at densities up to saturation, semiempirical mean-field approaches have been worked out. Based on the Hartree-Fock-Bogoliubov approximation and related quasiparticle concepts such as the Dirac-Brueckner-Hartree-Fock (DBHF) approach for the nuclear-matter EOS (see Ref. [25]), semiempirical approaches such as the Skyrme parametrization [26] or relativistic mean-field (RMF) model give an adequate description of the known properties of nuclear matter near the saturation density. For a discussion of different versions of these models, see, for instance, Refs. [14,15,22]. The mean-field potentials may be considered as density functionals that include various correlations beyond a microscopic Hartree-Fock-Bogoliubov approximation. In this work the density-dependent relativistic mean-field (DD-RMF) parametrization according to Typel (Refs. [27,28]) is used. Other parametrizations of the nucleon quasiparticle energies can alternatively be used to optimize the description of nuclear matter near saturation density.

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the chemical picture where bound states are considered as new species, to be treated on the same level as free particles, a consistent approach to treat few-body correlations and cluster formation has been worked out. Evaluating thermodynamic Green's functions [24], a cluster decomposition of the self-energy provides us with the possibility to take into account the contribution of different clusters *A*. Physical properties, including the thermodynamic relations (EOS) are obtained from the spectral function. The nucleons as well as the bound states (nuclei) are treated as quasiparticle energies, are modified by self-energy and (in the case of bound states) Pauli blocking. Detailed calculations have been performed for A = 1,2; see Ref. [31].

The inclusion of all light elements  $A \leq 4$  is important deuteron d (<sup>2</sup>H), triton t (<sup>3</sup>H), helion h (<sup>3</sup>He), and  $\alpha$  $(^{4}\text{He})$ —in addition to free neutrons (n) and protons (p). A theory for nuclear systems, assuming that clusters with A > 4 are irrelevant, can be applied to a wide range of the phase space at subsaturation densities; see Refs. [4,12,13,17] for an illustration of the parameter space  $\{T, n_B, Y_p\}$ , where such regions are shown. Solving the Bethe-Salpeter equation for the A-nucleon system, the constituents  $c = \{d, t, h, \alpha\}$  are considered as quasiparticles as discussed in Sec. III. The cluster quasiparticle energy  $E_c(\mathbf{P}; T, n_n^{\text{tot}}, n_p^{\text{tot}})$  depends not only of the center-of-mass (c.m.) momentum  $\mathbf{P}$ , but also the set of thermodynamic parameters  $\{T, n_n^{\text{tot}}, n_p^{\text{tot}}\}$  or, changing the set of thermodynamic variables,  $\{T, \mu_n, \mu_p\}$ , with the chemical potentials  $\mu_n, \mu_p$  as used in the grand-canonical ensemble. The Coulomb energy that is screened in dense matter can be treated rigorously in the QS approach [24]. For  $Z \leq 2$  the Coulomb contributions to the energy shift are small at subsaturation densities and can be omitted.

Previous investigations (see Refs. [8,32,33]) considered the in-medium shifts of the bound-state energies. In addition to the density and temperature dependence, the dependence on the total momentum of the cluster is essential. A consequence is the Mott effect: the bound states disappear at a certain density  $n_c^{\text{Mott}}(\mathbf{P}; T, Y_p)$ . To describe the low-density limit rigorously, excited states and continuum correlations have to be considered. This is taken into account by a virial expansion [34] of the EOS. The low-density region, where the contribution of the continuum correlations to the virial expansion has significant impact [35], was investigated recently in the context of the generalized RMF approach [36]. Introducing the quasiparticle concept, one has to be careful to avoid double counting because part of the continuum correlations is already implemented in the quasiparticle energy shift; see Ref. [37]. Similar to the bound-states case, the contribution of the scattering states to the EOS is modified by density effects as known from the generalized Beth-Uhlenbeck approach [31]. However, this contribution has not yet been investigated as a function of all variables {**P**;  $T, n_B, Y_p$ } for the light clusters, in contrast to the contribution of bound states where the quasiparticle energy shift is calculated for these variables.

Another shortcoming in previous studies is the calculation of Pauli blocking under the assumption of an uncorrelated medium. This has to be improved if one considers regions in the phase diagram where clusters are abundant. In particular, until now it was not possible to include it in the treatment of  $\alpha$  matter [38]. This problem should also be considered in the context of clustering in low-density nuclei; see Ref. [39]. Pairing can also be treated within a QS approach [31], but has not been included systematically in recent versions of the EOS.

The aim of the present study is to improve these shortcomings discussed above. The goal is to describe nuclear matter in the entire region of subsaturation densities, connecting the single-nucleon quasiparticle approach that reproduces the properties near  $n_{sat}$  to the low-density limit, where a clustervirial expansion [37] is possible. Correlations at densities larger than the Mott density are taken into account. Expressions for the contributions of continuum correlations  $v_c(\mathbf{P}; T, n_B, Y_p)$ will be given, which are calculated for A = 2 and estimated for A = 3,4; see Secs. IV and V D. The calculations for A = 2 are performed for a separable potential. Not only the low-density limit of the second virial coefficient, but also, within a generalized Beth-Uhlenbeck approach, the full dependence on the variables  $\{\mathbf{P}; T, n_B, Y_p\}$  is of relevance. Because of the small deuteron binding energy, the contribution of continuum correlations to the second virial coefficient is large.

Within a cluster-virial expansion [37], the virial coefficients for A = 3 in the low-density limit can be related to empirical scattering phase shifts in the corresponding breakup channels; see Ref. [40]. Future calculations may give more accurate values not only for the low-density limit of the virial coefficients for A = 3,4 but also their modification at finite densities to replace the estimates given in this work. Because of the relatively large binding energies for A = 3,4 compared with A = 2, the effect of the continuum correlations is less relevant.

Another problem is the treatment of correlations in the medium. The Pauli blocking is overestimated if the medium is approximated as uncorrelated. Although the formalism to include correlations has been worked out [37,41,42] (see Appendix B), the resulting cluster mean-field equations have not yet been solved in a self-consistent way. In contrast to the ideal Fermi distribution of free nucleons, the occupation of the phase space is changed if correlations in the medium are taken into account. A simple parametrization to modeling the phase-space occupation is proposed; see Sec. II C.

These improvements have already been used to interpret experimental results of heavy-ion collisions [1] but have not been published until now. Analyzing experiments to obtain the symmetry energy or the chemical constants, QS results are presented showing clustering at baryon densities up to  $0.03 \text{ fm}^{-3}$ . I collect in this work all inputs and parameters used in the QS approach so that results as presented, e.g., in Ref. [1], can be followed in detail. Moreover, I point out assumptions and estimates which demand more fundamental research in the future. For the present level of experimental accuracy, some of them are relevant, but other improvements will not lead to a significant change of the results.

The QS approach can be extended to describe further clusters with A > 4 (see Refs. [5,43]) but is not well worked out for this regime yet. An alternative approach to include heavy nuclei is the concept of the excluded volume (EV); see Ref. [11]. In a simple semiempirical approach, the effect of Pauli blocking is replaced by the strong repulsion determined

by the EV. The comparison between the EV model and the QS approach [44] gives qualitatively similar results, although in the EV model the center-of-mass motion of clusters is not systematically treated (for instance, effective mass and quantum condensation effects). In addition, light clusters such as the deuteron are not well described by a hard-core potential, not depending on the energy, and correlations in the continuum are not considered. However, to include heavier clusters, a combination of the QS approach for  $A \leq 4$  with the EV model or with Thomas-Fermi calculations for A > 4 [12,15,18,20,21,45,46] is promising and will be further worked out in the future.

The paper is organized as follows. After reviewing the basis relations of the QS approach in Secs. II and III, Pauli blocking in correlated matter is discussed in Sec. II C. New results are presented in Sec. IV, where continuum correlations and the virial coefficients as function of the thermodynamic variables  $\{T, n_B, Y_p\}$  and the c.m. momentum **P** are discussed. The explicit presentation of all relevant relations and parameter values should enable everybody to follow in detail the results given in Sec. V. Some general issues, which need to be resolved to devise an improved EOS, are discussed in Sec. VI.

# II. GREEN'S FUNCTIONS APPROACH AND QUASIPARTICLE CONCEPT

In Secs. II A and II B, some known relations are reviewed to introduce the relevant concepts, to give some definitions, and to indicate approximations performed in the evaluations. A new result is the use of an effective phase-space occupation number to take into account the effect of the correlated medium on the Pauli blocking (Sec. II C).

## A. Cluster decomposition of the equation of state

The total neutron number density  $n_n^{\text{tot}}$ , the total proton number density  $n_p^{\text{tot}}$ , and the temperature *T* are considered as independent thermodynamic variables. Weak interaction processes leading to  $\beta$  equilibrium are not considered. The chemical potentials  $\mu_n, \mu_p$  are an alternative to  $n_p^{\text{tot}}$  and  $n_n^{\text{tot}}$ in characterizing thermodynamic equilibrium of warm dense matter. The relations

$$\frac{1}{\Omega}N_n = n_n^{\text{tot}}(T,\mu_n,\mu_p), \quad \frac{1}{\Omega}N_p = n_p^{\text{tot}}(T,\mu_n,\mu_p), \quad (1)$$

are EOS that relate the set of thermodynamic quantities  $\{T, \mu_n, \mu_p\}$  to  $\{T, n_n^{\text{tot}}, n_p^{\text{tot}}\}$ . These EOS (chemical potentials) for warm dense matter are solved in this work. Further thermodynamic variables are consistently derived after a thermodynamic potential is found by integration; see Sec. V B and Appendix A.

The nuclear-matter EOS ( $\Omega$  is the system volume,  $\tau = \{n, p\}$ )

$$n_{\tau}^{\text{tot}}(T,\mu_{n},\mu_{p}) = \frac{1}{\Omega} \sum_{p_{1},\sigma_{1}} \int \frac{d\omega}{2\pi} \frac{1}{e^{(\omega-\mu_{\tau})/T} + 1} S_{\tau}(1,\omega) \quad (2)$$

is obtained from the spectral function  $S_{\tau}(1,\omega;T,\mu_n,\mu_p)$ , which is related to the self-energy  $\Sigma(1,z)$  (see Refs. [29,30]):

$$S_{\tau}(1,\omega) = \frac{2\mathrm{Im}\Sigma(1,\omega-i0)}{[\omega - E(1) - \mathrm{Re}\Sigma(1,\omega)]^2 + [\mathrm{Im}\Sigma(1,\omega-i0)]^2}.$$
(3)

The single-nucleon quantum state  $|1\rangle$  can be chosen as  $1 = {\mathbf{p}_1, \sigma_1, \tau_1}$ , which denotes wave number, spin, and isospin, respectively. The EOS (2) relates the total nucleon numbers  $N_{\tau}^{\text{tot}}$  or the particle densities  $n_{\tau}^{\text{tot}}$  to the chemical potentials  $\mu_{\tau}$  of neutrons or protons so that one can switch from the densities to the chemical potentials. However, if this EOS is known in some approximation, all other thermodynamic quantities are obtained consistently after calculating a thermodynamic potential as shown in Sec. V B.

The spectral function  $S_{\tau}(1,\omega;T,\mu_n,\mu_p)$  and the corresponding two-point correlation functions (density matrix) are quantities well-defined in the grand canonical ensemble characterized by  $\{T,\mu_n,\mu_p\}$ . The self-energy  $\Sigma(1,z;T,\mu_n,\mu_p)$  depends, besides the single-nucleon quantum state  $|1\rangle$ , on the complex frequency *z* and is calculated at the Matsubara frequencies. Within a perturbative approach it can be represented by Feynman diagrams. A cluster decomposition with respect to different few-body channels (*c*) is possible [24], characterized, for instance, by the nucleon number *A*, as well as spin and isospin variables.

Using the cluster decomposition of the self-energy which takes into account, in particular, cluster formation, one obtains

$$n_n^{\text{tot}}(T,\mu_n,\mu_p) = \frac{1}{\Omega} \sum_{1} \int \frac{d\omega}{2\pi} f_{1,0}(\omega) S_n(1,\omega)$$
$$= \frac{1}{\Omega} \sum_{A,\nu,\mathbf{P}} N f_{A,Z} [E_{A,\nu}(\mathbf{P};T,\mu_n,\mu_p)],$$
$$n_p^{\text{tot}}(T,\mu_n,\mu_p) = \frac{1}{\Omega} \sum_{1} \int \frac{d\omega}{2\pi} f_{1,1}(\omega) S_p(1,\omega)$$
(4)

$$= \frac{1}{\Omega} \sum_{A,\nu,\mathbf{P}} Zf_{A,Z}[E_{A,\nu}(\mathbf{P};T,\mu_n,\mu_p)],$$
  
denotes the c.m. momentum of the cluster (or, z

where **P** denotes the c.m. momentum of the cluster (or, for A = 1, the momentum of the nucleon). The internal quantum state  $\nu$  contains the proton number Z, and neutron number N = A - Z of the cluster,

$$f_{A,Z}(\omega; T, \mu_n, \mu_p) = \frac{1}{\exp[(\omega - N\mu_n - Z\mu_p)/T] - (-1)^A},$$
(5)

is the Bose or Fermi distribution function for even or odd A, respectively, that is depending on  $\{T, \mu_n, \mu_p\}$ . The integral over  $\omega$  is performed within the quasiparticle approach; the quasiparticle energies  $E_{A,\nu}(\mathbf{P}; T, \mu_n, \mu_p)$  are depending on the medium characterized by  $\{T, \mu_n, \mu_p\}$ . These in-medium modifications will be detailed in Secs. II B, II C, and III.

I review the contributions of the clusters  $(A \ge 2)$ , suppressing the thermodynamic variables  $\{T, \mu_n, \mu_p\}$ . In Eq. (4), the summation (integral) over the c.m. momentum **P** must be done numerically because the dependence of the in-medium

quasiparticle energies  $E_{A,\nu}(\mathbf{P}; T, \mu_n, \mu_p)$  on **P** is complex. The summation over  $\nu$  concerns the bound states as far as they exist, as well as the continuum of scattering states. One can introduce different channels (*c*) characterized, e.g., by spin and isospin quantum numbers. This intrinsic quantum number will be denoted by  $\nu_c$ , and one has in the nondegenerate case  $[\sum_{\mathbf{P}} \rightarrow \Omega/(2\pi)^3 \int d^3 P]$ 

$$n_{A,c} = \frac{1}{\Omega} \sum_{\nu_c, \mathbf{P}} f_{A,Z}[E_{A,\nu_c}(\mathbf{P})]$$
  
=  $e^{(N\mu_n + Z\mu_p)/T} \int \frac{d^3 P}{(2\pi)^3} \sum_{\nu_c} g_{A,\nu_c} e^{-E_{A,\nu_c}(\mathbf{P})/T}$   
=  $\int \frac{d^3 P}{(2\pi)^3} z_{A,c}^{\text{part}}(\mathbf{P}),$  (6)

with  $g_{A,c} = 2s_{A,c} + 1$  the degeneration factor in the channel *c*. The partial density of the channel *c* at **P**,

$$= e^{(N\mu_n + Z\mu_p)/T} \left\{ \sum_{\nu_c}^{\text{bound}} g_{A,\nu_c} \ e^{-E_{A,\nu_c}(\mathbf{P})/T} \times \Theta \Big[ -E_{A,\nu_c}(\mathbf{P}) + E_{A,c}^{\text{cont}}(\mathbf{P}) \Big] + z_{A,c}^{\text{cont}}(\mathbf{P}) \right\}, \quad (7)$$

contains the intrinsic partition function which can be decomposed in the bound-state contribution and the contribution of scattering states  $z_{A,c}^{\text{cont}}(\mathbf{P}; T, \mu_n, \mu_p)$ .

The summations of Eq. (7) over *A*, *c*, and **P** remain to be done for the EOS (4), and *Z* may be included in *c*. The region in the parameter space, in particular **P**, where bound states exist, is restricted as expressed by the step function  $\Theta(x) = 1, x \ge 0$ ; = 0 else. The continuum edge of scattering states is denoted by  $E_{A,c}^{\text{cont}}(\mathbf{P}; T, \mu_n, \mu_p)$ , e.g., defined in Eq. (22) below.

For instance, in the case A = 2 the deuteron is found in the spin-triplet, isospin-singlet channel ( $\{A,c\} \rightarrow d$ ) as a bound state (in the zero-density limit  $g_d = 3$ ,  $E_{2,T_l=0}(\mathbf{P}) = E_d(\mathbf{P}) = E_d^0 + \hbar^2 P^2/4m$ ,  $E_d^0 = -B_d = -2.225$  MeV). In addition, in the same channel one has also contributions from scattering states, i.e., continuum contributions, characterized by the relative momentum as internal quantum number. According to the Beth-Uhlenbeck formula [34] (see Ref. [24]), one has in the low-density limit

$$\int \frac{d^{3}P}{(2\pi)^{3}} z_{d}^{\text{part}}(\mathbf{P})$$

$$= \int \frac{d^{3}P}{(2\pi)^{3}} \left[ \sum_{\nu_{c}}^{\text{bound}} g_{A,\nu_{c}} e^{-E_{A,\nu_{c}}(\mathbf{P})/T} + z_{A,c}^{\text{cont}}(\mathbf{P}) \right]$$

$$= \frac{2^{3/2}}{\Lambda^{3}} \left[ g_{d} e^{-E_{d}^{0}/T} + \int_{0}^{\infty} \frac{dE}{\pi} e^{-E/T} \frac{d}{dE} \delta_{2,T_{I}=0}^{\text{tot}}(E) \right], \quad (8)$$

with  $\Lambda = (2\pi \hbar^2/mT)^{1/2}$  being the baryon thermal wavelength (the neutron and proton masses are approximated by  $m_\tau \approx m = 939.17 \text{ MeV}/c^2$ ) and  $\delta_{2,T_I=0}^{\text{tot}}(E) = \sum_{S,L,J} (2J + M_{T_I})^{1/2} (2J + M_{T_I})^{1/2}$ 

1) $\delta_{2s+1}L_J(E)$  the isospin-singlet ( $T_I = 0$ ) scattering phase shifts with angular momentum *L* as function of the energy *E* of relative motion. A similar expression can also be derived for the isospin-triplet channel (e.g., two neutrons) where, however, no bound state occurs; see also Ref. [35], where detailed numbers are given. The relation (8) gives an exact relation for the second virial coefficient in the low-density limit where in-medium effects are absent.

It should be noted that the ideal gas NSE is recovered if the summation over  $v_c$  is restricted to only the bound states (nuclei), neglecting the contribution of correlations in the continuum. Furthermore, for  $E_{A,v_c}(\mathbf{P}; T, \mu_n, \mu_p)$  the boundstate energies of the isolated nuclei are taken, neglecting the effects of the medium such as mean-field terms or contributions owing to correlations in the medium.

Note that the separation in Eqs. (7) and (8) into a bound state contribution and a contribution  $z_{A,c}^{\text{cont}}(\mathbf{P}; T, \mu_n, \mu_p)$  of continuum states is not unique. One can use another decomposition which follows after performing an integration by parts; see Eq. (37) below.

## B. Cluster mean-field approximation

For finite densities, the main problem is the medium modification of few-body properties which defines also  $E_{A,\nu_c}(\mathbf{P}; T, \mu_n, \mu_p)$  in the contribution (6) of the different components. Quasiparticles are introduced to describe the propagation of few-nucleon clusters (including A = 1) in warm dense matter. The Green's function approach describes the propagation of a single nucleon by a Dyson equation governed by the self-energy, and the few-particle states are obtained from a Bethe-Salpeter equation containing the effective interaction kernel. Both quantities, the effective interaction kernel and the single-particle self-energy, should be approximated consistently. Approximations which take cluster formation into account have been worked out [37,41]; the general scheme of the cluster mean-field approximation is outlined in Appendix B.

For the A-nucleon cluster, the in-medium Schrödinger equation

$$[E_{\tau_{1}}(\mathbf{p}_{1}; T, \mu_{n}, \mu_{p}) + \dots + E_{\tau_{A}}(\mathbf{p}_{A}; T, \mu_{n}, \mu_{p}) - E_{A\nu}(\mathbf{P}; T, \mu_{n}, \mu_{p})]\psi_{A\nu\mathbf{P}}(1, \dots, A) + \sum_{I',\dots,A'} \sum_{i < j} [1 - n(i; T, \mu_{n}, \mu_{p}) - n(j; T, \mu_{n}, \mu_{p})]V(ij, i'j') \times \prod_{k \neq i, j} \delta_{kk'}\psi_{A\nu\mathbf{P}}(1', \dots, i', \dots, j', \dots, A') = 0$$
(9)

is derived from the Green's function approach after the effective occupation numbers  $n(i; T, \mu_n, \mu_p)$  [Eq. (B5)] are introduced and exchange terms are neglected. This equation contains the effects of the medium in the single-nucleon quasiparticle shift

$$\Delta E_{\tau}^{\text{SE}}(\mathbf{p}; T, \mu_n, \mu_p) = E_{\tau}(\mathbf{p}; T, \mu_n, \mu_p) - \sqrt{m^2 c^4 + \hbar^2 c^2 p^2} + mc^2 \approx E_{\tau}(\mathbf{p}; T, \mu_n, \mu_p) - \frac{\hbar^2 p^2}{2m}$$
(10)

(nonrelativistic case), as well as in the Pauli blocking terms given by the occupation numbers  $n(1; T, \mu_n, \mu_p)$  in the phase space of single-nucleon states  $|1\rangle \equiv |\mathbf{p}_1, \sigma_1, \tau_1\rangle$ . Thus, two effects have to be considered, the quasiparticle energy shift and the Pauli blocking.

In the lowest order of perturbation theory with respect to the nucleon-nucleon interaction V(12, 1'2'), the influence of the medium on the few-particle states (A = 1, ..., 4) is given by the Hartree-Fock shift

$$\Delta E_{\tau_1}^{\rm HF}(\mathbf{p}_1) = \sum_2 V(12, 12)_{\rm ex} f_{1, \tau_2}(2)$$
(11)

and, consistently, the Pauli blocking terms

$$\Delta V_{12}^{\text{Pauli}}(12, 1'2') = -\frac{1}{2} \Big[ f_{1,\tau_1}(1) + f_{1,\tau_{1'}}(1') \Big] V(12, 1'2') \quad (12)$$

for A = 2, ..., 4; see Eqs. (B3) and (B4) neglecting the contributions with mass number B > 1.

Both terms (11) and (12) have a similar structure; besides the nucleon-nucleon interaction V, the single-nucleon Fermi distribution  $f_{1,\tau}(1) = f_{1,n/p}[E_{\tau}(\mathbf{p}_1); T, \mu_n, \mu_p]$  occurs. In this simplest approximation, only the free nucleons contribute to the self-energy shift and the Pauli blocking. The distribution function is the Fermi distribution with the parameter set  $\{T, \mu_n, \mu_p\}$ .

It is obvious that also the nucleons found in clusters contribute to the mean field, leading to the self-energy, but occupy also phase space and contribute to the Pauli blocking. The cluster mean-field (CMF) approximation [32,37,41] considers also the few-body T matrices in the self-energy and in the kernel of the Bethe-Salpeter equation. The CMF approximation leads to similar expressions (11) and (12), but with the free-nucleon Fermi distribution  $f_{1,\tau_1}(1)$  replaced by the effective occupation number (B5),

$$n(1) = f_{1,\tau_1}(1) + \sum_{B=2}^{\infty} \sum_{\bar{\nu},\bar{\mathbf{P}}} \sum_{2\dots B} B f_B[E_{B,\bar{\nu}}(\bar{\mathbf{P}};T,\mu_n,\mu_p)] \\ \times |\psi_{B\bar{\nu}\bar{\mathbf{P}}}(1,\dots,B)|^2,$$
(13)

which contains also the distribution function  $f_B[E_{B,\bar{\nu}}(\bar{\mathbf{P}})]$  for the abundance of the different cluster states and the respective wave functions  $\psi_{B\bar{\nu}\bar{\mathbf{P}}}(1,\ldots,B)$ . (The variable Z has not been given explicitly.) For the QS derivation, see the references given in Appendix B.

Because the self-consistent determination of  $n(1; T, \mu_n, \mu_p)$  for given  $\{T, \mu_n, \mu_p\}$  is very cumbersome, I consider appropriate approximations. In particular, I use the Fermi distribution with new parameters  $\{T_{\text{eff}}, \mu_n^{\text{eff}}, \mu_p^{\text{eff}}\}$  (effective temperature and chemical potentials),

$$n(1; T, \mu_n, \mu_p) \approx f_{1,\tau_1}(1; T_{\text{eff}}, \mu_n^{\text{eff}}, \mu_p^{\text{eff}}).$$
 (14)

These effective parameters make it possible to reproduce some moments of the occupation number distribution. For instance, besides the normalization (which gives the total neutron/proton number)

$$\sum_{\mathbf{p}_{1}} n(1; T, \mu_{n}, \mu_{p}) = N_{\sigma_{1}, \tau_{1}}^{\text{tot}} = \sum_{\mathbf{p}_{1}} f_{1, \tau_{1}} \big( 1; T_{\text{eff}}, \mu_{n}^{\text{eff}}, \mu_{p}^{\text{eff}} \big),$$
(15)

also

$$\sum_{1} p_{1}^{2} n(1; T, \mu_{n}, \mu_{p}) = \sum_{1} p_{1}^{2} f_{1,\tau} \left( 1; T_{\text{eff}}, \mu_{n}^{\text{eff}}, \mu_{p}^{\text{eff}} \right) \quad (16)$$

can be used to fix the values of  $T_{\text{eff}}, \mu_n^{\text{eff}}, \mu_p^{\text{eff}}$  as functions of  $\{T, \mu_n, \mu_p\}$  [47].

This ansatz contains the special case where the medium is described by noninteracting single-nucleon states. Then, the effective parameter values coincide with  $T, \mu_n, \mu_p$ . However, a correlated medium has a more diffuse Fermi surface. In the general case, the contributions of clusters according to Eq. (13) have to be taken into account.

## C. Medium modification of few-body properties in warm dense matter

For the A-nucleon cluster, the in-medium Schrödinger equation (9) is derived, depending on the occupation numbers  $n(i; T, \mu_n, \mu_p)$  of the single-nucleon states  $|i\rangle$ . As a consequence, the solutions [the energy eigenvalues  $E_{A\nu}(\mathbf{P}; T, \mu_n, \mu_p)$  and the wave functions] will also depend on the parameters which characterize the occupation numbers.

New variables  $\{T_{\text{eff}}, \mu_n^{\text{eff}}, \mu_p^{\text{eff}}\}\$  are introduced according to the approximation (14) to characterize the occupation number distribution. Because in the effective wave equation (9) the Pauli blocking  $1 - n(i; T, \mu_n, \mu_p) - n(j; T, \mu_n, \mu_p)$  depends on the surrounding medium only via the occupation number distribution, one can employ the calculations for the Fermi distribution (uncorrelated medium [32,33]) and replace the variables  $\{T, \mu_n, \mu_p\}$  with the new effective variables. According Eq. (14), these new variables are related to the original variables  $\{T, \mu_n, \mu_p\}$  so that the effects of Pauli blocking implicitly depend on the temperature *T* and the chemical potentials  $\mu_c$ . One can go a step further and switch from the chemical potentials to densities so that one uses  $\{T_{\text{eff}}, n_B, Y_p\}$  as variables to characterize the occupation number distribution,

$$n(1; T, \mu_n, \mu_p) \approx \tilde{f}_{1,\tau_1}(1; T_{\text{eff}}, n_B, Y_p).$$
 (17)

The tilde  $f_{1,\tau}(1; T_{\text{eff}}, n_B, Y_p)$  denotes a Fermi distribution as a function of densities instead the chemical potentials. Implicitly,  $\tilde{f}_{1,\tau}(1)$  depends on the effective parameter values  $\{T_{\text{eff}}, \mu_n^{\text{eff}}, \mu_p^{\text{eff}}\}$  so that the normalization holds; i.e.,  $\mu_{\tau}^{\text{eff}}(T_{\text{eff}}, n_B, Y_p)$  are the solutions of the normalization conditions (15).

The use of  $n_B = n_n^{\text{tot}} + n_p^{\text{tot}}$  and  $Y_p = n_p^{\text{tot}}/n_B$  realizes that all nucleon participate in the phase-space occupation [see Eq. (13)], and  $T_{\text{eff}}$  is a further parameter that takes into account the formation of correlations in the medium. As a consequence, the solutions [the energy eigenvalues  $E_{A\nu}(\mathbf{P}; T, n_B, Y_p)$  and the wave functions] will also depend on the parameters  $\{T_{\text{eff}}, n_B, Y_p\}$ , which now characterize the occupation numbers, but are functions of  $\{T, \mu_n, \mu_p\}$ .

From nuclear-matter calculations it is well known that because of correlations the occupation in phase space is more diffuse compared with the ideal Fermi gas, and tails in the single-nucleon distribution are related to the nucleon-nucleon interaction. For instance, the phase-space occupation function for various temperatures and densities was considered in Ref. [48]. At low densities, the phase-space occupation is determined by the composition of the nuclear matter and the wave function of the corresponding clusters. In particular, at decreasing temperatures the abundance of  $\alpha$  particles is increasing, and the occupation in phase space is determined by the internal momentum distribution of  $\alpha$  particles.

Based on the results for the phase-space occupation n(1) obtained in Ref. [48] for different values of T and  $n_B$ , I determined the effective temperature  $T_{\text{eff}}(T, n_B, Y_p)$ . For this,  $\tilde{f}_{1,\tau}(T_{\text{eff}}, n_B, Y_p)$  was fitted to the calculated values of n(1) so that not only the normalization  $n_n^{\text{tot}}, n_p^{\text{tot}}$  are fulfilled, but also the maximum of the first derivative (near the Fermi energy) is reproduced. A simple relation,

$$T_{\rm eff} \approx 5.5 \,\,\mathrm{MeV} + 0.5T + 60n_B \,\,\mathrm{MeV} \,\,\mathrm{fm}^3, \qquad (18)$$

was obtained as an approximation.

Obviously, the simple linear dependence on T and  $n_B$  is only a rough estimate, and a more complex dependence is expected for  $T_{\text{eff}}(T, n_B, Y_p)$  if a wide region in the parameter space is considered. At finite temperature, in the low-density limit all correlations disappear in the nuclear medium which can be treated as an ideal gas of nucleons. The linear increase of correlations and subsequently  $T_{\rm eff}(T, n_B, Y_p)$  with increasing  $n_B$  does not apply if degeneration sets in, and a nonlinear dependence on  $n_B$  is expected. At low temperature, the nuclear medium is described by  $\alpha$  matter, and the effective temperature describes the single-nucleon momentum distribution in the  $\alpha$  bound state. The simple fit formula (18) is applicable in the region 5 MeV < T < 15 MeV and densities  $n_B < n_{sat}/2$ of the parameter space. More detailed investigations are necessary to derive a more general expression for the effective temperature as function of  $T, n_B, Y_p$ . The present simple fit formula (18) may be considered as a first step in this direction.

To evaluate the dependence of the cluster energy eigenvalues  $E_{A\nu}(\mathbf{P}; T, n_B, Y_p)$  on  $\{T, n_B, Y_p\}$ , one has to solve the in-medium Schrödinger equation

$$[E_{\tau_{1}}(\mathbf{p}_{1}; T, n_{B}, Y_{p}) + \dots + E_{\tau_{A}}(\mathbf{p}_{A}; T, n_{B}, Y_{p}) - E_{A\nu}(\mathbf{P}; T, n_{B}, Y_{p})]\psi_{A\nu\mathbf{P}}(1, \dots, A) + \sum_{1',\dots,A'} \sum_{i < j} [1 - \tilde{f}_{1,\tau_{i}}(i; T_{\text{eff}}, n_{B}, Y_{p}) - \tilde{f}_{1,\tau_{j}}(j; T_{\text{eff}}, n_{B}, Y_{p})] \times V(ij, i'j') \prod_{k \neq i, j} \delta_{kk'}\psi_{A\nu\mathbf{P}}(1', \dots, A') = 0$$
(19)

obtained from Eq. (9), replacing the occupation numbers  $n(i; T, \mu_n, \mu_p)$  with a Fermi distribution  $\tilde{f}_{1,\tau_i}(i; T_{\text{eff}}, n_B, Y_p)$ . This equation contains the effects of the medium in the singlenucleon quasiparticle shift  $\Delta E_{\tau_1}^{\text{SE}}(\mathbf{P}; T, n_B, Y_p)$  [Eq. (10)], as well as in the Pauli blocking terms given by the occupation numbers  $\tilde{f}_{1,\tau_i}(i; T_{\text{eff}}, n_B, Y_p)$  in the phase space of singlenucleon states  $|i\rangle$ .

Obviously, the bound-state wave functions and energy eigenvalues  $E_{A\nu}(\mathbf{P}; T, n_B, Y_p)$  (Pauli blocking), as well as the scattering phase shifts, become dependent on the effective temperature  $T_{\text{eff}}$  and the densities  $n_{\tau}^{\text{tot}}$ . In particular, one obtains

the cluster quasiparticle shifts

$$E_{A,\nu}(\mathbf{P}) - E_{A,\nu}^{0}(\mathbf{P})$$
  
=  $\Delta E_{A,\nu}^{\text{SE}}(\mathbf{P}) + \Delta E_{A,\nu}^{\text{Pauli}}(\mathbf{P}) + \Delta E_{A,\nu}^{\text{Coulomb}}(\mathbf{P}),$  (20)

with the free contribution  $E_{A,\nu}^0(\mathbf{P}) = E_{A,\nu}^0 + \hbar^2 P^2/(2Am)$ . Expressions for the in-medium self-energy shift  $\Delta E_{A,\nu}^{\text{SE}}(\mathbf{P}; T, n_B, Y_p)$  and Pauli blocking  $\Delta E_{A,\nu}^{\text{Pauli}}(\mathbf{P}; T_{\text{eff}}, n_B, Y_p)$  are given in Sec. III B and Appendix C below. The Coulomb shift owing to screening effects is added, which can be approximated by the Wigner-Seitz expression. For the light elements with  $Z \leq 2$  considered here, the Coulomb corrections are small compared with the other contributions and are omitted.

Of special interest are the binding energies

$$B_{A,\nu}^{\text{cond}}(\mathbf{P}; T, n_B, Y_p) = -\left[E_{A,\nu}(\mathbf{P}; T, n_B, Y_p) - E_{A,\nu}^{\text{cont}}(\mathbf{P}; T, n_B, Y_p)\right], \quad (21)$$

with

$$E_{A,\nu}^{\text{cont}}(\mathbf{P}; T, n_B, Y_p)$$
  
=  $N E_n(\mathbf{P}/A; T, n_B, Y_p) + Z E_p(\mathbf{P}/A; T, n_B, Y_p),$  (22)

which indicate the energy difference between the bound state and the continuum of free (scattering) states at the same total momentum **P**. This binding energy determines the yield of the different nuclei according to Eq. (4), where the summation over **P** is restricted to that region where bound states exist, i.e.,  $B_{A,\nu}^{\text{bind}}(\mathbf{P}; T, n_B, Y_p) \ge 0$ . Note that the edge of the continuum states is determined by the decomposition to single-particle states. Other channels containing lighter clusters are already blocked out earlier because the respective Mott densities are smaller; see Sec. III C below.

In addition to the bound states, in solving Eq. (19), also continuum states have to be considered. The continuum states are also influenced by the medium effects, but the results are less obvious and demand more discussions. Some estimates are given in Sec. IV.

### **III. QUASIPARTICLE CONTRIBUTIONS TO THE EOS**

The contributions of different mass numbers A to the EOS (4) are analyzed. Before presenting new results with respect to the contribution of continuum correlations in the following section, known results concerning the contribution of bound states are briefly repeated, according to the intention to present all prerequisites for reproducing the calculations. Furthermore, to investigate continuum correlations, it is useful to review the treatment of the bound-state part.

The single-nucleon contribution A = 1 is extensively discussed; the quasiparticle picture is well elaborated and broadly applied. An exhaustive discussion of the two-nucleon contribution (A = 2) has been given in Ref. [31]. Besides the bound-state part, also the scattering states have been treated. A generalized Beth-Uhlenbeck equation has been considered where not only the low-density limit (second virial coefficient) is correctly reproduced, but also mean-field terms are consistently included avoiding double counting. The results can be applied to finite densities of warm dense matter up to saturation density. Then, all light clusters ( $A \leq 4$ ) are included. Besides the cluster-virial expansion in the low-density limit, the medium modifications which are increasing with increasing density are of interest, and the effect of correlations in the medium is discussed. The behavior of bound states has been investigated in previous work [32,33]. Some usable results are available, but the continuum contributions remain until now very difficult to treat. Some estimates and simple interpolation formulas are given in Sec. IV.

### A. Single-nucleon quasiparticle approximation

Before improving the low-density limit of the EOS considering the ideal gas NSE and cluster-virial expansion, the influence of the medium is discussed which is necessary to describe warm dense matter up to saturation density. First the approximation of the EOS (4) is considered where only the single-nucleon contributions are taken, i.e., the sum over A is reduced to A = 1, which contains the neutron (n) and proton (p) quasiparticle contribution to the EOS.

In the quasiparticle approximation, the imaginary part of  $\Sigma$  is neglected in Eq. (3). The spectral function is  $\delta$ -like, and the densities are calculated from Fermi distributions with the single-nucleon quasiparticle energies  $E_1(1) = \hbar^2 p_1^2/2m + \text{Re } \Sigma[1, E_1(1)] = \hbar^2 p_1^2/(2m) + \Delta E^{\text{SE}}(1)$  so that (spin factor 2)

$$n_{\tau}^{\rm qu}(T,\mu_n,\mu_p) = \frac{2}{\Omega} \sum_{\mathbf{p}} f_{1,\tau}[E_{\tau}(\mathbf{p};T,n_B,Y_p);T,\mu_n,\mu_p].$$
(23)

The quasiparticle approximation is well elaborated in nuclear physics; see Refs. [49,50]. Starting from a microscopic approach with suitable nucleon-nucleon interaction potentials, standard approximations for the single-nucleon self-energy shift  $\Delta E^{\text{SE}}(1)$  are the Hartree-Fock-Bogoliubov or the DBHF approximation; see Sec. I. In the spirit of the density-functional approach, semiempirical expressions such as the Skyrme forces or RMF approaches have been worked out. The relativistic quasiparticle energy

$$E_{\tau}(\mathbf{p}; T, n_B, Y_p) = \sqrt{[m_{\tau}c^2 - S(T, n_B, Y_p)]^2 + \hbar^2 c^2 p^2} + V_{\tau}(T, n_B, Y_p) - m_{\tau}c^2$$
(24)

gives in the nonrelativistic limit  $\Delta E_{\tau}^{\text{SE}}(0) = -S(T, n_B, Y_p) + V_{\tau}(T, n_B, Y_p)$  and  $m_{\tau}^*/m_{\tau} = 1 - S(T, n_B, Y_p)/(m_{\tau}c^2)$ . Explicit expressions for  $S(T, n_B, Y_p)$  and  $V_{\tau}(T, n_B, Y_p)$  in form of Padé approximations which are suitable for numerical applications, are given in Appendix D. They are obtained from the DD-RMF parametrization and can be replaced with alternative parametrizations [14,15,22].

Fitted to properties near the saturation density, the description of warm dense matter at densities near  $n_{sat}$  is adequate. No cluster formation can be described in the single-nucleon quasiparticle (mean field) approach. One has to go beyond this approximation [24] and has to treat the imaginary part of the self-energy  $\Sigma(1,z)$  in (3) to include cluster formation and to reproduce the correct low-density limit.

### B. Shifts of light cluster binding energies in dense matter

Coming back to the EOS (4), one has to add the contributions of clusters with  $A = \{2,3,4\}$ . We first consider the bound-state parts. In the low-density limit one can use the empirical binding energies  $B_c = -E_c^0$  (see below Table I, first line), as also used in the ideal gas NSE. In the case of  $c = \{d,t,h\}$  there is no excited bound state above the ground state. In the case of  $\alpha$ , binding energy  $B_{\alpha} = 28.3$  MeV, there exists an excited  $\alpha'$  state with excitation energy 20.2 MeV to be included into the partial density (7), which also contains the contribution of scattering states.

The contribution to the dispersion relation of the cluster quasiparticles according to Eq. (20) has to be discussed. The most significant medium effect is the Pauli blocking, which is also strongly dependent on temperature. The Pauli blocking shift of the binding energies  $\Delta E_c^{\text{Pauli}}(\mathbf{P}; T_{\text{eff}}, n_B, Y_p)$  [see Eq. (C1)] has been evaluated within a variational approach. The results are presented in Ref. [33], and a parametrization has been given which makes it possible to calculate the medium modification of the bound-state energies with simple expressions in good approximation; see Eq. (14) of Ref. [33]. The results for the Pauli-blocking medium shifts of the bound-state energies are collected in Appendix C.

The contribution of the single-nucleon energy shift to the cluster self-energy shift  $\Delta E_{A,\nu}^{SE}$  is easily calculated in the effective mass approximation, where the single-nucleon

$r_c$ binding energies, energies, energies stengths $n_c$ , and suppression parameter $\gamma_c$ for right nu	gnt nuclei.
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c	d	t	h	α
$\overline{B_c (\text{MeV})}$	2.225	8.482	7.718	28.3
$\lambda_c^{\rm eff}$ (MeV)	1287.4	1775.1	1724.3	2865
$n_c^{\text{Mott}}(T = 5 \text{ MeV}) \text{ (fm}^{-3})$	0.003 965 3	0.005 483 6	0.005 145 4	0.007 888 9
$n_c^{\text{Mott}}(T = 10 \text{ MeV}) (\text{fm}^{-3})$	0.007 987	0.010122	0.009 464 3	0.014 532
$n_c^{Mott}(T = 15 \text{ MeV}) \text{ (fm}^{-3})$	0.01197	0.015 118	0.014 141	0.021 162
$n_c^{Mott}(T = 20 \text{ MeV}) \text{ (fm}^{-3})$	0.015 861	0.020939	0.01992	0.027 892
$\gamma_c/T(T = 5 \text{ MeV}) \text{ (fm}^3)$	376.917	506.894	517.639	595.077
$\gamma_c/T(T = 10 \text{ MeV}) \text{ (fm}^3)$	187.62	274.613	281.421	323.049
$\gamma_c/T(T = 15 \text{ MeV}) \text{ (fm}^3)$	124.829	183.855	188.349	221.832
$\gamma_c/T(T=20 \text{ MeV}) \text{ (fm}^3)$	94.2282	132.748	133.707	168.309
$\gamma_c ({\rm MeV}{\rm fm}^3)$	1876.2	2746.1	2814.2	3230.5

quasiparticle energy shift

$$\Delta E_{\tau}^{\rm SE}(\mathbf{p}) = \Delta E_{\tau}^{\rm SE}(0) + \frac{\hbar^2 p^2}{2m^*} - \frac{\hbar^2 p^2}{2m}$$
(25)

can be represented by the energy shift  $\Delta E_{\tau}^{\text{SE}}(\mathbf{p} = 0)$  and the effective mass  $[m_{\tau}^*]^{-1} = [m_{\tau}]^{-1} + \partial^2 \Delta E_{\tau}^{\text{SE}}(\mathbf{p})/\partial p^2|_{\mathbf{p}=0}$ . One can use the empirical value [51]

$$\frac{m^*}{m} = 1 - 0.17 \frac{n_B}{n_{\text{sat}}}.$$
 (26)

In the rigid-shift approximation where  $m^* = m$ , the selfenergy shift  $\Delta E_{\tau}^{\text{SE}}$  cancels in the binding energy because the continuum is shifted by the same value. It can be absorbed in the chemical potential of the EOS (4).

In general, in the kinetic part of the the wave equation (19) which consists of the single-nucleon quasiparticle energies  $E_{\tau_i}(\mathbf{p}_i; T, n_B, Y_p)$ , one can introduce the c.m. momentum  $\mathbf{P}$  and the intrinsic motion described by Jacobi coordinates. In the effective mass approximation, the separation of the c.m. motion is simple because the single-particle dispersion relations are quadratic. The self-energy shift  $\Delta E_{A,\nu}^{SE}(\mathbf{P}; T, n_B, Y_p) = \Delta E_{A,\nu}^{SE,c.m.}(\mathbf{P}; T, n_B, Y_p) + \Delta E_{A,\nu}^{SE,intr.}(\mathbf{P}; T, n_B, Y_p)$  consists of the c.m. part  $\Delta E_{A,\nu}^{SE,c.m.}(\mathbf{P}; T, n_B, Y_p) = E_{A,\nu}^{cont}(\mathbf{P}; T, n_B, Y_p) - \hbar^2 P^2/(2Am)$ , which coincides with the edge of the continuum (22) for the intrinsic motion, and the intrinsic part

$$\Delta E_{A,\nu}^{\text{SE,intr}}(\mathbf{P}; T, n_B, Y_p) = E_{A,\nu}^{\text{kin,intr}} \left(\frac{m}{m^*} - 1\right). \quad (27)$$

The intrinsic part of the cluster self-energy shift  $\Delta E_{A,\nu}^{\text{SE,intr}}(\mathbf{P})$  is easily calculated for given wave functions [5,32] (see also Ref. [8]) within perturbation theory. Values for  $E_{A,\nu}^{\text{in,int}}$  for the light elements are given below in Table II. It results as the averages of  $\hbar^2/mq_1^2$  for A = 2,  $\hbar^2/m(q_1^2 + 3/4q_2^2)$  for A = 3, and  $\hbar^2/m(q_1^2 + 3/4q_2^3 + 2/3q_3^2)$  for A = 4, where  $\mathbf{q}_i$  denote the respective Jacobian momenta [32].

TABLE II. Parameter values for the Pauli blocking shift  $\Delta E_{\nu}^{\text{Pauli}}(\mathbf{P}; T, n_B, Y_p)$  [Eq. (C1)] for different nuclei ( $\nu = \{d, t, h, \alpha\}$ ).

Parameter	Units	<i>d</i> ( <sup>2</sup> H)	t ( <sup>3</sup> H)	h ( <sup>3</sup> He)	α ( <sup>4</sup> He)
$\overline{f_{\nu,1}}$	$MeV^{3/2}$ fm <sup>3</sup>	6792.6	20103.4	19 505.9	36 146.7
$f_{\nu,2}$	MeV	22.52	11.987	11.748	17.074
$f_{\nu,3}$	-	0.2223	0.85465	0.84473	0.9865
$f_{\nu,4}$	$\mathrm{fm}^{-1}$	0.2317	0.9772	0.9566	1.9021
$c_{\nu,0}$	MeV	2.752	11.556	10.435	150.71
$c_{\nu,1}$	MeV <sup>3</sup>	32.032	117.24	176.78	9772
$c_{\nu,2}$	MeV	0	3.7362	3.5926	2.0495
$c_{\nu,3}$	$MeV^2$	9.733	4.8426	5.8137	2.1624
$d_{\nu,1}$	$MeV^2 fm^6$	523757	108 762	90 996	5391.2
$d_{\nu,2}$	MeV	0	9.3312	10.72	3.5099
$d_{\nu,3}$	$MeV^2$	15.273	49.678	47.919	44.126
$u_{\nu}$	fm	11.23	25.27	25.27	44.92
$w_ u$	${\rm MeV^{-1}}~{\rm fm}$	0.145	0.284	0.27	0.433
$E_{ u}^{ m kin,intr.}$	MeV	10.338	23.735	23.021	51.575

The intrinsic part of the bound-state energies is introduced as

$$E_{A,\nu}^{\text{intr}}(\mathbf{P}; T, n_B, Y_p)$$

$$= E_{A,\nu}(\mathbf{P}; T, n_B, Y_p, T_{\text{eff}}) - E_{A,\nu}^{\text{cont}}(\mathbf{P}; T, n_B, Y_p)$$

$$= E_{A,\nu}^0 + \Delta E_{A,\nu}^{\text{SE,intr.}}(\mathbf{P}; T, n_B, Y_p) + \Delta E_c^{\text{Pauli}}(\mathbf{P}; T_{\text{eff}}, n_B, Y_p).$$
(28)

With Eq. (21), the intrinsic parts of the bound-state energies are the negative values of the binding energies,  $E_{A,\nu}^{\text{intr}}(\mathbf{P}) \equiv -B_{A,\nu}^{\text{bind}}(\mathbf{P})$ .

#### C. Mott points

A consequence of the medium modification is the disappearance of bound states with increasing density, which is of significance for the physical properties. To calculate the composition, one has to check for given parameter values  $\{T, n_B, Y_p\}$  whether the binding energy of the cluster with quantum numbers  $\{A, \nu, \mathbf{P}\}$  is positive. I denote the density  $n_{A,\nu}^{\text{Mott}}(T, Y_p)$  as Mott density [24] where the binding energy of a cluster  $\{A, \nu\}$  with c.m. momentum  $\mathbf{P} = 0$  vanishes, with (22) and (28)

$$E_{A,\nu}^{\text{intr}}(0; T, n_{A,\nu}^{\text{Mott}}, Y_p) = 0.$$
<sup>(29)</sup>

For baryon densities  $n_B > n_{A,\nu}^{\text{Mott}}(T,Y_p)$  I introduce the Mott momentum  $\mathbf{P}_{A,\nu}^{\text{Mott}}(T,n_B,Y_p)$ , where the bound state disappears,

$$E_{A,\nu}^{\text{intr}}\left(\mathbf{P}_{A,\nu}^{\text{Mott}};T,n_B,Y_p\right) = 0.$$
(30)

At  $n_B > n_{A,\nu}^{\text{Mott}}(T, Y_p)$ , the summation over the momentum to calculate the bound-state contribution to the composition is restricted to the region  $|\mathbf{P}| > |\mathbf{P}_{A,\nu}^{\text{Mott}}(T, n_B, Y_p)|$ .

Crossing the Mott point by increasing the baryon density, part of correlations survive as continuum correlations so that the properties change smoothly. Therefore, the inclusion of correlations in the continuum is of relevance.

### IV. VIRIAL EXPANSION AND CORRELATED MEDIUM

In the low-density limit, rigorous expressions for the EOS are obtained for the virial expansion. The second virial coefficient is related to experimental data such as the bound-state energies and scattering phase shifts, according to the Beth-Uhlenbeck formula [34]. The application to nuclear matter [24,37], as well as the generalized Beth-Uhlenbeck formula [31] and the cluster-virial expansion [6,13,37], make it possible to take into account continuum correlations for the EOS.

The virial coefficients are also determined by continuum correlations which are neglected in the ideal gas NSE. However, in particular for the deuteron contribution where the binding energy is small, their influence on the second virial coefficient is of relevance; see the comparison of QS with generalized RMF calculations in Ref. [8]. A detailed description of the virial expansion in the context of a RMF treatment has been given by Voskresenskaya and Typel [36]. Of interest is the extension of the virial expansion to higher densities up to  $n_{\rm sat}$ . For the two-nucleon case rigorous results

can be given, whereas for the treatment of higher order correlations only some estimates can be made. Expressions for the residual continuum contributions to the partial densities are presented, which depend on temperature, densities, and total momentum.

### A. Two-nucleon contribution

The virial expansion of the EOS (4) reads [24,31,34–36]

$$n_{n}^{\text{tot}}(T,\mu_{n},\mu_{p}) = \frac{2}{\Lambda^{3}} [b_{n}(T)e^{\mu_{n}/T} + 2b_{nn}(T)e^{2\mu_{n}/T} + 2b_{np}(T)e^{(\mu_{n}+\mu_{p})/T} + \cdots],$$

$$n_{p}^{\text{tot}}(T,\mu_{n},\mu_{p}) = \frac{2}{\Lambda^{3}} [b_{p}(T)e^{\mu_{p}/T} + 2b_{pp}(T)e^{2\mu_{p}/T} + 2b_{pn}(T)e^{(\mu_{n}+\mu_{p})/T} + \cdots].$$
(31)

Already the noninteracting, i.e., ideal Fermi gas of nucleons contains two effects in contrast to the standard low-density, classical limit.

- (i) The relativistic dispersion relation  $E_{\tau}(\mathbf{p}) = c\sqrt{(m_{\tau}c)^2 + (\hbar p)^2} m_{\tau}c^2$  results in a first virial coefficient  $b_{\tau} \neq 1$ . The value  $b_{\tau} = 1$  follows from the dispersion relation  $E_{\tau}(p) = \hbar^2 p^2 / 2m_{\tau}$ . For a more detailed investigation, see Ref. [36].
- (ii) The degeneration of the fermionic nucleon gas leads to the contribution  $-2^{-5/2}$  to  $b_{\tau\tau}$  [34].

The remaining part of the second virial coefficient is determined by the two-nucleon interaction. One can introduce different channels, in particular the isospin-triplet ( $T_I = 1$ , dineutron) and isospin-singlet ( $T_I = 0$ , deuteron) channels, which are connected with the spin-singlet and spin-triplet state, respectively, if even angular momentum is considered (for instance, *S*-wave scattering). The second virial coefficient in both channels is derived from  $b_{nn}$  and  $b_{np}$ . Empirical values are given as functions of *T* in Ref. [35] (isospin symmetry is assumed).

#### **B.** Generalized Beth-Uhlenbeck formula

The second virial coefficients  $b_{nn}$  and  $b_{np}$  cannot be directly used within a quasiparticle approach. Because part of the interaction is already taken into account when introducing the quasiparticle energy, one has to subtract this contribution from the second virial coefficient to avoid double counting; see Refs. [31,36,37]. Expanding the density with respect to the fugacities within the quasiparticle approximation picture (23) and (24), one can identify the residual isospin-triplet contribution  $v_{2,T_{I}=1}^{0}(T)$  from the neutron matter case as (the index 0 denotes the zero-density limit)

$$n_{B,\text{neutron m.}}^{\text{tot}}(T,\mu_n,\mu_p) = n_n^{\text{qu}}(T,\mu_n,\mu_p) + \frac{2^{5/2}}{\Lambda^3} e^{2\mu_n/T} v_{2,T_I=1}^0(T) + \cdots, \quad (32)$$

and the residual isospin-singlet contribution  $v_{2,T_{I}=0}^{0}(T)$  from the symmetric matter case ( $\mu_{p} = \mu_{n}$ ) according to

$$u_{B,\text{symmetr.m.}}^{\text{uct}}(T,\mu_{n},\mu_{p})$$

$$= n_{n}^{\text{qu}}(T,\mu_{n},\mu_{p}) + n_{p}^{\text{qu}}(T,\mu_{n},\mu_{p}) + \frac{2^{5/2}3}{\Lambda^{3}}e^{(\mu_{n}+\mu_{p})/T}$$

$$\times \left[e^{-E_{d}^{0}/T} - 1 + v_{2,T_{I}=0}^{0}(T) + v_{2,T_{I}=1}^{0}(T)\right] + \cdots, \quad (33)$$

where dots indicate higher orders in densities. The residual second virial coefficients  $v_c^0(T)$  are given by [31]

$$v_c^0(T) = \frac{1}{\pi T} \int_0^\infty dE \ e^{-E/T} \left\{ \delta_c(E) - \frac{1}{2} \sin[2\delta_c(E)] \right\}.$$
 (34)

(The index *c* denotes the isospin channel. For the two-nucleon system considered here, the isospin channel  $T_I = 0$  contains the deuteron *d*,  $T_I = 1$  the dineutron system.) Comparing Eq. (33) with the ordinary Beth-Uhlenbeck formula (8), there are two differences.

- (i) After integration by parts, the derivative of the scattering phase shift is replaced with the phase shift, and according to the Levinson theorem for each bound state the contribution -1 appears.
- (ii) The contribution  $-\frac{1}{2}\sin[2\delta_c(E)]$  appears to avoid double counting [31,37] when introducing the quasiparticle picture. *E* denotes the relative energy in the c.m. system.

The EOS (4) is not free of ambiguities with respect to the subdivision into bound-state contributions and continuum contributions; compare Eqs. (33) and (34) with Eqs. (7) and (8). The continuum correlations in  $b_{\tau,\tau'}(T)$  are reduced to the residual part  $v_c^0(T)$  if the quasiparticle picture is introduced. The remaining part of the continuum contribution in Eq. (8) is absorbed in the quasiparticle shift. This has been discussed in detail in Refs. [31,36,37].

To give an approximation for  $v_c^0(T)$ , I performed calculations within the generalized Beth-Uhlenbeck approach [31] for a simple separable potential,

$$V_{c}(12,1'2') = -\lambda_{c}e^{-\frac{(\mathbf{p}_{1}-\mathbf{p}_{2})^{2}}{4\gamma^{2}}}e^{-\frac{(\mathbf{p}_{1}'-\mathbf{p}_{2})^{2}}{4\gamma^{2}}}\delta_{\mathbf{p}_{1}+\mathbf{p}_{2},\mathbf{p}_{1}'+\mathbf{p}_{2}'}\delta_{\sigma,\sigma'}\delta_{\tau,\tau'},$$
(35)

with  $\lambda_d = 1287.37$  MeV for the deuteron (isospin 0) channel,  $\gamma = 1.474$  fm<sup>-1</sup> (see Ref. [33]), adapted to binding energy and point r.m.s. radius of the deuteron. After evaluating the *T* matrix, the scattering phase shifts are obtained, and  $v_d^0(T)$ has been evaluated. For details, see Ref. [31]. The result is approximated by

$$v_d^0(T) = v_{2,T_I=0}^0(T) \approx 0.308\,57 + 0.653\,27\,e^{-0.102\,424\,T/\text{MeV}}.$$
  
(36)

A similar calculation has been performed for the isospintriplet channel. The empirical value for the *n*-*n* scattering length (-18.818 fm) is reproduced with the interaction potential (35),  $\lambda_{T_I=1} = 814.2$  MeV, leaving  $\gamma$  unchanged. Also, the effective range (2.834 fm) is well approximated. The resulting value  $v_{2,T_I=1}^0(T) \approx 0.16$  is nearly independent of *T*. Thus, for the EOS (4) one has the residual contribution of continuum correlations in the isospin-triplet channel as well as in the isospin-singlet channel. The contribution of the isospin-triplet channel  $v_{2,T_l=1}^0(T)$  gives only a small contribution to the free-nucleon densities and will be omitted in the present work. [Note that according Eq. (34) the lowest orders of  $\delta_c(E)$  are compensated because of the introduction of the quasiparticle shift of the nucleons.] The residual continuum correlations in the isospin-singlet channel  $v_d^0(T)$  are part of the partial density of the deuteron channel. The latter changes smoothly at the Mott point where the bound-state contributions vanish.

The contribution of bound states to the EOS is not simply given by the term  $e^{-E_c^0/T}$  with the bound-state energy  $E_c^0$ , as known, for instance, from the NSE. At the same time one has to take into account the contribution of continuum correlations (scattering states). Only the total contribution of the channel *c* to the partial densities is well defined. The subdivision in the bound-state contribution and the scattering state contribution to the density is not unique. An alternate expression for the contribution of bound states is  $e^{-E_c^0/T} - 1$ , which remains smooth when the binding energy goes to zero (for instance, at the Mott point).

To discuss this issue more clearly, I consider the twonucleon isospin-singlet (d) channel. The partial density  $z_d^{\text{part}}(\mathbf{P}; T, n_B, Y_p)$  (7) of the d channel (switching from the variables  $\{T, \mu_n, \mu_p\}$  to the set  $\{T, n_B, Y_p\}$ ) reads in the lowdensity limit

$$z_{d}^{\text{part}}(\mathbf{P}; T, n_{B} = 0, Y_{p}) = e^{(\mu_{n} + \mu_{p})/T} e^{-\hbar^{2}P^{2}/(4mT)} g_{d} \Big[ e^{-E_{d}^{0}/T} - 1 + v_{2, T_{I}=0}^{0}(T) \Big].$$
(37)

Compared with Eq. (8), the term  $e^{-E_d^0/T} - 1$  occurs as consequence of the Lewison theorem. The residual second virial coefficient  $v_{2,T_I=0}^0(T)$  is given as an integral over the relative energy *E* in Eq. (34). One can implement the term  $e^{-E_d^0/T} - 1$  into the integral over *E* if the phase shift  $\delta_{2,T_I=0}(E) = \pi \Theta(E - E_d^0)$  is defined for E < 0 and the integral over *E* starts from  $-\infty$ ; see Ref. [52].

To illustrate the relevance of the continuum contributions in the *d* channel, these extended phase shifts are shown in Fig. 1. The calculations are performed for various densities (zero density is almost identical with  $n_B = 0.0001 \text{ fm}^{-3}$ ) at T = 4 MeV, using the separable interaction (35). For other values of *T* and a more detailed discussion, see Ref. [52]. Together with the Boltzmann factor  $e^{-E/T}$  in Eq. (34), the negative region of *E* gives the contribution  $e^{-E_d^0/T} - 1$  to this integral (now  $-\infty$  as lower limit of integration), which is small if the binding energy is small. The relative importance of the two parts of the integral, the bound part (E < 0) and the part of the residual continuum correlations (E > 0), is clearly shown. As discussed in the following section, both parts do not jump at the Mott point where the bound-state energy goes to zero.

Similar to the deuteron case, I assume that the expression

$$z_{c}^{\text{part}}(\mathbf{P}; T, n_{B} = 0, Y_{p})$$

$$\approx e^{(N\mu_{n} + Z\mu_{p})/T} e^{-\hbar^{2}P^{2}/(2AmT)} g_{c} \left[ e^{-E_{c}^{0}/T} - 1 + v_{2,T_{I}=0}^{0}(T) \right]$$
(38)



FIG. 1. (Color online) Role of continuum correlations in the *d* channel. Extended phase shifts, containing a contribution at negative intrinsic energies *E* describing the bound state part, are presented for baryon densities of the nuclear medium  $n_B = 0.0001, 0.003, 0.01, 0.03, 0.1 \text{ fm}^{-3}$  and T = 4 MeV.

can be taken to continue the contribution of bound states to the continuum of scattering states for the other light elements t,h. In the  $\alpha$  case, there is also an excited state of the ground state, excitation energy  $E_{\alpha'} = E_{\alpha} + 20.2$  MeV. Within our estimations, the two bound states lead to larger continuum contribution,

$$z_{\alpha}^{\text{part}}(\mathbf{P}; T, n_{B} = 0, Y_{p})$$

$$\approx e^{(2\mu_{n} + 2\mu_{p})/T} e^{-\hbar^{2} P^{2}/(8mT)}$$

$$\times \left[ e^{-E_{\alpha}^{0}/T} + e^{-E_{\alpha'}^{0}/T} - 2 + 2 v_{2,T_{I}=0}^{0}(T) \right]. \quad (39)$$

To motivate the ansatz (38) and (39), one can consider the effective interaction between the constituent nucleons of the cluster which are comparable with the nucleon-nucleon interaction in d. As in the deuteron case, one can represent the total contribution to the partial density (7) of channel c as integral over the intrinsic energy E; see Eq. (34), which is extended to negative energies to include the bound-state part. According to the Levinson theorem, the integrand has the value  $\pi$  in this region (E < 0) and goes smoothly to zero at positive energies. The detailed behavior at E > 0 may differ from the deuteron case, and different channels for the decomposition of clusters with A > 2 are possible. It is only a rough approximation that all residual virial coefficients  $v_c^0(T)$  can be estimated by  $v_{2,T_l=0}^0(T)$ . However, the results for the EOS are not very sensitive to the continuum contributions for A = 3,4. In the high-temperature region, continuum correlations are of relative importance in the deuteron channel because of the small binding energy of 2.225 MeV. The other clusters  $\{t, h, \alpha\}$ are more strongly bound so that the contribution of continuum correlations is of less relevance for the EOS.

The more precise determination of the residual virial coefficients  $v_c^0(T)$  for A = 3,4 would be an interesting issue of future work. Within the cluster-virial expansion, empirical scattering phase shifts can be considered to calculate the residual virial coefficients. For instance, virial coefficients for

the scattering of nucleons with the A = 3 nuclei are given in Ref. [40]. Using measured and calculated data, the <sup>3</sup>He -nand <sup>3</sup>H -p scattering contributions of the virial expansion are obtained. Because both combinations belong to the  $\alpha$  channel, these scattering data can be used to find an alternate estimate for the residual virial coefficient  $v_{\alpha}^{0}(T)$ . For T = 10 MeV, the values 0.781 for  $b_{p3He}$ , 0.803 for  $b_{n3H}$ , and 0.198 for  $b_{n3He}$ are given there. The latter (together with the estimated same amount for  $b_{p3H}$ ) contribute to the  $\alpha$  channel as 0.396 and is not very different from the estimate 0.543 according to Eq. (36) for  $v_{d}^{0}$ . Of course, a better treatment of the continuum contributions in the A = 3,4 channels is desirable, but not solved until now. Anyhow, the contributions of continuum correlations from the A = 3,4 channels are small at the conditions considered here.

## C. Extrapolation to saturation densities, deuteron case

Using the quasiparticle concept, the virial expansion introduced at low densities can be extended to arbitrary subsaturation densities. Using Eqs. (28) and (22) to introduce the intrinsic energy, the partial density (7) of the channel c (A has been dropped) with c.m. momentum **P** reads

$$z_{c}^{\text{part}}(\mathbf{P}; T, n_{B}, Y_{p})$$

$$= e^{[N\mu_{n} + Z\mu_{p} - NE_{n}(\mathbf{P}/A; T, n_{B}, Y_{p}) - ZE_{p}(\mathbf{P}/A; T, n_{B}, Y_{p})]/T}$$

$$\times g_{c} \left\{ \left[ e^{-E_{c}^{\text{intr}}(\mathbf{P}; T, n_{B}, Y_{p})/T} - 1 \right] \Theta \left[ -E_{c}^{\text{intr}}(\mathbf{P}; T, n_{B}, Y_{p}) \right] + v_{c}(\mathbf{P}; T, n_{B}, Y_{p}) \right\}$$

$$(40)$$

(the set of variables  $\{T, n_B, Y_p\}$  is used). The residual continuum contribution  $v_c(\mathbf{P}; T, n_B, Y_p)$  depends on the nucleon densities.

For A = 2, the second virial coefficient was investigated within a generalized Beth-Uhlenbeck approach starting from the quasiparticle approach [31]. The cluster binding energy as well as the in-medium scattering phase shifts are modified by self-energy and Pauli blocking shifts; see Eqs. (9) and (20). The calculations for realistic nucleon-nucleon interaction [31] show the following.

- (i) At the Mott point, the bound state disappears abruptly, but at the same time the scattering phase shifts jump by  $\pi$  so that the total contribution (8) to the virial coefficient changes smoothly. In particular, the EOS which relates the total baryon density to the chemical potentials remains smooth.
- (ii) Near the saturation density, approximately only the single-nucleon quasiparticle contribution to the density (4) remains. The correlated partial densities  $[z_{A,c}^{part}(\mathbf{P})$  with A > 1] becomes very small when the baryon density approaches the saturation density. However, part of the correlations is already included in the quasiparticle approach. For instance, two-nucleon correlations are treated in the Brueckner approximation for the self-energy.

To estimate the density dependence of the residual virial coefficient  $v_d(\mathbf{P}; T, n_B, Y_p)$  (34), the in-medium wave equation (9) has been solved for A = 2 with the separable potential (35); for details see Ref. [31]. The Pauli blocking term was taken

in the Tamm-Dancoff form  $[1 - f_{1,\tau_i}(i)][1 - f_{1,\tau_j}(j)]$  [53], so that pairing has been neglected. The *T* matrix has been solved taking into account the fermionic Pauli blocking terms. From the *T* matrix, the in-medium scattering phase shifts are obtained. For illustration, results for the scattering phase shifts at various densities  $n_B$  are shown in Fig. 1. The phase shifts are extended to negative *E* to include the contribution of bound states. Of interest is the behavior near the Mott point where the bound state part continuously goes to zero.

The contribution of residual continuum correlations (34) to the EOS according to the generalized Beth-Uhlenbeck expression has been evaluated as function of T and  $n_B$  contained in the Pauli blocking terms (symmetric matter  $Y_p = 0.5$ ). The result at  $\mathbf{P} = 0$  is approximated by

$$v_d(\mathbf{P} = 0; T, n_B, Y_p) \approx \left\{ 1.24 + \left[ \frac{1}{v_{2, T_I = 0}(T)} - 1.24 \right] e^{\gamma_d n_B/T} \right\}^{-1}, \quad (41)$$

where  $\gamma_d = 1876.2 \text{ MeV fm}^3$  and  $v_{2,T_l=0}(T)$  given by Eq. (36). At high temperatures, the dominant part of the *d* component is caused by the scattering states because the binding energy is small compared with the temperature, and the residual virial coefficient describing continuum correlations is of relevance in the deuteron case. For the simultaneous treatment of the bound-state and scattering-state contribution, see also Ref. [52]. The dependence of  $Y_p$  has been neglected.

One can interpret this result (40) as follows: The contribution  $e^{-E_d(P;T,n_B,Y_p)/T} - 1$  of the bound state (*d*) is decreasing with increasing density and disappears at the so-called Mott density. The bound state merges with the continuum of scattering states and forms a resonance so that there remains a contribution to the baryon density. When the density is further increasing, the resonance moves to higher energies and becomes broader. Consequently, the contribution to the continuum states is strongly reduced.

Note that to describe pairing at high densities and very low temperatures, the Tamm-Dancoff form of the Pauli blocking used, for instance, in the Brueckner theory, must be replaced with the Feynman-Galitsky form  $[1 - f_{1,\tau_i}(i) - f_{1,\tau_j}(j)]$  according Eq. (9); see Ref. [31].

## **D.** Estimates for higher clusters A = 3,4

In contrast to the deuteron case  $(c \rightarrow d)$ , no simple way is known to estimate the continuum contribution of the other clusters with A = 3,4. I took  $Y_p = 0.5$ , neglected the dependence on  $Y_p$ , and estimated the residual virial contribution of the continuum  $v_c(\mathbf{P}; T, n_B, Y_p)$  at  $\mathbf{P} = 0$ .

All bound states behave quite similarly; the binding energy is decreasing with increasing density. The shift of the quasiparticle cluster bound-state energies was considered elsewhere [33]; see Appendix C. Similar to the deuteron case, it can be expected that also for the clusters with A = 3,4 a contribution to the residual virial coefficient remains when the bound state is dissolved. To estimate this contribution, I considered a two-particle system (for A > 2 there are several possibilities) with an effective interaction of separable Gaussian type [33] and fixed range parameter  $\gamma = 1.474$  fm<sup>-1</sup>, Eq. (35), but with effective coupling parameter  $\lambda_c^{\text{eff}}$  which reproduces the binding energy  $B_c$  of cluster c. The corresponding parameter values are given in Table I. Changing the strength  $\lambda_c^{\text{eff}}$ , at the critical value  $\lambda_c^{\text{crit}} = 885.996$  MeV, the bound state merges with the continuum. From the strict evaluation of the bound-state (quasiparticle) energy [33], the so-called Mott densities  $n_c^{\text{Mott}}(T, Y_p)$  (29) are known where the bound states at  $\mathbf{P} = 0$  disappear; see Table I. As before, calculations are preformed for  $\mathbf{P} = 0$ . Finite values for  $\mathbf{P}$  are discussed in Sec. V D.

I calculated the relation between the coupling strength  $\lambda_c$  of the separable potential (35) and the residual virial  $v_c(T)$  without any in-medium effects and found a simple relation  $v_c(T) \propto \lambda_c^4$  in good approximation for all values T under consideration. However, one can search for an effective interaction strength which mimics the shift of the binding energies, caused by the Pauli blocking as a density effect. This reduced effective interaction strength  $\lambda_c(n_B) = \lambda_c^{\text{eff}} e^{-\gamma_c n_B/(4T)}$  and determined  $\gamma_c$  from the known value  $\lambda_c^{\text{eff}}$  at zero density, as well as the value  $\lambda_c(n_c^{\text{Mott}}) = \lambda_c^{\text{crit}}$  at the Mott density  $n_c^{\text{Mott}}(T, Y_p)$ , where the bound state disappears.

With the expression (36), the fit formula

$$v_{c}(\mathbf{P} = 0; T, n_{B}, Y_{p}) \approx \left\{ 1.24 + \left[ \frac{1}{v_{2, T_{l} = 0}(T)} - 1.24 \right] e^{\gamma_{c} n_{B}/T} \right\}^{-1}$$
(42)

for the residual virial coefficients is obtained. Parameter values are found in Table I.

#### V. RESULTS

First, all the expressions are collected which are used for the calculations in this section. Equations (4) are solved considering the different contribution with  $A \leq 4$ , i.e., besides the free nucleons *n*, *p* also the channels related to *d*, *t*, *h*,  $\alpha$ . The intrinsic quantum number  $\nu_c$  refers to the bound states as far as they exist and to the scattering states. The summation over **P** is replaced with an integral,  $\frac{1}{\Omega} \sum_{\mathbf{P}} \rightarrow \int d^3 P / (2\pi)^3$ .

The main ingredients are the medium modified energies  $E_{A,\nu}(\mathbf{P}; T, n_B, Y_p)$ . They are determined as function of the total nucleon densities,

$$n_n^{\text{tot}} = (1 - Y_p)n_B, \quad n_p^{\text{tot}} = Y_p n_B,$$
 (43)

and a further parameter  $T_{\text{eff}}(T, n_n^{\text{tot}}, n_p^{\text{tot}})$  [Eq. (18)] that takes the correlations in the medium into account when calculating the Pauli blocking effect. Consequently, Eqs. (4) have the form

$$n_n^{\text{tot}} = \sum_{c=n,p,d,t,h,\alpha} N_c n_c (T,\mu_n,\mu_p;n_n^{\text{tot}},n_p^{\text{tot}}),$$

$$n_p^{\text{tot}} = \sum_{c=n,p,d,t,h,\alpha} Z_c n_c (T,\mu_n,\mu_p;n_n^{\text{tot}},n_p^{\text{tot}}).$$
(44)

For given  $\{T, n_n^{\text{tot}}, n_p^{\text{tot}}\}$ , a self-consistent solution of (44) must be found which determines  $\mu_n, \mu_p$ . Then the EOS  $\mu_n(T, n_n^{\text{tot}}, n_p^{\text{tot}})$  and  $\mu_p(T, n_n^{\text{tot}}, n_p^{\text{tot}})$  are found.

More explicitly, Eqs. (44) read  $n_n^{\text{tot}} = n_n + n_d + 2n_t + n_h + 2n_{\alpha}$  and  $n_p^{\text{tot}} = n_p + n_d + n_t + 2n_h + 2n_{\alpha}$ . The contribution of free neutrons and protons (A = 1) to the total density is given by

$$n_{\tau}(T,\mu_{n},\mu_{p};n_{n}^{\text{tot}},n_{p}^{\text{tot}}) = \frac{1}{\pi^{2}} \int_{0}^{\infty} dP \frac{P^{2}}{e^{[E_{\tau}(\mathbf{P};T,n_{B},Y_{p})-\mu_{\tau}]/T} + 1}.$$
(45)

The single-nucleon quasiparticle energies  $E_{\tau}(\mathbf{P}; T, n_B, Y_p)$  are taken from a RMF approach (24). A parametrization of a particular approach (DD-RMF) is given by Eqs. (D1) and (D3).

The contribution of the deuteron channel is (nondegenerated case)

$$n_{d}(T,\mu_{n},\mu_{p},n_{n}^{\text{tot}},n_{p}^{\text{tot}}) = \frac{3}{2\pi^{2}} \int_{0}^{\infty} dP P^{2} e^{[-E_{n}(\mathbf{P}/2;T,n_{B},Y_{p})-E_{p}(\mathbf{P}/2;T,n_{B},Y_{p})+\mu_{n}+\mu_{p}]/T} \\ \times \{ \left[ e^{-E_{d}^{\text{intr}}(\mathbf{P};T,n_{B},Y_{p})/T} - 1 \right] \Theta \left[ -E_{d}^{\text{intr}}(\mathbf{P};T,n_{B},Y_{p}) \right] + v_{d}(\mathbf{P};T,n_{B},Y_{p}) \},$$
(46)

with the intrinsic in-medium bound-state energy [negative binding energy  $-B_d^{\text{bind}}(\mathbf{P})$  (21)] [see Eq. (28)],

$$E_d^{\text{intr}}(\mathbf{P}; T, n_B, Y_p) = E_d^0 + \Delta E_d^{\text{SE,intr}}(\mathbf{P}; T, n_B, Y_p) + \Delta E_d^{\text{Pauli}}(\mathbf{P}; T_{\text{eff}}, n_B, Y_p).$$
(47)

The contribution of the c.m. motion to the kinetic energy is given by  $E_n(\mathbf{P}/2; T, n_B, Y_p) + E_p(\mathbf{P}/2; T, n_B, Y_p)$ . Expressions for  $\Delta E_d^{\text{SE,intr}}(\mathbf{P}; T, n_B, Y_p)$  are given by Eq. (27) and for  $\Delta E_d^{\text{Pauli}}(\mathbf{P}; T_{\text{eff}}, n_B, Y_p)$  by Eq. (C1) with Eq. (18). Beyond the Mott density  $n_d^{\text{Mott}}(T, Y_p)$  [Eq. (29)], bound states arise only for c.m. momenta  $|\mathbf{P}|$  larger than the Mott momentum  $|\mathbf{P}_d^{\text{Mott}}(T, n_B, Y_p)|$  [Eq. (30)]. One must not solve these relations but can use the  $\Theta$  function in Eq. (46), which indicates the region where a bound state exists. The merge with the continuum is smooth because of the subtraction of 1. The intrinsic energy which is the difference between the bound-state energy  $E_d(\mathbf{P}, T, n_B, Y_p)$  and the edge of the continuum of scattering states  $E_n(\mathbf{P}/2; T, n_B, Y_p) + E_p(\mathbf{P}/2; T, n_B, Y_p)$  [see Eq. (22)] goes to zero at the Mott point and is compensated for by the term -1. Above the Mott point, the residual virial contribution  $v_d(\mathbf{P}; T, n_B, Y_p)$  (41) to the partial density in the deuteron channel remains. It is strongly decreasing with increasing density.

Similar expressions are also obtained for the other light elements contributing, as cluster states, to the density. In particular,

$$n_{t}(T,\mu_{n},\mu_{p},n_{n}^{\text{tot}},n_{p}^{\text{tot}}) = \frac{1}{\pi^{2}} \int_{0}^{\infty} dP P^{2} e^{[-2E_{n}(\mathbf{P}/3;T,n_{B},Y_{p})-E_{p}(\mathbf{P}/3;T,n_{B},Y_{p})+2\mu_{n}+\mu_{p}]/T} \\ \times \{ \left[ e^{-E_{t}^{\text{intr}}(\mathbf{P};T,n_{B},Y_{p})/T} - 1 \right] \Theta \left[ -E_{t}^{\text{intr}}(\mathbf{P};T,n_{B},Y_{p}) \right] + v_{t}(\mathbf{P};T,n_{B},Y_{p}) \},$$
(48)  
$$n_{t}(T,\mu_{t},\mu_{t},\mu_{t}) = \frac{1}{\pi^{2}} \int_{0}^{\infty} dP P^{2} e^{[-E_{n}(\mathbf{P}/3;T,n_{B},Y_{p})-2E_{p}(\mathbf{P}/3;T,n_{B},Y_{p})+\mu_{n}+2\mu_{p}]/T}$$

$$n_{h}(T,\mu_{n},\mu_{p},n_{n},n_{p}) = \frac{1}{\pi^{2}} \int_{0}^{\infty} dT T e^{-E_{h}^{intr}(\mathbf{P};T,n_{B},Y_{p})/T} - 1 \Big] \Theta \Big[ -E_{h}^{intr}(\mathbf{P};T,n_{B},Y_{p}) \Big] + v_{h}(\mathbf{P};T,n_{B},Y_{p}) \Big],$$
(49)  
$$n_{\alpha} \Big(T,\mu_{n},\mu_{p},n_{n}^{tot},n_{p}^{tot}) = \frac{1}{2\pi^{2}} \int_{0}^{\infty} dP P^{2} e^{[-2E_{n}(\mathbf{P}/4;T,n_{B},Y_{p})-2E_{p}(\mathbf{P}/4;T,n_{B},Y_{p})+2\mu_{n}+2\mu_{p}]/T}$$

$$\times \left\{ \left[ e^{-E_{\alpha}^{\text{intr}}(\mathbf{P};T,n_{B},Y_{p})/T} - 1 \right] \Theta \left[ -E_{\alpha}^{\text{intr}}(\mathbf{P};T,n_{B},Y_{p}) \right] + \left[ e^{-E_{\alpha'}^{\text{intr}}(\mathbf{P};T,n_{B},Y_{p})/T} - 1 \right] \Theta \left[ -E_{\alpha'}^{\text{intr}}(\mathbf{P};T,n_{B},Y_{p}) \right] + 2v_{\alpha}(\mathbf{P};T,n_{B},Y_{p}) \right\}.$$
(50)

The intrinsic in-medium bound-state energy  $E_c^{\text{intr}}$  [see Eq. (28)] and the values for the shifts  $\Delta E_c^{\text{SE,intr}}(\mathbf{P}; T, n_B, Y_p)$  and  $\Delta E_c^{\text{Pauli}}(\mathbf{P}; T_{\text{eff}}, n_B, Y_p)$  are given by Eqs. (27) and (C1). For the  $\alpha$ -like contribution, the excited state at  $E_{\alpha'}^0 = -8.1$  MeV has been taken into account, with shifts estimated by the values of the shifts for the ground state at  $E_{\alpha}^0 = -28.3$  MeV. The residual virial contribution of continuum states  $v_c(\mathbf{P}; T, n_B, Y_p)$ is estimated with  $\mathbf{P} = 0$  by Eq. (42).

## A. EOS and critical point

The self-consistent solution of Eqs. (44) is shown in Fig. 2  $(n_B = n_n^{\text{tot}} + n_p^{\text{tot}}, Y_p = n_p^{\text{tot}}/n_B)$ . Isotherms of the chemical potential  $\bar{\mu} = g = (1 - Y_p)\mu_n + Y_p\mu_p$  are shown for fixed asymmetry  $Y_p = 0.5$  (symmetric matter) as function of the baryon density  $n_B$ . The temperatures are chosen as 5, 10, 15, and 20 MeV. The solution for T = 1 MeV is also shown for



FIG. 2. (Color online) Baryon chemical potential  $\bar{\mu}$  as function of the baryon density  $n_B$  for symmetric matter ( $Y_p = 0.5$ ). Isotherms are shown for T = 1, 5, 10, 15, and 20 MeV. The QS result (solid line) is compared with the RMF solution which considers only the contributions with A = 1 in Eq. (4); see also Eq. (23) (thin line) and the ideal gas NSE solution (dashed). (Inset) Comparison with the QS calculations (Pauli blocking in uncorrelated matter) given in Ref. [8] (thin lines).

discussion, but in this case the formation of larger cluster is of importance.

For comparison, the pure mean-field (RMF) solution (4) neglecting all contributions A > 1 is also shown. It dominates at low densities where (because of entropy) all bound states dissociate, but becomes a good approximation at high densities where all bound states are blocked out and dissolved. The thermodynamics of the RMF approximation is modified in the region where clusters are formed. The chemical potential is lowered when correlations are taken into account.

The region where the mean-field approach is not sufficient depends strongly on *T*. For T = 20 MeV deviations owing to cluster formation appear below  $n_B = 0.07$  fm<sup>-3</sup>; for T = 5 MeV they appear below  $n_B = 0.03$  fm<sup>-3</sup>. At the low-density region, the deviation from the mean-field solution (which coincides approximately with the free-nucleon solution) is attributable to cluster formation as described by the massaction law (NSE). It is well understood and also strongly depending on *T*. At low temperatures (compare T = 1 MeV) clustering occurs already at very low densities.

The ideal gas NSE is also shown in Fig. 2 what gives the correct behavior in the low-density limit. Cluster formation is described by the NSE, but deviations from  $\bar{\mu}$  are shown as soon as the mean-field effects arise at about  $n_B = 10^{-3}$  fm<sup>-3</sup>.

A comparison with former QS calculations [8] is shown in the inset of Fig. 2. The improved treatment of residual continuum contributions to the partial densities as well as the modification of the Pauli blocking owing to cluster formation in the medium makes the clusters more stable. In particular at low temperatures, the RMF solution without clustering is approximated only at higher densities. The general features are not changed, but the region where correlations and bound states are relevant is extended to higher densities, resulting in a lowering of the chemical potential.

Thermodynamic stability requires  $\partial \bar{\mu} / \partial n_B \ge 0$ . As seen in Fig. 2, below a critical temperature a phase transition appears, and a Maxwell construction can be applied. For the pure mean-field (RMF) solution (4) neglecting all contributions A > 1, the critical point is at  $T_{\rm cr}^{\rm RMF} = 13.72$  MeV,  $n_{B,{\rm cr}}^{\rm RMF} = 0.0486$  fm<sup>-3</sup>. Taking clustering with  $A \le 4$  into account, our QS approach gives  $T_{\rm cr}^{\rm QS} = 12.42$  MeV,  $n_{B,{\rm cr}}^{\rm QS} = 0.063$  fm<sup>-3</sup>. The lowering of the critical temperature, if clustering is taken into account,

is a general feature of many-particle systems. The lowering of  $T_{\rm cr}$  owing to clustering has been obtained for the QS approach in Ref. [24] and, in contrast to the generalized RMF, also in Ref. [8]. Calculations of  $T_{\rm cr}$  with the Skyrme interaction, accounting for clustering, have been performed some time ago [41]; see also Refs. [13,17].

A region of metastability is seen for low temperatures near  $n_B \approx 0.02 \text{ fm}^{-3}$ . Note that the results at very low temperatures have to be improved taking into account quantum condensates like pairing and quartetting. This is also possible within the QS approach, introducing, e.g., the pair amplitude and performing a Bogoliubov transformation to new quasiparticles. For some results, see Refs. [38,39,54]. At low temperatures, also clusters with A > 4 have to be taken into account.

### B. Thermodynamic potential: The free energy

There are different relations between thermodynamic variables, so-called EOS. The present work focused on the density as function of the temperature and chemical potentials (1); others are the thermodynamic EOS for the pressure or the caloric EOS for the internal energy. For further examples, see Ref. [8]. I do not discuss here the various thermodynamic quantities but consider only the free energy per nucleon  $F_A = F/(N_n + N_p)$  as function of the natural variables ( $\{T, n_B, Y_p\}$ ), which is a thermodynamic potential; see Appendix A. All other thermodynamic quantities such as pressure, entropy, and internal energy can be derived from the thermodynamic potential.

Isotherms of  $F_A$  for symmetric matter ( $Y_p = 0.5$ ) are shown in Fig. 3 as function of the baryon density. For comparison, also the results of former QS calculations neglecting correlations in the continuum [8] are shown. The account of continuum correlations in the partial densities and in the Pauli blocking, as performed in the present work, gives, in general, rather small effects and does not change the overall picture, with exception of the low-temperature region. However, light clusters ( $A \leq 4$ )



FIG. 3. (Color online) Free energy per nucleon  $F_A$  as function of the baryon density  $n_B$  for symmetric matter ( $Y_p = 0.5$ ). Isotherms are shown for T = 1,5,10,15,20 MeV. The QS result (solid lines) is compared with former QS calculations [8] neglecting continuum correlations (dashed lines).

can survive up to larger densities, and, consequently, the free energy per nucleon becomes lower in the region 0.001 fm<sup>-3</sup>  $\leq n_B \leq 0.1$  fm<sup>-3</sup>.

### C. Composition of symmetric matter

Of interest is the composition; i.e., the mass fractions  $X_c = A_c n_c/n_B$ . They are shown for symmetric matter ( $Y_p = 0.5$ ) at different temperatures as function of the baryon density  $n_B$  in Fig. 4,  $c = \{n, p, d, t, h, \alpha\}$ . In the low-density region, the mass fractions evolve in proportional to the mass-action law (NSE), whereas at higher densities medium effects become of relevance for the QS approach. The bound states are dissolved at the Mott density. Whereas within the ideal gas NSE the mass fractions  $X_n$ ,  $X_p$  of the free nucleons are continuously decreasing with density, because of Pauli blocking the single-quasiparticle mass fractions increase with density for  $n_B > 0.02 \text{ fm}^{-3}$ . Correspondingly, the mass fractions of the clusters are strongly decreasing at high densities.

At low densities, the discrepancies between the QS and the ideal gas NSE results are attributable to the partial densities (7) which contain also the continuum correlations. Compared with the ideal gas NSE, the QS mass fractions  $X_d, X_t, X_h$  are reduced because of the contribution  $-1 + v_c(0; T, n_B, Y_p)$ ; see Eqs. (33), (38), and (42). Thus, the contribution of the clusters to the total density is smaller than expected from the NSE approach. For  $X_{\alpha}$ , the QS mass fraction is larger than the ideal gas NSE result because the excited state  $\alpha'$  has also been taken into account; see Eq. (39).

At lower temperatures, the role of correlations and cluster formation is increasing; see Figs. 4(a) and 4(b). Whereas above  $T_{\rm cr}$  the two-particle correlations dominate, heavier clusters, in particular  $\alpha$ -like correlations, give an increasing contribution to the composition of warm dense matter at decreasing temperatures. For instance, at T = 5 MeV the mass fraction  $X_{\alpha}$ is large in the density range 0.001 fm<sup>-3</sup> <  $n_B$  < 0.03 fm<sup>-3</sup>.

In this intermediate density region, heavier clusters A > 4 may be formed that are not included in the present work. Moreover, the thermodynamic instability in that region leads to a first-order phase transition of the liquid  $\leftrightarrow$  gas type. Droplet formation and formation of pasta states may occur; see Refs. [12,15,17]. The inclusion of Coulomb interaction is indispensable, but the theory of heavier clusters and phase transition is not a subject of this work.

For illustration, also the case T = 1 MeV is considered in Fig. 5. Up to densities of  $n_B \approx 0.02$  fm<sup>-3</sup>,  $\alpha$ -like correlations dominate and are dissolved owing to the Pauli blocking terms. At higher densities, neutrons and protons as single-nucleon quasiparticles describe the internal structure, well-described by RMF and other theories. At very low temperatures, quantum condensates [38,39] appear which are not considered in the present work. However, as already mentioned, at T = 1 MeV the formation of clusters with A > 4 becomes relevant.

### D. P dependence of Pauli blocking

In addition to Secs. VA–VC, where only the medium modified continuum states with  $\mathbf{P} = 0$  have been taken into account, the residual continuum contributions are now



FIG. 4. (Color online) Composition of symmetric matter ( $Y_p = 0.5$ ) at (a) T = 5 MeV, (b) T = 10 MeV, (c) T = 15 MeV, and (d) T = 20 MeV. The mass fraction  $X_c$  is shown as a function of the density  $n_B$ . The QS solution (solid lines) is compared with the ideal gas NSE solution (dashed lines).

considered as function of **P**. Like the in-medium shift of the binding energy, the medium modification of scattering states is strongly depending on **P** because the Pauli blocking changes quickly with the c.m. momentum **P**. At large values of  $|\mathbf{P}|$  the Pauli blocking and, correspondingly, the reduction of the mass fraction of the clusters become weaker.

For arbitrary **P**, the partial densities  $n_c(T, n_B, Y_p)$  [Eqs. (46), (48), (49), and (50)] can be calculated with

the residual virial coefficients  $v_c(\mathbf{P}; T, n_B, Y_p)$  now depending on **P**. The approximation (42) for the residual continuum contributions contains the parameter  $\gamma_d(\mathbf{P}; T, n_B, Y_p)$ , which depends on **P**. Using the same method given in Sec. IV D for  $\mathbf{P} = 0$ , i.e., scaling the reduction of the binding energy for increasing  $n_B$  with the known value for  $n_c^{\text{Mott}}(\mathbf{P}, T, Y_p)$  according to Ref. [33], one finds the expressions

$$\gamma_{d}(\mathbf{P}, T, n_{B}, Y_{p}) = 1873.2 \text{ MeV fm}^{3} \exp[-P^{2} \text{ fm}^{2}/(1.8463 + 0.1617 \ T \ \text{MeV}^{-1} + 0.17 \ P^{2} \ \text{fm}^{2})],$$
  

$$\gamma_{t}(\mathbf{P}, T, n_{B}, Y_{p}) = 2773.2 \ \text{MeV fm}^{3} \ \exp[-P^{2} \ \text{fm}^{2}/(4.6671 + 0.3037 \ T \ \text{MeV}^{-1} + 0.19 \ P^{2} \ \text{fm}^{2})],$$
  

$$\gamma_{h}(\mathbf{P}, T, n_{B}, Y_{p}) = 2843.5 \ \text{MeV fm}^{3} \ \exp[-P^{2} \ \text{fm}^{2}/(4.6793 + 0.28486 \ T \ \text{MeV}^{-1} + 0.19 \ P^{2} \ \text{fm}^{2})],$$
  

$$\gamma_{\alpha}(\mathbf{P}, T, n_{B}, Y_{p}) = 3268.8 \ \text{MeV fm}^{3} \ \exp[-P^{2} \ \text{fm}^{2}/(9.7514 + 0.6922 \ T \ \text{MeV}^{-1} + 0.24 \ P^{2} \ \text{fm}^{2})].$$
(51)

For comparison, in Fig. 6 the composition of symmetric matter ( $Y_p = 0.5$ ) at T = 10 MeV is calculated neglecting the **P** dependence of the residual continuum contributions and taking it into account. There are larger differences at higher densities because now the Pauli blocking effect is reduced for increasing |**P**|. Consequently, the correlations are stabilized and the mass fractions of the clusters are larger.

At higher densities, also further corrections have to be considered: Correlations in the medium as expressed by  $T_{\text{eff}}$  to replace T in the exponent of Eq. (42) will further reduce the Pauli blocking, with the consequence of increasing mass fractions, in particular  $X_d$ . However, the use of the Feynman-Galitzky expression  $[1 - f_{1,\tau_i}(i) - f_{1,\tau_j}(j)]$  instead of the Tamm-Dancoff expression  $[1 - f_{1,\tau_i}(i)][1 - f_{1,\tau_j}(j)]$ 



FIG. 5. (Color online) Composition of symmetric matter ( $Y_p = 0.5$ ) at T = 1 MeV. The mass fraction  $X_c$  is shown as function of the density  $n_B$ . The QS solution (solid lines) is compared with the ideal gas NSE solution (dashed lines). The mass fractions of d, t, h are very small and are not seen here.

for the Pauli blocking in Eq. (9) will reduce the mass fraction  $X_d$ . A systematic investigation was performed in Ref. [31], but only two-nucleon correlations  $(c \rightarrow d)$  have been considered, and the occupation numbers in the Pauli blocking (9) was given by the uncorrelated, free quasiparticles.

The self-consistent treatment of correlations in the medium demands further work, beyond the introduction of an effective chemical potential and an effective temperature (18) to calculate the Pauli blocking. Possibly, the fits for  $T_{\text{eff}}$ and  $v_c(\mathbf{P}; T, n_B, Y_p)$  have to be improved for  $n_B > n_{\text{sat}}/2$ . Note that a consistent treatment of nuclear matter at higher densities has also to take into account the formation of heavy nuclei, in particular at low temperatures, and thermodynamic



FIG. 6. (Color online) Composition of symmetric matter ( $Y_p = 0.5$ ) at T = 10 MeV. The QS solution (solid lines), same as in Fig. 4(b), is compared with the solution (dashed lines), where the **P** dependence of the Pauli blocking for the residual continuum contributions [Eq. (51)] is taken into account.

instability which leads to a phase transition. Therefore, in the region where details of the contribution of continuum correlations considered in this subsection influence the light cluster abundances, also further effects like heavy cluster formation and phase instability (pasta phases) interfere with the contribution of light elements to the composition of warm dense matter and have to be taken into account to derive the EOS.

#### VI. DISCUSSION

The present work aims at deriving the EOS for warm dense matter in the subsaturation region, incorporating the known low-density virial expansions, as well as mean-field theories near saturation density. In the context of a systematic QS approach, the single-nucleon quasiparticle description (e.g., RMF theory) is improved by including few-body ( $A \leq 4$ ) correlations. The QS approach provides a many-particle description of self-energy effects, Pauli blocking, and correlations in the continuum. In the low-density region, the rigorous results of the virial expansion are reproduced. It is challenging to work out a generalized Beth-Uhlenbeck approach which takes all light clusters into account. Based on a quasiparticle concept, this approach is valid also near the saturation density. Our study presents some steps in this direction. They should be improved as indicated below.

Extending previous work [32,33], I estimated the effects of continuum correlations, in particular the residual contributions of the continuum states to the EOS and the modification of Pauli blocking in a correlated nuclear medium. Results are given for the EOS (chemical potentials) and the composition at selected parameter values. A thermodynamic potential (free energy) is calculated which can be used to evaluate other thermodynamic variables, such as pressure, internal energy, entropy, and symmetry energy. The quantitative results for the EOS are sensitive to the contributions of continuum correlations. Based on the solution of the two-nucleon problem, estimates for the residual contributions of the continuum states are presented depending on  $\{T, n_B, Y_p\}$  and the c.m. momentum P; see Secs. IV B and VD. Within a clustervirial expansion [37], future work is needed to improve the description of contributions owing to continuum correlations, considering in-medium scattering phase shifts for different decay channels.

The treatment of Pauli blocking is of fundamental relevance for determining the formation of correlations in warm dense matter. The approximation (18) for the Pauli blocking in a correlated medium is only a simple fit that should be improved. For instance, at low temperatures,  $\alpha$  matter is formed, and quantum condensates may occur. Pairing is not included in my approach because the Tamm-Dancoff expression was used instead of the Feynman-Galitsky expression for the Pauli blocking in the Bethe-Salpeter equation (9). Also, quartetting [38] is not reproduced, but there are some recent results which consider the energy as function of density [54], including quantum condensates.

A related problem arises in nuclear structure calculations [52,53]. In particular,  $\alpha$ -like correlations appear in low-density isomers (e.g., the Hoyle state [39]) and in the low-density region at the surface of heavy nuclei which are  $\alpha$  emitters (for instance <sup>212</sup>Po [53]); see also [45]. Here a local density theory can be used to implement the results of the QS approach to the EOS. I expect that a more general and sophisticated approach to treat few-body correlations in warm dense matter (determining Pauli blocking, Secs. II B and II C) will be worked out in future, which is also of interest for nuclear structure calculations.

In addition to the parametrizations of the residual continuum contributions to the partial densities and the Pauli blocking in correlated matter discussed above, there are other items to be improved in further works. A main disadvantage is the omission of larger clusters (A > 4) which form at low temperatures and high densities. It restricts the region of applicability of the present results. A systematic QS approach to describe these correlations in warm dense matter is rather cumbersome; see Ref. [43]. As a semiempirical treatment [11], the EV model may be introduced. Thomas-Fermi calculations [12,15,18,20,21,45,46] provide us with a microscopic treatment of large nuclei in a dense medium. This may be improved by considering the intrinsic partition function, in particular the continuum contributions. Furthermore, the region of phase instability can be treated, and Coulomb corrections are important and must be included. So-called nuclear pasta phases are discussed to derive the EOS also within the region of thermodynamic instability; see Refs. [12,15,17,18].

The free energy and other thermodynamic variables derived from the thermodynamic potential are of interest in astrophysics where warm dense matter can occur. In particular, the physics of core-collapse supernovae enters the parameter region where cluster formation with  $A \leq 4$  in the subsaturation region occurs [2]. The presence of clusters modifies the thermodynamic properties and affects, for instance, the neutrino transport [6,12,40,55]. Whereas previous approaches [3,4] considered only  $\alpha$ -particle formation, recently also other light elements have been taken into account, within a QS model [5] or using the EV concept [11]. The systematic investigation of correlations and formation of light elements as presented in this work is relevant not only for the EOS but also for the calculation of microscopic processes describing the evolution of those astrophysical objects.

In heavy-ion collision (HIC) a description is required which takes medium effects into account beyond the ideal gas NSE. Recently, different versions of the EOS were compared with laboratory results [1]. The QS approach which takes cluster formation  $A \leq 4$  into account agrees well with the experimental data. Continuum correlations described by residual virial coefficients  $v_c(\mathbf{P}; T, n_B, Y_p)$  (42) and the effective phase-space occupation number  $\tilde{f}_{1,\tau}(1; T_{\text{eff}}, n_B, Y_p)$  (17) for the Pauli blocking energy shift, as presented in this work, have been used recently to calculate the chemical constants and the symmetry energy [1].

Results for equilibrium EOS have been used for HIC [1] to calculate the yields  $(n, p, d, t, h, \alpha)$  of the expanding fireball within the freeze-out concept. The question arises how the continuum correlations are assigned to the different yields of light elements. For instance, the residual continuum correlations in the isospin-singlet channel  $v_d^0(T)$  were taken into account for the deuteron yield. The partial density of correlations in the

isospin-triplet channel contributes solely to the free-nucleon yields because no stable bound state is formed in this channel. On a more fundamental level, a nonequilibrium approach is necessary to determine the fate of continuum correlations when the fireball is expanding. Future work is necessary to devise a transport theory for HIC, which is compatible with the thermodynamic properties and EOS, described in this work, as equilibrium solution.

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## APPENDIX A: THERMODYNAMIC POTENTIAL FOR WARM DENSE MATTER

In this work, the EOS (1) (chemical potentials as function of  $\{T, n_B, Y_p\}$ ) for warm dense matter is solved. Note that there exist different EOS that refer to further thermodynamic variables like the pressure, the internal energy, or the entropy. To get all thermodynamic quantities consistently, one can derive a thermodynamic potential. For instance, for fixed  $Y_p$ the free energy  $F(T, \Omega, N_n, N_p) = \Omega f(T, n_B, Y_p)$  is found by integration,

$$f(T, n_B, Y_p) = f(T, n_0, Y_p) + \int_{n_0}^{n_B} \bar{\mu}(T, n', Y_p) dn', \quad (A1)$$

where

$$G/N_{B} = \bar{\mu}(T, n_{B}, Y_{p})$$
  
=  $(1 - Y_{p})\mu_{n}[T, (1 - Y_{P})n_{B}, Y_{p}n_{B}]$   
+  $Y_{p}\mu_{p}[T, (1 - Y_{P})n_{B}, Y_{p}n_{B}]$  (A2)

is the free enthalpy per baryon.  $\mu_{\tau}(T, n_n^{\text{tot}}, n_p^{\text{tot}})$  are the solutions of the EOS (4),  $\tau = \{n, p\}$ , and  $\lim_{n_0 \to 0} f(T, n_0, Y_p)$  follows from the solution of the free energy density for the ideal classical gas.

## APPENDIX B: GENERAL EXPRESSION FOR THE CMF APPROXIMATION

The chemical picture gives the motivation to extend the mean-field approximation for the case of cluster formation [32,37,41]. Bound states are considered as new species, to be treated on the same footing as free particles.

I repeat expressions presented in Ref. [41]. The self-energy of the *A*-particle cluster is calculated to first order in the interaction with the single particles (n, p) as well as with the *B*-particle cluster states  $(d,t,h,\alpha)$  in the medium, but with full antisymmetrization of the normalized wave functions of both clusters *A* and *B* [37,41]. The notation  $\{A, v, \mathbf{P}\}$  is used for the particle number, internal quantum number (including proton number *Z*), and center of mass momentum for the cluster under consideration and  $\{B, \overline{v}, \overline{\mathbf{P}}\}$  for a cluster of the surrounding medium. For the *A*-particle problem, the effective

# G. RÖPKE

wave equation is derived as

$$[E(1) + \cdots E(A) - E_{A,\nu}(\mathbf{P})]\psi_{A\nu\mathbf{P}}(1,\dots,A) + \sum_{\substack{1',\dots,A'}}\sum_{i< j}^{A} V_{ij}^{A}(1,\dots,A,1',\dots,A')\psi_{A\nu\mathbf{P}}(1',\dots,A') + \sum_{\substack{1',\dots,A'}} V_{matter}^{A,mf}(1,\dots,A,1',\dots,A')\psi_{A\nu\mathbf{P}}(1',\dots,A') = 0,$$
(B1)

with the kinetic energy  $E(1) = \hbar^2 p_1^2 / 2m_1$  and the interaction  $V_{ij}^A(1, \ldots, A, 1', \ldots, A') = V(12, 1'2')\delta_{33'}, \ldots, \delta_{AA'}$ . The effective potential  $V_{\text{matter}}^{A,\text{mf}}(1, \ldots, A, 1', \ldots, A')$  describes the influence of the nuclear medium on the cluster bound states and has the form

$$V_{\text{matter}}^{A,\text{mf}}(1,\ldots,A,1',\ldots,A') = \sum_{i}^{A} \Delta E^{\text{SE}}(i)\delta_{11'},\ldots,\delta_{AA'} + \sum_{i,j}' \Delta V_{ij}^{A}(1,\ldots,A,1',\ldots,A'),$$
(B2)

with

$$\Delta E^{\text{SE}}(1) = \sum_{2} V(12, 12)_{\text{ex}} n(2) - \sum_{B=2}^{\infty} \sum_{\bar{\nu}\bar{\mathbf{P}}} \sum_{2\dots B} \sum_{1'\dots B'} f_B[E_{B,\bar{\nu}}(\bar{\mathbf{P}})] \\ \times \sum_{i< j}^{m} V_{ij}^B(1, \dots, B, 1', \dots, B') \psi_{B\bar{\nu}\bar{\mathbf{P}}}(1, \dots, B) \psi^*_{B\bar{\nu}\bar{\mathbf{P}}}(1', \dots, B'),$$
(B3)

$$\Delta V_{12}^{A}(1,\ldots,A,1',\ldots,A') = -\left\{\frac{1}{2}[n(1)+n(1')]V(12,1'2') + \sum_{B=2}^{\infty}\sum_{\bar{\nu}\bar{\mathbf{P}}}\sum_{\bar{2},\ldots,\bar{B}}\sum_{\bar{2}',\ldots,\bar{B}'}f_{B}[E_{B,\bar{\nu}}(\bar{\mathbf{P}})] \times \sum_{j}^{B}V_{1j}^{B}(1\bar{2},'\ldots,\bar{B}',1'\bar{2},\ldots,\bar{B})\psi_{B\bar{\nu}\bar{\mathbf{P}}}(2\bar{2},\ldots,\bar{B})\psi_{B\bar{\nu}\bar{\mathbf{P}}}(2'\bar{2}',\ldots,\bar{B}')\right\}\delta_{33'},\ldots,\delta_{AA'}, \quad (B4)$$

$$n(1) = f_1(1) + \sum_{B=2}^{\infty} \sum_{\bar{\nu}\bar{\mathbf{P}}} \sum_{2,\dots,B} B f_B[E_{B,\bar{\nu}}(\bar{\mathbf{P}})] |\psi_{B\bar{\nu}\bar{\mathbf{P}}}(1,\dots,B)|^2,$$
(B5)

where the variable Z in the cluster distribution function (5) has not been given explicitly. Equation (9) follows if all exchange terms are omitted so that only (B5) remains to describe medium effects.

### APPENDIX C: SHIFTS OF BOUND-STATE ENERGIES OWING TO PAULI BLOCKING

The cluster quasiparticle energies have been calculated from Eq. (19) as function of  $\{T, n_n^{\text{tot}}, n_p^{\text{tot}}\}$ , using a variational approach. The single-nucleon occupation numbers are approximated by Fermi distributions  $\tilde{f}_{1,\tau}(\mathbf{p}; T_{\text{eff}}, n_B, Y_p)$  at the effective temperature  $T_{\text{eff}}$  and normalized to the densities  $n_n^{\text{tot}}, n_p^{\text{tot}}$ . These parameters determine the effect of Pauli blocking leading to the bound-state energy shift  $\Delta E_{A,\nu}^{\text{Pauli}}(\mathbf{P}; T_{\text{eff}}, n_B, Y_p)$  [Eq. (20)]. For the calculations, see Ref. [33], where results for the Fermi function depending on  $\{T, n_B, Y_p\}$  are derived. Expressions obtained for this parameter set are given below. To perform the calculations in Sec. V, the variable T has to be replaced with  $T_{\text{eff}}$ , which now is relevant for the Pauli blocking expression.

The shifts of bound-state energies owing to Pauli blocking are approximated by  $(v = \{d, t, h, \alpha\}$  is used for the component c)

$$\Delta E_{\nu}^{\text{Pauli}}(\mathbf{P}; T, n_B, Y_p) = c_{\nu}(\mathbf{P}; T) \left\{ 1 - \exp\left[ -\frac{f_{\nu}(\mathbf{P}; T, n_B)}{c_{\nu}(\mathbf{P}; T)} y_{\nu}(Y_p) n_B - d_{\nu}(\mathbf{P}; T, n_B) n_B^2 \right] \right\}.$$
(C1)

In the term linear in  $n_B$ ,  $f_v(\mathbf{P}; T, 0)$  is given by first-order perturbation theory with respect to the density, using the unperturbed wave functions of the free nuclei. Motivated by the exact solution for A = 2 with the interaction potential (35) (for details, see Ref. [33]) the following fit for arbitrary  $n_B$  and v is used:

$$f_{\nu}(\mathbf{P};T,n_{B}) = f_{\nu,1} \exp\left[-\frac{P^{2}/\hbar^{2}}{4(f_{\nu,4}^{2}/f_{\nu,3}^{2})(1+T/f_{\nu,2}) + u_{\nu}n_{B}}\right] \frac{1}{T^{1/2}} \frac{2f_{\nu,4}}{P/\hbar} \operatorname{Im}\left(\exp\left\{f_{\nu,3}^{2}(1+f_{\nu,2}/T)\left[1-i\frac{P/\hbar}{2f_{\nu,4}(1+T/f_{\nu,2})}\right]^{2}\right\}\right) \times \operatorname{erfc}\left\{f_{\nu,3}(1+f_{\nu,2}/T)^{1/2}\left[1-i\frac{P/\hbar}{2f_{\nu,4}(1+T/f_{\nu,2})}\right]\right\}\right).$$
(C2)

The parameter values  $f_{\nu,i}$  and  $u_{\nu}$  are given in Table II.

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	$S_{i,j,k}$	i = 1	i = 2	<i>i</i> = 3	i = 4	<i>i</i> = 5
	k = 0	4462.35	204 334	125 513	49.0026	241.935
j = 0	k = 2	1.63811	-11043.9	-64680.5	-1.76282	-19.8568
	k = 4	0.293 287	-46439.7	-4940.76	-10.6072	-48.3232
j = 1	k = 0	-7.22458	7293.23	1055.3	1.701 56	6.6665
	k = 2	0.92618	-49220.9	-19422.6	-11.1142	-52.6306
	k = 4	-0.679 133	35263	15 842.8	7.926 04	38.1023
j = 2	k = 0	0.009 755 76	-209.452	132.502	-0.0456724	-0.112 997
	k = 2	-0.0355021	2114.07	572.292	0.473 553	2.15092
	k = 4	0.026 292	-1507.55	-555.762	-0.337016	-1.575 97

TABLE III. Coefficients  $s_{i,j,k}$  for the Padé approximation of the scalar self-energy  $S(T, n_B, \delta)$ .

The dependence on the asymmetry  $Y_p$  is given by the expression  $y_v(Y_p)$  in Eq. (C1) with  $y_d(Y_p) = y_\alpha(Y_p) = 1$ , for triton  $y_t(Y_p) = (\frac{4}{3} - \frac{2}{3}Y_p)$ , and for helion  $y_h(Y_p) = (\frac{2}{3} + \frac{2}{3}Y_p)$ . The term

$$c_{\nu}(\mathbf{P};T) = c_{\nu}(0;T) = c_{\nu,0} + \frac{c_{\nu,1}}{(T - c_{\nu,2})^2 + c_{\nu,3}}$$
(C3)

is not depending on P, but

$$d_{\nu}(\mathbf{P}; T, n_B) = d_{\nu}(0; T, n_B) \exp\left[-\frac{P^2/\hbar^2}{w_{\nu}Tn_B}\right],$$
  
$$d_{\nu}(0; T, n_B) = \frac{d_{\nu,1}}{(T - d_{\nu,2})^2 + d_{\nu,3}},$$
 (C4)

is depending on **P** with the parameter  $w_{\nu}$ . The corresponding parameter values are given in Table II.

## APPENDIX D: NUCLEON QUASIPARTICLES

The single-nucleon quasiparticle dispersion relation (24)  $E_{\tau}(\mathbf{p}) = \hbar^2 p^2 / (2m_{\tau}) + \Delta E_{\tau}^{\text{SE}}(\mathbf{p}) = \Delta E_{\tau}^{\text{SE}}(0) + \hbar^2 p^2 / (2m_{\tau}^*) + \mathcal{O}(p^4)$  is parametrized by various density functionals. An improved parametrization of the DD-RMF model [8,37] is given here in form of a Padé approximation. The variables are temperature *T*, baryon number density  $n_B = n_n^{\text{tot}} + n_p^{\text{tot}}$ , and the asymmetry parameter  $\delta = 1 - 2Y_p$  with the total proton fraction  $Y_p = n_p^{\text{tot}}/n_B$ . The intended relative accuracy in the parameter value range T < 20 MeV,  $n_B < 0.16$  fm<sup>-3</sup> is 0.001.

The scalar self-energy (identical for neutrons and protons) is approximated as

$$S(T, n_B, \delta) = \frac{s_1(T, \delta) n_B + s_2(T, \delta) n_B^2 + s_3(T, \delta) n_B^3}{1 + s_4(T, \delta) n_B + s_5(T, \delta) n_B^2}, \quad (D1)$$

with coefficients

$$s_{i}(T,\delta) = s_{i,0}(\delta) + s_{i,1}(\delta) T + s_{i,2}(\delta) T^{2},$$
  

$$s_{i,j}(\delta) = s_{i,j,0} + s_{i,j,2} \delta^{2} + s_{i,j,4} \delta^{4},$$
(D2)

with baryon number densities  $n_B$  in fm<sup>-3</sup> and temperatures T as well as the self-energies S, V in MeV. Parameter values are given in Table III.

TABLE IV. Coefficients  $v_{i,j,k}$  for the Padé approximation of the vector self-energy  $V_p(T,n_B,\delta) = V_n(T,n_B,-\delta)$ .

	$v_{i,j,k}$	i = 1	i = 2	<i>i</i> = 3	i = 4	<i>i</i> = 5
	k = 0	3403.94	-345.863	335 53.8	2.7078	18.7473
	k = 1	-490.15	1521.62	4298.76	-0.162553	4.094 836 4
j = 0	k = 2	-0.021 314 3	-2658.72	3692.23	-0.308454	-0.0308012
5	k = 3	0.007 607 59	-408.013	-1083.14	-0.174442	-0.751981
	k = 4	0.026 510 9	-132.384	-728.086	-0.0581052	-0.585746
	k = 0	-0.000978098	29.309	-192.395	0.016 145 6	-0.102959
	k = 1	-0.000142646	-8.80748	-52.0101	-0.00145171	-0.044524
j = 1	k = 2	0.001 769 29	-236.029	-141.702	-0.0689643	-0.308021
	k = 3	0.000 437 52	13.7447	-57.9237	-0.0000398794	-0.019 092 1
	k = 4	-0.00321724	111.538	-11.4749	0.031 799 6	0.086 952 9
	k = 0	0.000 065 160 9	3.633 22	15.2158	0.001 051 79	0.011 804 9
	k = 1	0.000 009 816 8	0.016 349 5	3.866 52	0.000 192 765	0.002 114 1
j = 2	k = 2	-0.0000394036	6.882 56	-0.785201	0.002 037 28	0.007 054 8
	k = 3	0.000 038 140 7	-0.369704	1.596 25	0.000 005 614 67	0.000 565 564
	k = 4	0.000 110 931	-3.28749	2.0419	-0.000932046	-0.00182714

The vector self-energy  $V_p(T, n_B, \delta) = V_n(T, n_B, -\delta)$  is approximated as

$$V_p(T, n_B, \delta) = \frac{v_1(T, \delta) n_B + v_2(T, \delta) n_B^2 + v_3(T, \delta) n_B^3}{1 + v_4(T, \delta) n_B + v_5(T, \delta) n_B^2},$$
(D3)

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with coefficients

$$v_{i}(T,\delta) = v_{i,0}(\delta) + v_{i,1}(\delta) T + v_{i,2}(\delta) T^{2},$$
  

$$v_{i,j,k}(\delta) = v_{i,j,0} + v_{i,j,1} \delta + v_{i,j,2} \delta^{2} + v_{i,j,3} \delta^{3} + v_{i,j,4} \delta^{4}.$$
(D4)

Parameter values are given in Table IV.

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