Ensemble in-equivalence in supernova matter within a simple model

F. Gulminelli\textsuperscript{1,2} and Ad. R. Raduta\textsuperscript{3}

\textsuperscript{1} CNRS, UMR6534, LPC , F-14050 Caen cédex, France
\textsuperscript{2} ENSICAEN, UMR6534, LPC , F-14050 Caen cédex, France
\textsuperscript{3} NIPNE, Bucharest-Magurele, POB-MG6, Romania

A simple, exactly solvable statistical model is presented for the description of baryonic matter in the thermodynamic conditions associated to the evolution of core-collapsing supernova. It is shown that the model presents a first order phase transition in the grandcanonical ensemble which is not observed in the canonical ensemble. Similar to other model systems studied in condensed matter physics, this ensemble in-equivalence is accompanied by negative susceptibility and discontinuities in the intensive observables conjugated to the order parameter. This peculiar behavior originates from the fact that baryonic matter is subject to attractive short range strong forces as well as repulsive long range electromagnetic interactions, partially screened by a background of electrons. As such, it is expected in any theoretical treatment of nuclear matter in the stellar environment. Consequences for the phenomenology of supernova dynamics are drawn.

PACS numbers: 64.10.+h, 64.60.-i, 26.50.+x, 26.60.-c

I. INTRODUCTION

Standard thermodynamics is based on the assumption that the physical properties of a system at equilibrium do not depend on the statistical ensemble which is used to describe it. Under this condition thermodynamics is unique and the different thermodynamic potentials are related via simple linear Legendre transforms. It is however well known that the equivalence between the different statistical ensembles can only be proved\textsuperscript{1} at the thermodynamic limit and under the hypothesis of short range interactions, while non-standard thermostatistic tools have been developed during the years to deal with non-extensive and long-range interacting systems\textsuperscript{2,3}.

The issue of ensemble in-equivalence, namely the possible dependence of the observed physics on the externally applied constraints, has been typically associated to phase transitions, more precisely to phase separation quenching due to the external constraint. A well-known example in the literature concerns the possible occurrence of negative heat capacity in finite systems, which has been widely studied theoretically\textsuperscript{4} and has also given rise to different experimental applications in nuclear and cluster physics\textsuperscript{5}. In this specific example the phase separation is quenched by the microcanonical conservation constraints, leading to the thermodynamic anomaly of a non-monotonous equation of state.

Concerning macroscopic systems, different model applications have shown fingerprints of ensemble in-equivalence\textsuperscript{3,6–10} but phenomenological applications are scarce. In this paper we show that the dense matter which is produced in the explosion of core-collapse supernova and in neutron stars is an example of a physical system which displays this in-equivalence.

We will limit our discussion to finite temperature $T \approx 10^{10} K$ and nuclear sub-saturation $10^{10} < \rho < 10^{14}$ g cm\textsuperscript{-3} densities, thermodynamic conditions which are known to be largely explored in the dynamics of supernova matter and in the cooling phase of proto-neutron stars\textsuperscript{11,12}. The baryonic component of this stellar matter is given by a statistical equilibrium of neutrons and protons, the electric charge of the latter being screened by an homogeneous electron background.

If the electromagnetic interactions are ignored, this gives the standard model of nuclear matter, which is known to exhibit first and second order phase transitions with baryonic density as an order parameter, meaning that the transition concerns a separation between a dense (ordered) and a diluted (disordered) phase\textsuperscript{13}. It is however known since decades to the astrophysical community that the situation is drastically different in stellar matter, where microscopic dishomogeneities are predicted at almost all values of temperature, density and proton fraction and thermodynamical quantities continuously change at the phase transition\textsuperscript{14,13}. This specific situation of stellar matter respect to ordinary nuclear matter has been shown to be due to Coulomb frustration which quenches the first order phase transition\textsuperscript{14,13}. However, the thermodynamic consequences of this specific thermodynamics with long range interactions have never been addressed to our knowledge.

In this work we will show that these dishomogeneities imply ensemble in-equivalence, making neutron star matter the first astrophysical example to our knowledge of ensemble in-equivalence at the thermodynamic limit. Additionally,
we will show that a consistent treatment of this specific thermodynamics can have sizeable effects in the equations of state which are currently used to describe the supernova phenomenology.

In a recent paper [17] we have proposed a phenomenological hybrid model for supernova matter which was numerically solved by Monte-Carlo simulations. Since convergence is always an issue in Monte-Carlo calculations, we propose in this paper an analytic version of the same model. In order to have analytical results, we will limit to the simplest version of the model where a schematic nuclear energy functional is used. It is clear that more sophisticated energy functionals will have to be implemented in order to have quantitative predictions for the supernova simulations.

However, the qualitative conclusions of this paper will only depend on the sign (attractive or repulsive) of the interactions and on the size dependence (in terms of volume and surface) of the nuclear binding energy. As such, they will not depend on the details of the model.

II. THE MODEL

Stellar matter at temperature lower than the typical nuclear binding energy \( E_b \approx 8 \text{ MeV/nucleon} \approx 10^{11} \text{ K} \), and density \( \rho \) lower than the saturation density of nuclear matter \( \rho_0 \approx 0.16 \text{ fm}^{-3} \approx 1.6 \cdot 10^{14} \text{ g cm}^{-3} \), can be viewed as a statistical mixture of free protons and neutrons with loosely interacting nuclear clusters at internal density \( \rho_0 \), immersed in an homogeneous electron background density \( \rho_e \) which neutralizes the total positive charge density \( \rho_p \) over macroscopic length scales, \( \rho_e = \rho_p \). Nucleons bound in clusters can be described by a phenomenological free energy functional depending on the cluster size \( a = n + z \) and chemical composition \( i = n - z \) as well as on the temperature of the medium:

\[
f_{a,i}^{\beta} = e_{a,i} + \langle e_{a,i}^* \rangle_\beta - T_s^{\beta}.
\]

For nuclear (fermionic) clusters both the average cluster excitation energy \( \langle e_{a,i}^* \rangle_\beta \) and entropy \( s_{a,i}^{\beta} \) can be evaluated in the low temperature Fermi gas approximation

\[
\langle e_{a,i}^* \rangle_\beta = c_0 a T^2;
\]

\[
s_{a,i}^{\beta} = \left( 2 c_0 T + c_s a^{-1/3} h(T) \right) a,
\]

The surface term \( c_s a^{2/3} h(T) \) in Eq. (6) effectively accounts for the entropy increase at finite temperature due to surface excitations, producing a vanishing surface free energy at a given temperature, corresponding to the critical point \( \beta_C = T_C^{-1} \) of nuclear matter. The cluster energy \( e_{a,i} \) is modified with respect to the energy of the nucleus in the vacuum \( e_{a,i}^0 \) because of the electromagnetic interaction with the electron background which neutralizes the proton charge. In the Wigner- Seitz approximation the functional results [18]

\[
e_{a,i} = e_{a,i}^0 - c_C z^2 a^{-1/3} \left( \frac{3}{2} \left( \frac{\rho_p}{\rho_0} \right)^{1/3} - \frac{1}{2} \left( \frac{\rho_p}{\rho_0} \right)^{1/2} \right)
\]

where \( \rho_p = \rho_e \) is the proton density and \( \rho_0 \geq \rho_p \) the corresponding saturation value. The minimal scale at which charge neutrality is verified, is called a Wigner- Seitz cell.

We use in the following a simple liquid-drop parameterization for the cluster energies \( e_{a,i}^0 \) [17]:

\[
e_{a,i}^0 = \left( c_V a + c_s a^{2/3} \right) \left( 1 - c_I \frac{r^2}{a^2} \right) + c_C z^2 a^{-1/3}.
\]

but shell and pairing corrections can be readily incorporated [14]. Density dependent correction terms accounting for the nuclear interaction with the free nucleons [24][23] are also expected to improve the predictive power of the model, as well as a more sophisticated form for the cluster internal entropy using realistic \( a \) and \( i \) dependent densities of states [17]. Since none of these improvements is expected to change the qualitative results of this paper, we are not including them here to keep an analytically solvable model.

As a first approximation, one can consider that the the system of interacting nucleons is equivalent to a system of non-interacting clusters, nuclear interaction being completely exhausted by clusterization [24]. This classical model of clusterized nuclear matter is known in the literature as nuclear statistical equilibrium (NSE) [25][28]. This simple model can only describe diluted matter at \( \rho \ll \rho_0 \) as it can be found in the outer crust of neutron stars, while nuclear...
interaction among nucleons and clusters has to be included for applications at higher density, when the average inter-particle distance becomes comparable to the range of the force.

In our model, interactions among composite clusters are taken into account in the simplified form of a hard sphere excluded volume. Since the nuclear density is (approximately) constant inside the clusters, the volume occupied by each species \((a, i)\) is given by \(V_{a, i} = a n_{a, i}/\rho_0\), where \(n_{a, i}\) is the abundance of the species \((a, i)\). The volume fraction available to the clusters then reads:

\[
\frac{V_F}{V} = 1 - \sum_{a>i,i} a \frac{n_{a,i}}{\rho_0 V} = 1 - \frac{\rho_{cl}}{\rho_0},
\]

where \(\rho_{cl}\) is the total density of nucleons bound in clusters. A slightly different expression has been used in Refs. 17, 19, which however does not change the results presented in this paper.

In addition to the excluded volume effect for the clusters, the inter-particle nuclear interaction is also considered for the nucleons not bound in clusters. The free nucleons self-energy is computed in the self-consistent Hartree-Fock approximation with a phenomenological realistic effective interaction [29]. The energy density can be expressed as a function of the density of neutrons \(\rho_n\) and protons \(\rho_p\) which are not bound in clusters as:

\[
e^{(HM)} = \frac{\hbar^2}{2m_0}(\tau_n + \tau_p) + t_0(x_0 + 2)(\rho_n + \rho_p)^2/4 - t_0(2x_0 + 1)(\rho_n^2 + \rho_p^2)/4 + t_3(x_3 + 2)(\rho_n + \rho_p)^{r+2}/24 - t_3(2x_3 + 1)(\rho_n + \rho_p)^r(\rho_n^2 + \rho_p^2)/24 + (t_1(x_1 + 2) + t_2(x_2 + 2))(\rho_n + \rho_p)(\tau_n + \tau_p)/8 + (t_2(2x_2 + 1) - t_1(2x_1 + 1))(\rho_n \tau_n + \rho_p \tau_p)/8,
\]

where \(m_0\) is the nucleon mass, \(t_0, t_1, t_2, t_3, x_0, x_1, x_2, x_3, \sigma\) are Skyrme parameters and \(\tau_n, \tau_p\) represent the neutron and proton kinetic energy density. We use the SKM* [29] parameterization for the numerical applications.

At density \(\rho \geq \rho_0\) the whole baryonic matter is expected to be homogeneous and described by eq. (4). The transition from inhomogeneous to homogeneous matter is physically realized in stellar matter at the interface between the crust and the core of a neutron star. As we can see from eq. (4), in our model at proton densities \(\rho_p = \rho_{0p}\) the Wigner-Seitz correction exactly compensates the Coulomb self-energy of the cluster and the total Coulomb energy vanishes, reflecting matter homogeneity at supersaturation densities. In this regime the asymptotic cluster energy represents the energy density of asymptotic neutral nuclear matter

\[
\lim_{a \to \infty} \frac{e_{a,i}(\rho_p = \rho_{0p})}{a} = \frac{1}{\rho} \epsilon^{(HM)}(\rho_n, \rho_{0p}),
\]

where \(\rho = \lim_{A,V \to \infty} A/V = \rho_n + \rho_p, \mu = \lim_{I,V \to \infty} I/V = \rho_n - \rho_p, \text{ and } A, I\) are the total number of particles and chemical asymmetry. The crust-core transition can thus be seen equivalently as the melting of clusters inside dense homogeneous matter, or as the emergence of a percolating cluster of infinite size.

Charge neutrality is imposed globally but local charge dishomogeneities at the scale of the Wigner-Seitz cell naturally appear in the thermodynamic conditions where matter is clustered. In turn, this gives rise to a long range monopole component of the Coulomb potential which extends over domains of the order of the cluster size, and which can potentially become macroscopic in the limit of very extended clusters close to the crust-core transition. As we will show in detail, these long range Coulomb correlations are at the origin of the specific thermodynamics.

**Grandcanonical formulation**

Considering that the center of mass of composite fragments can be treated as a classical degree of freedom, their grandcanonical partition sum reads [17, 19]

\[
Z_{\beta, \mu_1}^{a>1} = \prod_{a>1, i \neq (-a,a)} \exp z_{a,i}
\]

The partition sum associated to a cluster composed of \(n\) neutrons and \(z\) protons in a volume \(V\) is given by

\[
z_{a,i} = V_F \left( \frac{2\pi a m_0}{\beta \hbar^2} \right)^{3/2} \exp \left[ - \beta \left( f_{a,i} - \mu_{a,i} \right) \right]
\]
Here, $V_F$ is the free volume associated to the cluster center of mass given by eq. (6), and the cluster chemical potential is a linear combination of the isoscalar and isovector chemical potentials $\mu$, $\mu_I$ which have to be introduced in the presence of two conserved charges

$$\mu_{a,i} = \mu a + \mu_I i.$$  

Fermi statistics cannot be neglected when treating $a = 1$ fragments (protons and neutrons). This component of the baryonic partition sum is thus included in the finite temperature Hartree-Fock approximation [17]

$$Z_{a=1}^{\beta,\mu,\mu_I} = Z_{a=1}^{\beta,\mu,\mu_I} \exp \left[ -\beta \left( \frac{\partial}{\partial \beta} \ln Z_{a=1}^{\beta,\mu,\mu_I} + V e^{HM} \right) \right]$$

where the non-interacting part of the partition sum can be expressed as a functional of the kinetic energy density $\tau_q$ for neutrons ($q = n$) or protons ($q = p$):

$$\ln Z_{a=1}^{\beta,\mu,\mu_I} = \frac{2\beta V}{3} \sum_{q=n,p} \frac{\partial e^{HM}}{\partial \tau_q}$$

(13)

with:

$$\tau_q = \frac{8\pi}{\hbar^3} \int_0^\infty \frac{1}{\hbar^2} \frac{p^3 dp}{1 + e^{\beta (e_q - \mu_q)}}.$$  

(14)

The number density of free protons and neutrons $\rho_{fq} = \partial_{\beta \mu} \ln Z_{a>1}^{\beta,\mu,\mu_I} / V$ determines the single particle energy which enters in the self-consistency equation (14) according to,

$$e_q = p^2 \frac{\partial e^{HM}}{\partial \tau_{fq}} + \frac{\partial e^{HM}}{\rho_{fq}}.$$  

(15)

The computation of all thermodynamical variables is straightforward using the standard grandcanonical expressions for the global baryonic partition sum $Z = Z_{a>1}^{\beta,\mu,\mu_I} Z_{a=1}^{\beta,\mu,\mu_I}$. In particular the total baryonic pressure is simply $\beta p = \ln Z_{a=1}^{\beta,\mu,\mu_I} / V$, the multiplicity of the different clusters is given by

$$n_{a,i} = \frac{\partial \ln Z_{a=1}^{\beta,\mu,\mu_I}}{\partial \beta \mu_{a,i}} = z_{a,i}$$

(16)

and the total baryonic density is the sum of the clusterized ($a > 1$) and the unbound ($a = 1$) component

$$\rho = \rho_p + \rho_n = \sum_{a,i} a \frac{n_{a,i}}{V} + \rho_f = \rho_{cl} + \rho_f$$

(17)

where $\rho_f = \rho_{fp} + \rho_{fn}$ is the total density associated to the nucleons which are not bound in clusters.

Expression Eq. (14) includes the electrons self-energy inside the Wigner-Seitz cell. This means that in the global stellar partition sum the remaining electron contribution will be factorized $Z_{tot} = Z_{bar}^{\beta,\mu,\mu_I} Z_{el}^{\beta,\mu,e}$, where $Z_{bar}^{\beta,\mu,\mu_I}$ is given by Eq. (9) and $Z_{el}^{\beta,\mu,e}$ is a trivial ideal Fermi gas contribution which has no influence on the thermodynamics and will not be discussed further [18].

The functional relation between the different grandcanonical variables is represented in Fig. 1 for a representative given value of $T$ and $\mu_I$, relevant for the astrophysical applications. The constrained entropy per baryon $s_{\beta,\mu_I} = \sigma_{\beta,\mu_I}/\rho$ is evaluated from the Legendre transform of the partition sum in the region where the density is defined:

$$\sigma_{\beta,\mu_I}(\rho) = \ln Z_{\beta,\mu,\mu_I} / V - \beta \mu \rho,$$

(18)

and shown in panel (a) as a function of the volume per baryon or inverse density $v = 1/\rho$. The first derivative of this function is the baryonic pressure $P$ given in panel (b). The first derivative of the entropy density $\sigma_{\beta,\mu_I}$ with respect to the density gives the other equation of state, namely the chemical potential $\mu = P/\rho - s_{\beta,\mu_I}/\beta$, represented in panel (c). Finally phase equilibrium is best spotted by looking at the phase diagram given by the relation between intensive variables, as shown in panel (d).
The grandcanonical thermodynamics leads to a first order phase transition. This can be inferred from the characteristic two-humped structure of the constrained entropy, which is better evidenced by subtraction of a straight line, as well as by the crossing of the two equations of state (panel (d)). In the presence of a first order phase transition only in the ensemble where the order parameter is fixed (here: the canonical ensemble) the phase transition region is accessible, while it is jumped over in the ensemble where the order parameter is fixed only in average (here: the grandcanonical). As a consequence, a discontinuity is observed in the equations of state covering a huge range of baryonic densities relevant for the description of supernova dynamics.

The equilibrium solution in the phase transition region corresponds to a linear combination of the two pure phases following Gibbs rules. This construction is exactly equivalent to a one-dimensional Maxwell construction if we work in an ensemble where all intensive parameters are fixed but one, and it is represented by the dashed lines in Fig. 1 [30, 31]. We note on passing that this simplification demands to work in the non-standard ensemble \((T, \rho, \mu_I)\). In astrophysical applications it is customary to work rather with the parameters \((T, \rho, y_p)\), where \(y_p = \rho_p/\rho\) is the proton fraction. Within this ensemble, a full two-dimensional Gibbs construction is needed to correctly calculate the coexistence zone. The use of a Maxwell construction in the ensemble \((T, \rho, y_p)\) is a mistake, yet it is often used in the literature [18, 19].
The construction of a convex entropy envelope allows to recognize that inside the density region, indicated by dotted lines, the obtained grandcanonical solutions do not correspond to an equilibrium, since a higher entropy solution can be obtained by making a linear combination of the two (dense and diluted) solutions marked by a filled circle, that is by a first order phase transition. The pressure and chemical potential associated to the metastable branch on the low density side are also represented in Fig. 1. From the pressure viewpoint (panel (b)) such solutions appear equivalent to a phase coexistence (dashed line), but this is not true in terms of chemical potential (panel (c)).

The presence of metastable solutions was never discussed in the framework of NSE models to our knowledge. It can be understood from the fact that, for chemical potentials higher than the Fermi energy of dense uniform matter \( \mu \geq \epsilon_F \approx -16 \text{MeV} \), the equilibrium condition can be obtained either as a mixture of clusters and homogeneously distributed nucleons \( \mu^{a=1} = \mu^{a=1} = \mu \), or alternatively letting the clustered component to vanish \( (\mu^{a=1} = \mu \text{ and } \rho_d = 0) \). This gives a second stationary entropy solution which appears to correspond to the absolute entropy maximum, and which renders metastable the clustered solution at lower density.

The ending point of the metastable branch can be worked out easily. Indeed from Eq. (11) we can see that, for any temperature \( \beta^{-1} \) and isovector chemical potential \( \mu_I \), it exist a limiting value of chemical potential \( \mu_{max} \) for which the cluster multiplicities \( n_{A,1} \) asymptotically diverge. This value is determined by the condition of an asymptotically negative Gibbs free energy

\[
\lim_{a \to \infty} f_{a,i}^\beta - \mu a - \mu_i i < 0
\]

combined with the requirement that the Coulomb energy vanishes in the limit of an infinitely extended homogeneous cluster:

\[
\frac{1}{V} \sum_{a,i} a - i \cdot n_{a,i} = \rho_{pp}
\]

For chemical potentials above \( \mu_{max} \), clustered partitions become unstable due to the emergence of a liquid phase.

Coming back to the discontinuity shown in the equations of state in Figure 1 in standard thermodynamics the fact that the Gibbs construction is a posteriori made to fill up the coexistence region is not a limitation, because ensemble equivalence guarantees that the very same linear combination solution would have been obtained if we had worked in the canonical ensemble, explicitly constraining the density.

Because of the complexity of the phenomenology of stellar matter we have not proposed an Hamiltonian treatment of the problem. However the phenomenological free energy functional Eq. (12) we have used implicitly contains the effect of the attractive short range nuclear forces, scaling proportionally to the number of particles in the thermodynamic limit, and repulsive long range Coulombic forces, scaling proportionally to the square of the number of particles and only partially screened. None of the possible improvements on the nuclear energy functional would change these very general scaling behaviors. It has been argued in ref. 16 that this generic frustration effect should lead to a quenching of the first order phase transition. We have shown that the phase transition is observed in the grandcanonical ensemble. We turn therefore to explore the possibility that ensemble in-equivalence might be at play in the stellar environment, with the thermodynamic anomalies associated to the thermodynamics of long range interactions.

**Canonical formulation**

A fully canonical formulation of our model would imply the use of two independent extensive variables, the proton and neutron density \( (\rho_p, \rho_n) \) or equivalently the isoscalar and isovector density \( (\rho, \rho_I) \). It is however well established that, contrary to other physical systems like binary alloys and molecular mixtures where phase transitions can also imply separation of the species, the isovector density is not an order parameter of the nuclear matter phase transition. Since the in-equivalence effect we are looking for is associated to the phenomenon of phase coexistence, we thus expect to see it even if we keep a grandcanonical treatment for the isovector density.

The effect we are looking for is due to the long range Coulomb interaction, which vanishes in homogeneous matter. This Coulomb interaction is neglected in the computation of the abundances of \( a = 1 \) particles which are modelized as homogeneously distributed. For this reason we will also stick to a grandcanonical formulation for \( a = 1 \) particles according to Eq. (13), and assume that the approximate Legendre transformation Eq. (18)

\[
\ln Z_{\beta,\mu}^{a=1}(\rho) = \ln Z_{\beta,\mu,\nu}^{a=1} - \beta \mu \rho V,
\]

which is exact in the mean-field approximation we have employed, is physically correct. For the same reason we will consider that the standard thermodynamic assumption of total canonical entropy being additive among independent
components, is verified as expected at the thermodynamic limit within ensemble equivalence:

$$\sigma^{\text{can}}_{\beta,\mu_I}(\rho) = \ln Z_{\beta,\mu_I}^{a=1}(\rho_f) + \lim_{V \to \infty} \frac{1}{V} \ln Z_{\beta,\mu_I}^{a>1}(V \rho_{cl})$$

where the density repartition between the clustered $\rho_{cl}$ and unbound $\rho_f$ component Eq. (17) is uniquely defined by the condition of having a single chemical potential $\mu$ for both components. Possible extra deviations from ensemble equivalence originating from the $a=1$ contribution would need a more sophisticated model where the polarization of the free protons would be explicitly accounted for [19]. For simplicity, in the following we will refer to this hybrid $(\beta, \mu_I, \rho)$ ensemble as to the "canonical" ensemble.

To derive the expression of the canonical partition sum, we start from the general statistical mechanics relation which links the different statistical ensembles, restricted to composite clusters $a > 1$ only (the subscript $a > 1$ is omitted hereafter for simplicity):

$$Z_{\beta,\mu,\mu_I} = \sum_{A>1} Z_{\beta,\mu_I}(A) \exp (\beta \mu A)$$

Identification with Eq. (9) gives,

$$Z_{\beta,\mu_I}(A) = \sum_{\{n_a\} \atop \sum a n_a = A} \prod_{a>1} \omega^{n_a}_{a} n_a!$$

where $n_a = \sum_i n_{ia}$ is the occupation number of size $a$ and the sum is restricted to combinations $\{n_a\} \equiv \{n_2, \ldots , n_A\}$ satisfying the canonical constraint,

$$\sum_{a=2}^{A} a n_a = A.$$

The weight of the different cluster size is given by,

$$\omega_a = \sum_{z=0}^{a} \omega_{a,a-2z} \exp(\beta \mu_I (a - 2z)),$$

and the weight of each nuclear species is determined by the free energy functional we have assumed,

$$\omega_{a,i} = V_F \left( \frac{2 \pi a m_0}{\beta h^2} \right)^{3/2} \exp \left( -\frac{\beta f_{\beta a,i}}{a} \right).$$

Following Ref. [35] we introduce an auxiliary canonical partition sum $Z_{\beta,\mu_I}^m(A)$ defined by the additional constraint that the cluster multiplicity is fixed to $m$, $\sum_a n_a = m$. With the help of relation (24) we get,

$$Z_{\beta,\mu_I}^{m-1}(A - a) = \frac{< n_a >_m}{\omega_a} Z_{\beta,\mu_I}^m(A),$$

where $< n_a >_m$ is the average multiplicity of size $a$ under the additional constraint of total multiplicity $m$. Explicitly implementing the canonical constraint Eq. (25) we arrive to the recursion relation,

$$Z_{\beta,\mu_I}^m(A) = \frac{1}{A} \sum_{a=2}^{A} a \omega_a Z_{\beta,\mu_I}^{m-1}(A - a),$$

which is valid for any value of $A$. Summing over all the possible $m$ values, we can see that the same relation holds for the unconstrained canonical partition sum

$$Z_{\beta,\mu_I}(A) = \frac{1}{A} \sum_{a=2}^{A} a \omega_a Z_{\beta,\mu_I}(A - a).$$

This expression can be recursively computed with the initial condition $Z_{\beta,\mu_I}(2) = \omega_2$. The computational problem however arises that going towards the thermodynamic limit the evaluation of the double sum implied by Eq. (26) becomes numerically very heavy. Starting from a sufficiently high minimal value $a_{\text{min}}$ we therefore develop a continuous approximation for Eq. (26),

$$\omega_{a>a_{\text{min}}} \approx \frac{1}{2} \int_{-a}^{a} dy \exp g(y).$$
This integral is calculated in the saddle point approximation:

\[ g(i) = \ln \omega_{a,i} + \beta \mu_I i \approx \ln \omega_{a,<i>} + \beta \mu_I < i > - \frac{(i - < i >)^2}{2\sigma_a^2}. \]  

(32)

where the most probable isotopic composition \(< i >\) of a cluster of size \(a\) depends on the temperature according to,

\[ \mu_I = \left. \frac{\partial f_{a,i}}{\partial i} \right|_{i = < i >}, \]  

(33)

and the associated dispersion is given by

\[ \frac{1}{\sigma_a^2} = \beta \left. \frac{\partial^2 f_{a,i}}{\partial i^2} \right|_{i = < i >}. \]  

(34)

The global weight of size \(a\) finally results,

\[ \omega_{a > a_{min}} \approx \omega_{a,<i>} \sqrt{2\pi \sigma_a^2} \exp(\beta \mu_I < i >) / 2 \]  

(35)

and the value of \(a_{min}\) is chosen such that Eq. (35) and Eq. (26) give estimation differing less than 5%. The canonical thermodynamical potential \(\sigma_{\beta,\mu_I}^N\) is then defined by Eq. (22), with the identification \(Z_{\beta,\mu_I} \equiv Z_{\beta,\mu_I}^{a>1}\).

Ensembles are equivalent if this function coincides with the entropy density \(\sigma_{\beta,\mu_I}(\rho)\) defined by the Legendre transform of the grandcanonical partition sum Eq. (18). More precisely, ensemble equivalence demands that the thermodynamic quantities as calculated from the canonical partition sum,

\[ \mu_{\text{can}} = -\frac{1}{\beta} \frac{\partial \sigma_{\beta,\mu_I}^\text{can}}{\partial \rho}, \]

\[ p_{\text{can}} = \frac{\rho \sigma_{\beta,\mu_I}^\text{can}}{\beta} + \mu \rho, \]

\[ \epsilon_{\text{can}} = -\frac{\partial \sigma_{\beta,\mu_I}^\text{can}}{\partial \beta}, \]  

(36)

coincide with the corresponding grandcanonical quantities. The canonical thermodynamics, in the same thermodynamic conditions as in Fig. 1, is displayed in Fig. 2. We can see that the canonical calculation allows to interpolate between the dense and dilute branches observed in the grandcanonical ensemble as expected. However the interpolation is not linear, meaning that the chemical potential continuously varies as a function of the density. The discontinuity in the entropy slope at high density leads to a jump in the intensive observables close to the saturation density, in complete disagreement with the grandcanonical solution [3]. Even more interesting, the entropy presents a convex intruder, the behavior of the equations of state is not monotonous and a clear back-bending is observed, qualitatively similar to the phenomenon observed in first order phase transitions in finite systems [4].

The canonical partition sum Eq. (30) is only defined for finite values of the total number of particles \(A\). The doubt therefore arises that this non-trivial behavior and the similarity with the finite systems thermodynamics might be due to a non achievement of the thermodynamic limit. Fig. 3 shows that this is not the case, and the canonical calculation is convergent. In this figure the chemical potential (a), pressure (b) and cluster size distribution (c) are represented for different values of the total number of particles \(A\) at a given density inside the in-equivalence region.

We can see that indeed a very large size has to be used before this limit is achieved. As a rule of thumb, the total system size has to typically be approximately ten times bigger than the most probable cluster size in order to have convergent results, meaning that the equivalent of a Wigner-Seitz cell contains in average \(\approx 10\) dominant clusters. This can be understood considering that at finite temperature the distribution is very large, and the often used single-nucleus approximation [18] is not realistic.

As it can be seen in Fig. 3, the grandcanonical equilibrium prediction for this thermodynamic condition would correspond to a macroscopic liquid fraction in equilibrium with essentially free particles (dashed line). An explicit computation of the coexistence region in the canonical ensemble shows that this is not the case, as the cluster sizes do not scale with the total system size \(A\). As one may notice, this liquid fraction is replaced by a finite, though large, nucleus with a characteristic radius of the order of only \(5 - 10\) fm.

This finding is in agreement with all the theoretical microscopic modelizations which are naturally elaborated inside a single Wigner-Seitz cell within a fixed number of particles [34, 38]. All these canonical studies agree in predicting that matter is clusterized for all subsaturation densities and the cluster size and composition evolve continuously
FIG. 2: Constrained entropy (a), pressure (b),(c) and chemical potential (b)(d) evaluated in the canonical ensemble in the same thermodynamic conditions as in Fig. 1. The pressure and chemical potential discontinuity is indicated by a dotted line.

with the density, which is incompatible with a modelization based on phase coexistence \[40\] where only the relative proportion of the two phases varies through the phase transition.

As it has been argued in Refs. \[16\], the quenching of the phase transition is due to the high electron incompressibility. Because of the charge neutrality constraint over macroscopic distances, an intermediate density solution given by a linear combination of a high density homogeneous region and a low density clustered region would imply an infinite repulsive interaction energy due to the electron density discontinuity at the (macroscopic) interface \[16\].

This argument requires electrons to be completely incompressible. Since the electron incompressibility, while high, is not infinite, it could have been argued that a slightly modified coexistence region should be observed, where the liquid fraction would be constituted by large but still mesoscopic clusters, such that the interface energy would not diverge. The comparison between canonical and grandcanonical shown in Fig. \[1\] \[2\] \[3\] demonstrates that this is not true: the presence of microscopic, instead than macroscopic, fluctuations, qualitatively change both the thermodynamics and the composition of matter.
FIG. 3: Convergence study of the canonical ensemble. The baryonic chemical potential (a), baryonic pressure (b) and cluster multiplicity per unit volume as a function of the cluster size are represented at a representative density inside the ensemble in-equivalence region, by varying the total system size. Thick line in panel (c): cluster multiplicity distribution in the grandcanonical ensemble.

FIG. 4: (a) Cluster distributions as a function of the density in the ensemble in-equivalence region; (b) mass fraction of unclusterized matter as a function of the total baryonic density, in the same thermodynamic conditions as in (a). The dashed line gives the saturation density of nuclear matter.

III. PHENOMENOLOGICAL CONSEQUENCES OF ENSEMBLE IN-EQUIVALENCE

It is important to remark that in the density region where the grandcanonical ensemble is defined, the predictions of the ensembles coincide. The in-equivalence is observed in the intermediate density region, where the grandcanonical first order phase transition is not observed in the canonical ensemble. Since in this density domain the grandcanonical ensemble is not defined, there is no ambiguity on which ensemble should be chosen, meaning that the phenomenology of star matter has to be described with canonical thermodynamics.

A closer look at the cluster distribution in the in-equivalence region can be obtained from the left part of Fig.
which displays the cluster distributions as a function of the density in the ensemble in-equivalence region. We can see that this distribution varies continuously, as it is expected physically, with very heavy nuclei and a very wide size distribution at the highest densities corresponding to the inner crust. These very massive nuclei disappear at a density close to saturation density, which defines the density corresponding to the crust-core transition in the model. This sudden process is at the origin of the non differentiable point observed in the entropy in Fig. 2. The resulting discontinuity in chemical potential and pressure is therefore a physical effect in the framework of this model.

A word of caution is however necessary. It is well known from star matter literature that close to saturation density deformed extended nuclei are energetically favored, the so called ”pasta” phases. We expect that adding a deformation degree of freedom to the cluster energy functional would smooth this discontinuity.

The right part of Fig. 4 represents the mass fraction of unclustered matter (free nucleons and homogeneous dense matter) as a function of the density. Homogeneous matter dominates at the very low densities which physically correspond to the neutron star atmosphere, while clusters become increasingly dominant at higher density, until they melt into the homogeneous liquid core. Even in the absence of a first order phase transition, a very sharp behavior is obtained defining a relatively precise value for the crust-core transition density.

Besides the relevance of the issue of ensemble in-equivalence from the statistical physics viewpoint, it is interesting to remark that the use of grandcanonical thermodnamics can lead to important qualitative and quantitative discrepancies in the computation of different physical quantities of interest for the astrophysical applications. This is demonstrated in Fig. 5 which shows the cluster distribution for a chosen thermodynamic condition (temperature $T = 1.6$ MeV, baryonic density $\rho = 3.3 \cdot 10^{11}$ g cm$^{-3}$, proton fraction $Y_p = 0.41$) which is typical for the dynamics of supernova matter after the bounce and before the propagation of the shock wave. We can see that the dominant cluster size is around $A = 60$, which is a particularly important size in the process of electron capture which determines the composition of the resulting neutron star. It is clear that it is very important to correctly compute the abundances of such nuclei.

Conversely in a grandcanonical formulation, as the widely used nuclear statistical equilibrium (NSE) calculations, these partitions are simply not accessible as they fall in the phase transition region. An approach consisting in taking the metastable grandcanonical prediction and considering only the nuclei of size such that the chosen total density is obtained, as in Ref. 19, is shown by the dashed line in Fig. 5. It is clear that such approach completely misses the correct cluster distribution. Alternatively, hybrid canonical-grandcanonical formulations are routinely used in the astrophysical community. Such approaches do not share the drawback of grandcanonical NSE calculations, but they always introduce artificial Maxwell constructions to fill the high density part of the equation of state. Moreover, they never address the fluctuations in the cluster composition, clusterized matter being modeled by a single representative nucleus. It is clear from Fig. 6 that this approximation is highly questionable at finite temperature, where distributions are wide, the largest cluster does not coincide with the average one nor with the most probable. The model we have presented overcomes all these problems. It is clear that many improvements are still necessary in this model before it can be considered as a reliable quantitative prediction for astrophysical simulations. Both improvements on the cluster energy functional and inclusion of deformation degrees of freedom are in progress to this aim. However we believe that the main results presented in this paper, namely the absence of phase transition due to Coulomb frustration and the dominance of microscopic clusters with a large and continuous distribution of size extending over most of the subsaturation region, are general results which will not change with a more sophisticated model.

**IV. CONCLUSIONS**

To conclude, in this paper we have shown that dense stellar matter as it can be found in core-collapse supernova and in the crust of neutron stars is a macroscopic physical example of ensemble in-equivalence. A first-order phase transition is observed in the grandcanonical ensemble, but when the region corresponding to the discontinuity is explored explicitly constraining the density in the canonical ensemble, the macroscopic dishomogeneities associated to phase coexistence are seen to be replaced by microscopic dishomogeneities leading to cluster formation. As a consequence, the transition observed in the physical system is continuous. This phenomenon is due to the long range Coulombic interactions which quench the phase transition, thus giving rise to a thermodynamics qualitatively similar to the one of finite systems including thermodynamic anomalies. Specifically, the relation between density and chemical potential is non monotonous implying negative susceptibility.

Accounting for this specificity can have sizeable effects in the computation of different quantities of interest for supernova dynamics.

This paper has been partly supported by ANR under the project NEXEN and by IFIN-IN2P3 agreement nr. 07-44.
Ad. R. R acknowledges partial support from the Romanian National Authority for Scientific Research under grant PN-II-ID-PCE-2011-3-0092 and kind hospitality from LPC-Caen.

[1] L. Van Hove, Physica 15 (1949) 951; C.N. Yang and T.D. Lee, Phys. Rev. 87, 404 (1952); K.Huang, Statistical Mechanics, John Wiley and Sons Inc. (1963), chap.15.2 and appendix C.
[2] C. Tsallis, Introduction to Nonextensive Statistical Mechanics: Approaching a Complex World, Springer, NY (2009).
[3] T. Dauxois, S. Ruffo, E. Arimondo and M. Wilkens (eds.), Dynamics and Thermodynamics of Systems With Long Range Interactions, Lect. Notes in Phys.602, Springer (2002); A. Campa, T. Dauxois, S. Ruffo, Phys. Rep. 480, 57 (2009).
[4] P. Chomaz et al., Phys. Rev. Lett. 85, 3587 (2000); D.H.E. Gross, ‘Microcanonical Thermodynamics: Phase Transitions in Finite Systems’, Lecture Notes in Physics, vol. 66, World Scientific (2001).
[5] M. D’Agostino et al., Phys. Lett. B 473, 219 (2000); M. Schmidt et al., Phys. Rev. Lett. 86, 1191 (2001); F. Gobet et al., Phys. Rev. Lett. 89, 183403 (2002).
[6] R. Bachelard et al., Phys. Rev. Lett. 101, 260603 (2008); S. Ruffo, Eur. Phys. J. B 64, 355 (2008).
[7] F. Bouchet and J. Barré, J. Stat. Phys. 118, 1073 (2005).
[8] F. Baldovin and E. Orlandini, Phys. Rev. Lett. 96, 240602 (2006).
[9] S. Gupta, D. Mukamel, Phys. Rev. Lett. 105, 040602 (2010).
[10] F. Gulminelli and Ph. Chomaz, Phys. Rev. E 66, 046108 (2002).
[11] F. S. Kitaura, J. M. Lattimer, J. P. Swesty, F. Douchin, P. Haensel and J. Meyer, Astrophys. J. 650, 345 (2006).
[12] A. Marek and H. Th. Janka, Astrophys. Journ. 694, 664 (2009).
[13] D. Vautherin, Adv. Nucl. Phys. 9, 153 (1996); S. Shlomo and V. M. Kolomietz, Rep. Prog. Phys. 68, 1 (2005); F. Douchin, P. Haensel and J. Meyer, Nucl. Phys. A 665, 419 (2000); A. Rios, Nucl. Phys. A 845, 58 (2010).
[14] J. M. Lattimer and M. Prakash, Science Vol. 304 no. 5670, 536 (2004).
[15] P. Haensel, A.Y. Potekhin, D.G. Yakovlev, ‘Neutron stars: equation of state and structure’, Springer, Berlin (2007).
[16] P. Napiótkowski et al., Phys. Rev. Lett. 98, 131102 (2007); C. Ducoin et al., Phys. Rev. C 75, 065805 (2007).
[17] A. Arcones et al., Phys. Rev. C 78, 015806 (2008).
[18] S. Heckel, P. P. Schneider and A. Sedrakian, Phys. Rev. C 80, 015805 (2009).
