# Phase transitions from nuclei to stars

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## ABSTRACT

In these lectures we review the present status of knowledge of the nuclear thermal as well as quantum phase transitions.

Examples in nuclear physics concern in particular shape transitions, vanishing of pairing correlations at high excitation, nuclear multifragmentation as well as deconfinement to the quark-gluon plasma. For all these phenomena conceptual and formal challenges arise, associated to the definition and classification of phase transitions in finite, open and transient systems. In these lectures we discuss the theoretical methods allowing one to extend the standard formalism of phase transitions to these non-standard situations.

The thermodynamics of phase transitions in nuclei is associated to new physics phenomena, very different to the ordinary macroscopic phase transition behaviors. In particular when non-extensive systems as atomic nuclei are subject to of phase transitions, the different statistical ensembles are not equivalent, meaning that the observed physics depends on the externally applied constraints. In this context we show that an extensive external constraint on the order parameter leads to phase separation quenching as well as to thermodynamic anomalies. Two different applications in nuclear physics are worked out, namely the possible occurrence of negative heat capacity in nuclear multifragmentation, and the phase transition quenching in the core-crust transition of neutron stars.

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## I. INTRODUCTION

Phase transitions are ubiquitous phenomena in nature. In the macroscopic world, they are univocally defined by a qualitative modification of the system properties occurring at well defined values of the control variables, which are typically given by external macroscopic fields. Pressure, temperature, external magnetic or electric fields are standard examples of such fields. If a phase transition occurs, the system response to the applied field shows a sudden change, leading to discontinuities and/or divergences in the associated thermodynamic variables, namely compressibility, heat capacity and susceptibility for the examples given above.

Coming to the microscopic world, it is clear that these concepts cannot be used as such to describe phenomena occurring in an isolated quantum object with a small number of constituents as an atomic nucleus. Yet the notion of phase transition is currently evoked in nuclear physics when addressing the changes of nuclear shape along the isotopic table, the vanishing of pairing correlations at excitation energy overcoming a few MeV, the observation of multifragmentation in heavy ion collisions in the Fermi energy domain, the ephemeral exploration of deconfinement in the ultrarelativistic regime.

The above cited state changes associated to the nuclear phenomenology are very different in nature.

In particular, the concept of a bulk limit can still be invoked in the case of the quark-gluon plasma, for which Lattice QCD predicts a well defined phase diagram with first and second order phase transitions, that can be unambiguously defined with the same theoretical tools which are used for ordinary low temperature matter with atomic and molecular degrees of freedom. It is clear that nuclear collisions are out of equilibrium and transport models have to be developed to connect the experimental observations with the underlying equation of state, but still the observed phenomenology can be considered as an (ephemeral) realization of the new deconfined phase which can be understood in bulk terms. The challenge there is more to extract partonic information out of the final hadronic state, than to compute finite size corrections to thermodynamic variables[1].

From this point of view, the situation is more complex in the case of pairing quenching and fragmentation. In both cases a macroscopic analogue exists: superfluid to normal fluid, and normal fluid to vapour. However the theoretical description of the associated bulk systems (BCS and finite temperature mean field respectively) misses fundamental properties of the nuclear systems which are studied in the laboratory, namely conservation laws and Coulombic interactions. In these conditions, the link between the phenomenology observed in the laboratory and the properties of the different nuclear bulk phases as they can be realized in astrophysical objects as neutron stars, is far from being direct.

The case of shape transitions is again different, because in this case no bulk limit exists in a rigourous sense. In most books or review articles, such phenomena are analyzed in the framework of quantum phase transitions, and as such they are considered as completely different with respect to thermal transitions[2]. However most thermal phase transitions are perfectly defined at zero temperature, meaning that a unified conceptual description of these different phenomena does exist. Indeed the thermodynamic limit is an issue also when studying shape transitions: in the framework of the interacting boson model (IBM) , which is the standard theoretical guideline in this field, the physical number of particles is replaced by a more abstract number of bosons which is requested to fulfill the thermodynamic limit[3].

A detailed quantitative description of these very different phenomena requires the construction of Hamiltonian (or Lagrangian) models adapted to the very different degrees of freedom which are implied, and is far beyond the scope of these lectures. The purpose of this course is to review the generic statistical tools which, when applied to the specific many-body treatment, allow identifying, classifying and characterizing the possible phase transitions in the microscopic nuclear world. As we develop in the next section, this requires the use of some information theory concepts in the framework of quantum statistical mechanics.

## II. THERMAL AND QUANTUM PHASE TRANSITIONS IN MICROSCOPIC PHYSICS

The main well-known characteristics of phase transitions can be introduced from the viewpoint of information theory. This formalization of statistical mechanics allows one to univocally associate phase transitions to non analyticities in the partition sum, which reflects in specific topologic properties of the entropy functional, and leads to a simple definition of first order and continuous transitions. The advantage of this formalism is that, contrary to other thermodynamic tools, partition functions are well defined for any arbitrary number of particles, allowing an extension of the definition of phase transitions to the domain of finite systems[4].

As we will show in this section, quantum and thermal phase transitions can be treated on an equal footing, and this formalism has been successfully applied to the different phase transitions of nuclear matter in the bulk limit.

### A. Concepts and definitions

From a microscopic viewpoint, each realization of a physical system with N degrees of freedom is characterized by a microstate or pure state $|\Psi>$. For complex systems, the exact state is often impossible to define and each realization $(n)$ is associated to a probability $p^{(n)}$. Then, it is preferable to deal with mixed states, or *macrostates*, or *statistical ensembles*, described by the density

$$\hat{D} = \sum_n |\Psi^{(n)} > p^{(n)} < \Psi^{(n)}| \tag{1}$$

Given a set of observables $\hat{A}_l$, that is operators defined on the appropriate Hilbert space, the information which can be associated to the system is the ensemble of observations $< \hat{A}_l >= \sum_n p^{(n)} < \Psi^{(n)}|\hat{A}_l|\Psi^{(n)} >$. If the information is complete at a given time, the same is true at any time, since the dynamical evolution of microstates is governed by a deterministic equation, the Liouville Von Neumann equation.

However in complex systems initial conditions are never known exactly and a solution of the Liouville Von Neumann equation is out of scope, and even redundant. Because of the complexity of the density operator, a complete knowledge of the state of the system (that is: of the ensemble of the $p^{(n)}$) requires only the knowledge of a limited set of pertinent observables.

This lack of information can be quantified by introducing the Shannon entropy[5]

$$S = -\sum_n p^{(n)} \ln p^{(n)} = -Tr\hat{D}\ln\hat{D} \tag{2}$$

Then the set of $p^{(n)}$ giving the optimal state of the system can be computed within a variational approach consisting in the maximization of the Shannon entropy $S$, under the constraint of the pertinent information $\{< \hat{A}_l >\}$. Indeed any other probability distribution would introduce an extra source of information, which contradicts our initial statement that the information on the system is contained in the applied constraints. Conservation laws can also be seen as particular constraints characterized by the fact that the expectation value of the associated operators $\hat{B}_j$ is the same for all microstates, $B_j^{(n)} \equiv < \Psi^{(n)}|\hat{B}_j|\Psi^{(n)} >= B_j \; \forall n$.

The maximization of the entropy under the constraint of the available information is easily done with the Lagrange multipliers technique, giving[4]

$$\hat{D}_{\vec{\alpha},\vec{B}} = \frac{1}{Z_{\vec{\alpha},\vec{B}}} \sum_{\vec{B}^{(n)}=\vec{B}} |\Psi^{(n)} > e^{-\sum_l \alpha_l A_l^{(n)}} < \Psi^{(n)}| \tag{3}$$

where the sum is limited to the microstates satisfying the conservation laws $B_j^{(n)} = B_j \forall j$, and we have introduced the shorthand notation $\vec{B} = \{B_j\}_{j=1,\ldots,m}, \vec{\alpha} = \{\alpha_l\}_{l=1,\ldots,r}$ for the $m$ conservation laws (or *extensive variables*) and the $r$ Lagrange multipliers associated to observables known in average (or *intensive variables*). The normalization of the density matrix is accounted by the definition of the partition sum

$$Z_{\vec{\alpha},\vec{B}} = Tr\{\vec{B}^{(n)} = \vec{B}\} e^{-\sum_l \alpha_l \hat{A}_l} \tag{4}$$

The Shannon entropy associated to the minimum bias or *equilibrium state* can be obtained from the partition sum via a Legendre transform:

$$S_{<\hat{\vec{A}}>,\vec{B}} = \ln Z_{\vec{\alpha},\vec{B}} + \sum_{l=1}^{r} \alpha_l < \hat{A}_l > \tag{5}$$

A special case occurs in the case of divergence of one of the Lagrange parameters, $\overline{\alpha} \to \infty$. In this case $\ln Z$ diverges but the quantity $\lim_{\overline{\alpha} \to \infty} \frac{1}{\overline{\alpha}} \ln Z_{\vec{\alpha},\vec{B}}$ is still defined. For this reason, it is customary to introduce a *thermodynamic potential* $\Omega = \frac{1}{\overline{\alpha}} \ln Z_{\vec{\alpha},\vec{B}}$ which allows addressing all the possible values of the Lagrange $\overline{\alpha}$. There is no principle restriction to the choice of the specific $\overline{\alpha}$ giving the scale of the thermodynamic potential, but because of the special importance of the Hamiltonian operator in physical problems, a wise choice is to choose $\overline{\alpha} = -\beta$, where the inverse temperature $\beta = T^{-1}$ is the conjugate of the Hamiltonian. As we will show in the following, this choice is necessary to recover standard thermodynamics as a limiting case of the information theory approach.

The link between extensive and intensive observables is given by the so-called *equations of state*:

$$\begin{aligned} < \hat{A}_l > &= -\frac{\partial \ln Z_{\vec{\alpha},\vec{B}}}{\partial \alpha_l} && (6) \\ \alpha_l &= \frac{\partial S_{<\hat{\vec{A}}>,\vec{B}}}{\partial < \hat{A}_l >} && (7) \\ \beta_k &= \frac{\partial \ln Z_{\vec{\alpha},\vec{B}}}{\partial B_k} && (8) \end{aligned}$$

Using the Legendre transform eq.(5), the entropy maximization under constraints can equivalently be seen as a minimization of the thermodynamical potential with respect with the imposed observables:

$$\Omega(< \hat{\vec{A}} >, \vec{B}) \equiv \frac{1}{\overline{\alpha}} \ln Z_{\vec{\alpha},\vec{B}} = \frac{1}{\overline{\alpha}} S_{<\hat{\vec{A}}>,\vec{B}} - \sum_{l=1}^{r} \frac{\alpha_l}{\overline{\alpha}} < \hat{A}_l >= min \tag{9}$$

The equilibrium solution can thus be seen as a minimization problem in the multidimensional observables space.

In most physical situations, for a given value of the intensive control parameters, the system properties are univocally defined, that is the conjugated extensive variables have a unique well defined value given by the associated equation of state. Moreover in any finite system the partition sum eq.(4) is a finite sum of exponential functions, that is an analytic (infinitely differentiable) function. This implies that equations of state (6),(7),(8) are continuous analytic functions, meaning that the system properties vary continuously with the control variables.

This is not the case in the presence of a phase transition. The existence of a qualitative change of the bulk system properties at the transition point means that a non-analyticity has to develop in the partition sum. A phase transition can thus be microscopically defined as a non-analyticity (discontinuity or divergence) in at least one of the partial derivatives of the logarithm of the partition sum (or thermodynamic potential ) in the bulk limit, $\lim_{N\to\infty} \partial^n_{\alpha_l} \ln Z$. The order of the derivative where the non-analyticity occurs is defined as the order of the phase transition, and the conjugated observable(s) is (are) the order parameter(s) of the transition.

Specifically, a *first order phase transition* corresponds to a discontinuity in one of the first order derivatives of $\ln Z$. According to eq.(6), this implies a discontinuity or jump in the conjugated extensive variable $< \hat{A} >$ at the transition point $\alpha = \alpha_t$. A phase transition with latent heat (as solid-liquid, or liquid-gas) is an example of a first order phase transition, where energy is the order parameter. It is however important to stress that first order phase transitions are not necessarily associated to a latent heat: to give a single well-known example, a ferromagnetic material below the Curie temperature experiences a magnetization jump passing from positive to negative magnetic field without any discontinuity in the energy density, that is with no latent heat.

Transitions which are not first order are called *continuous*. A particularly interesting case concerns *second order phase transitions* where one of the second order derivatives of the thermodynamic potential respect to an intensive variable diverges. Such transitions exhibit *criticality*, with their universality character and the associated divergence of fluctuations and correlations[6]. Specifically, a second order phase transition associated to a critical point is defined by a divergent generalized susceptibility

$$\lim_{\alpha_l=\alpha_c} \frac{\partial^2 \ln Z_{\vec{\alpha},\vec{B}}}{\partial \alpha_l^2}|_{\alpha_l=\alpha_c} = \infty \tag{10}$$

where the susceptibility is defined as the response of the order parameter to the conjugated external field (see eq.(6))

$$\chi_{\vec{\alpha},\vec{B}} \equiv \frac{\partial^2 \ln Z_{\vec{\alpha},\vec{B}}}{\partial \alpha_l^2} = \frac{\partial < \hat{A}_l >}{\partial \alpha_l} \tag{11}$$

Using the definition eq.(4) of the partition sum it is easy to show that the susceptibility is a measure of the fluctuations of the order parameter

$$\chi_{\vec{\alpha},\vec{B}} == < \left( \hat{A}_l - < \hat{A}_l > \right)^2 > . \tag{12}$$

A second order phase transition is thus characterized by a divergence of the fluctuations of the order parameter. In most physical situations it is useful to consider averages limited to finite portions of space, but large enough such as to have negligible correlations among the different spatial regions. Then fluctuations will also be localized in space, $\sigma_{\hat{A}_l}(\vec{r}) =<$

$\left(< \hat{A}_l(\vec{r}) > - < \hat{A}_l >\right)^2 >$ and we can introduce a correlation function as

$$\chi = \int d\vec{r} \int d\vec{r}' G(\vec{r} - \vec{r}') \tag{13}$$

$$= \int d\vec{r} \int d\vec{r}' \left(< \hat{A}_l(\vec{r}) > - < \hat{A}_l >\right) \left(< \hat{A}_l(\vec{r}') > - < \hat{A}_l >\right). \tag{14}$$

Assuming $G(\vec{s}) \propto \exp(-s/\xi)$, we can see that the correlation length also diverges at the transition point: a critical point is characterized by correlations over all length scales which develop even in systems with short range interactions.

A particularly simple result can be obtained if a series developement of the thermodynamical potential eq.(9) can be done in powers of the order parameter(s) around the transition point. In this case, which is known as the Landau theory[7], the occurrence of a phase transition and its order can be inferred from the sign of the different expansion parameters. Let us take the simplest case of a single scalar order parameter $< \hat{\Phi} >$. If $< \hat{\Phi} >$ is a conservation law, the thermodynamic potential $-T \ln Z_{\vec{\alpha},\hat{\Phi}}$ is already an explicit function of $< \hat{\Phi} >$. If it is known only in average, we can considered the associated constrained entropy obtained via the Legendre transform eq.(9)

$$-\ln Z_{\vec{\alpha},\alpha_\phi} = -S_{\vec{\alpha},<\hat{\Phi}>} + \alpha_\phi < \hat{\Phi} >= \Omega_{\vec{\alpha}}(< \hat{\Phi} >) \tag{15}$$

Then the expansion reads

$$\Omega_{\vec{\alpha}}(< \hat{\Phi} >) = \Omega_0 + A_{\vec{\alpha}} < \hat{\Phi} >^2 + B_{\vec{\alpha}} < \hat{\Phi} >^3 + C_{\vec{\alpha}} < \hat{\Phi} >^4 + \ldots \tag{16}$$

Analyzing the behavior of this function for transitions between a more symmetric ($< \hat{\Phi} >= 0$) and a less symmetric ($< \hat{\Phi} >\neq 0$) phase, it is found that first-order phase transitions form continuous lines in the intensive parameter space, while second-order transitions occur either along continuous lines or at isolated points. The former is the case if the coefficient $B_{\vec{\alpha}}$ vanishes identically for all $\alpha$'s. If this is not so, the conditions for the second-order transition in the simplest case, read as $A_{\vec{\alpha}} = 0$, $B_{\vec{\alpha}} = 0$, and $C_{\vec{\alpha}} > 0$, giving an isolated solution $\vec{\alpha} = \vec{\alpha}_c$.

### B. Thermal versus quantum

One of the appealing characteristics of the microscopic definition of phase transitions based on information theory is that thermal transitions, that is transitions involving excited states, and quantum transitions, that is transitions occurring in the ground state, can be treated on an equal footing.

A standard textbook example of a quantum phase transition is given by interacting spins with an antiferromagnetic interaction in the presence of an external magnetic field $\vec{h}$. Such a system is described by the Heisenberg Hamiltonian

$$\hat{H} = \sum_{i\neq j} J_{ij} \vec{\hat{s}}_i \cdot \vec{\hat{s}}_j - \vec{h} \cdot \sum_i \vec{\hat{s}}_i \tag{17}$$

where $J_{ij} = J$ for a simple constant antiferromagnetic coupling. If we consider a single pair of spins one-half, the thermodynamic potential at zero temperature is readily calculated

$$-\left(T \ln Z\right)_{T=0,h} = -\lim_{\beta\to\infty} \frac{1}{\beta} \ln Tr e^{-\beta \hat{H}} =< \hat{H} >_{GS}= \begin{cases} \hbar^2 J/4 & |\vec{h}| < J/2; \\ -3\hbar^2 J/4 - |\vec{h}| & |\vec{h}| > J/2. \end{cases} \tag{18}$$

Following eq.(6), we can see that this very simple system exhibits a first order phase transition with a magnetization jump at the transition point $h = J/2$, signalling a transformation from a singlet to a fully polarized state. A numerical resolution of the Heisenberg model for the many body case reveals[2] that this singlet-triplet transition towards the thermodynamic limit splits into two transitions with the appearence of an intermediate state characterized by a uniform magnetization parallel to the field and antiferromagnetic order perpendicular to it. It is however interesting to remark that the transition can be unambiguously spotted already from the two-body system.

This simple example shows that there is no principle difference between quantum and thermal phase transitions in the framework of information theory, where temperature is just a Lagrange multiplier among others.

Concerning specific nuclear physics applications, J.Jolie and collaborators[8] have considered quadrupole deformations in the framework of the Interacting Boson Model. Using a standard two-dimensional parametrization of the IBM-1 Hamiltonian:

$$\hat{H}_{\eta,\chi} = c\left(\eta\hat{n}_d + \frac{\eta-1}{N}\hat{Q}_\chi \cdot \hat{Q}_\chi\right) \tag{19}$$

where $\hat{n}_d$ is the d-boson number operator, $\hat{Q}_\chi$ is the quadrupole operator and $N$ stands for the total number of bosons, they have considered a series expansion of the IBM energy functional according to eq.(16) as a function of the deformation parameter $\beta$, using the dimensionless IBM couplings $\eta, \chi$ as intensive control parameters. Using the results from Landau theory described above, they have shown that the IBM exhibits an isolated second order phase transition and three continuous lines of first-order phase transitions and the same must be true for any collective model where the potential can be expanded as in Eq.(16).

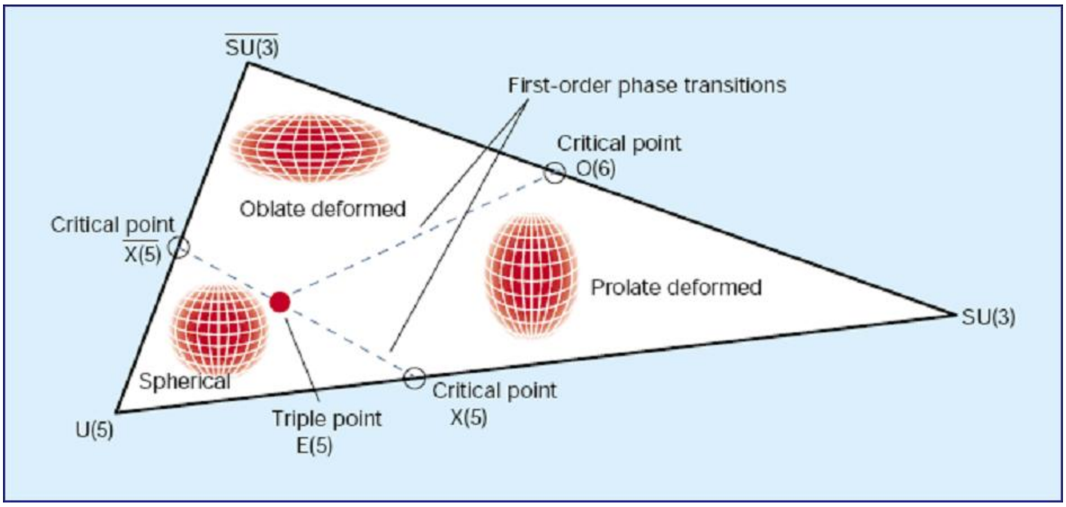

FIG. 1: *The extended Casten triangle of the IBM model and its different phases. The solid dot in the center represents the second-order transition between spherical nuclei (Phase I) and deformed nuclei with prolate (Phase II) and oblate (Phase III) forms. The dashed lines correspond to first-order phase transitions. Figure extracted from ref[8]*

## C. The thermodynamic limit and ensemble equivalence

Thermodynamics is a limiting case of statistical mechanics. Indeed if we consider a macroscopic system $V \to \infty$, and assume that the only pertinent information is given by the energy $\hat{A}_1 = \hat{H}$ and the particle number $\hat{A}_2 = \hat{N}$, we immediately recover the standard textbook thermodynamics in the microcanonical $(V, E, N)$, canonical $(V, T, N)$ and grancanonical $(V, T, \mu)$ ensemble, where $\beta = T^{-1}$ is the conjugate of the energy $E =< \hat{H} >$, and $-\beta\mu$ is the conjugate of the particle number $N =< \hat{N} >$.

Equation (4) shows that in general the thermodynamic potential depends on the applied constraints. This means that in principle the grancanonical $Z_{V,\beta,\mu}$, canonical $Z_{V,\beta,<\hat{N}>}$ and microcanonical $Z_{V,<\hat{H}>,<\hat{N}>}$ partition sums are different functions. However very simple relations between these quantities can be worked out at the thermodynamic limit.

This limit requires that any extensive variable should scale proportionally to the system volume, in particular $\ln Z_{V,\beta,\mu} \to V \ln z_{\beta,\mu}$ and $\ln Z_{V,\beta,<\hat{N}>} \to V \ln z_{\beta,\rho}$ with $\rho = \lim_{V\to\infty} < \hat{N} > /V$. Under the hypothesis of short range interactions, it is possible to show[6, 9] that the relation linking the partition sum to the associated entropy in a given ensemble coincides with the transformation between different ensembles, namely

$$\ln z_{\beta,\rho} = \ln z_{\beta,\mu} - \beta\mu\rho \tag{20}$$

This relation, which is readily generalized to any couple of conjugated variables at the thermodynamic limit ($\ln z_{\epsilon,\rho,\mu} = \ln z_{\beta,\rho,\mu} + \beta\epsilon$, etc), shows that at the thermodynamic limit the different ensembles differ only by linear transformations. Replacing in eqs.(6,7) we can see that identical equations of state are extracted from the two ensembles, leading to the unicity of thermodynamics.

This fundamental property implies that the thermal properties of a system are unically defined from its microscopic structure and do not depend on the externally applied constraints, nor on the type of observation which is made on the system[9]: taking the example of water as a system and energy as an observable, ensemble equivalence implies that the same thermodynamics is observed if water is heated up in a kettle (energy fixed) or inside an oven (temperature fixed).

In the recent years it has however appeared that this fundation principle breaks down in at least two situations: finite systems and long range interactions[10]. In these situations, eq.(20) may be violated and ensemble inequivalence arises. Interesting enough, the dependence of statistical properties on the observations made on the system, that is the emergence of subjectivity in the domain of thermodynamics, is systematically associated to the presence of phase transitions.

As we will show in great detail in the next chapters, both situations occur in nuclear physics, making the study of the atomic nucleus a unique laboratory for thermodynamic anomalies.

### D. Non-standard statistical ensembles

At the thermodynamic limit, the equation of state (6) in the canonical ensemble implies

$$P = \frac{\partial T \ln Z_{V,T,N}}{\partial V} = T \ln z_T(\rho), \tag{21}$$

showing that the thermodynamic potential (with a minus sign) has the physical meaning of a pressure for any finite temperature. At zero temperature it is easy to show that

$$\lim_{\beta\to\infty} \frac{1}{\beta} \ln Tr_\mu e^{-\beta(\hat{H}-\mu\hat{N})} =< H >^c_{GS} (\rho) \tag{22}$$

where the trace is taken with constant $\mu$, and $< H >^c_{GS}$ represents the minimal energy corresponding to the particle density imposed by the chosen $\mu$ constraint. This means that the thermodynamic potential at zero temperature corresponds to the system energy density.

Because of this specific meaning of the equation of state (6) at the thermodynamic limit, in the literature the term "equation of state" is typically reserved to the functional dependence of the pressure (at finite temperature) or of the energy density (at zero temperature) on the particle density.

It is however important to stress that out of the thermodynamic limit and/or in the presence of other constraints, the pressure is just an intensive observable among others, and the tools of statistical mechanics allow one to extend considerably the equilibrium theory out of the standard domain of classical thermodynamics.

Specifically, constraining observables can be defined as any set of operators on the Hilbert space. In standard thermodynamics constraints are typically chosen as conserved variables, that is operators commuting with the Hamiltonian. Particle number and angular momentum (orbital or intrinsic) are standard examples. The use of non-commuting operators and time-odd observables greatly increases the domain of phenomena that can be addressed.

In the following we will consider a few model examples to illustrate the power of description of the present approach.

### *1. The incomplete momentum relaxation ensemble*

Let us first consider a symmetric heavy-ion head-on collision with a too short reaction time to fully relax the incoming momentum.

This typically out-of-equilibrium phenomenon can be studied with the tools of statistical mechanics by introducing the observation of an additional one body state variable, the memory of the initial momenta $< \tau \hat{p}_z >$, where $\hat{p}_z$ is the momentum along the beam axis and $\tau = -1(+1)$ for the particles initially belonging to the target (projectile).

The maximization of the entropy leads to the partition sum of the incomplete momentum relaxation ensemble (IMRE)

$$Z_{\beta,\alpha} = Tr\ e^{\left(-\beta \hat{H} + \alpha \sum_{i=1}^{N} \tau_i \hat{p}_{iz}\right)} \tag{23}$$

where the indice $i$ stands for the $i$-th particle and $N$ is the total (conserved) particle number. $\alpha$ and $\beta$ are the Lagrange multipliers associated to the constraint of the incomplete stopping $< \tau \hat{p}_z >$ and of the total center of mass energy $< \hat{H} >$.

The average kinetic energy per particle is given by a thermal component $< e_{th} >= 3/(2\beta)$ plus a flow $< e_{fl} >= p_0^2/(2m)$ while the equation of states related to $\alpha$ leads to $< \tau \hat{p}_z >= N p_0$. The degree of transparency can be measured from the ratio $< e_{fl} > / < e_{th} >$ which is nothing but the quadrupolar deformation in momentum space, $\Delta p^2/p^2 = (< p_z^2 > - < p_x^2 >)/3 < p_x^2 >$.

In the limit $p_0 = 0$ the IMRE reduces to the usual canonical ensemble while in the general case it can be interpreted as two thermalized sources with a non zero relative velocity $2\vec{p}_0/m$ along the beam axis $\vec{u_z}$. In actual heavy ion experiments the centrality selection criteria imply a sorting of data according to the total deposited energy or to variables which are strongly correlated to it. This means that a total energy conservation has to be implemented to eq.(23). In this case the equations of state are not analytical but can still be numerically evaluated.

To understand the effect of transparency on the evaluation of thermodynamical quantities the Lattice Gas hamiltonian has been used in ref.[11], where occupied sites on a three dimensional cubic lattice interact via a constant attractive closest neighbors coupling $\epsilon$. This simple but numerically solvable model is isomorphous to the ferromagnetic Ising model in the grancanonical ensemble and constitutes therefore a paradigm of standard equilibrium statistical mechanics with first and second order phase transitions. The upper part of Fig. 2 shows the cluster size distributions for a temperature corresponding to the transition temperature in the canonical ensemble, and different degrees of transparency.

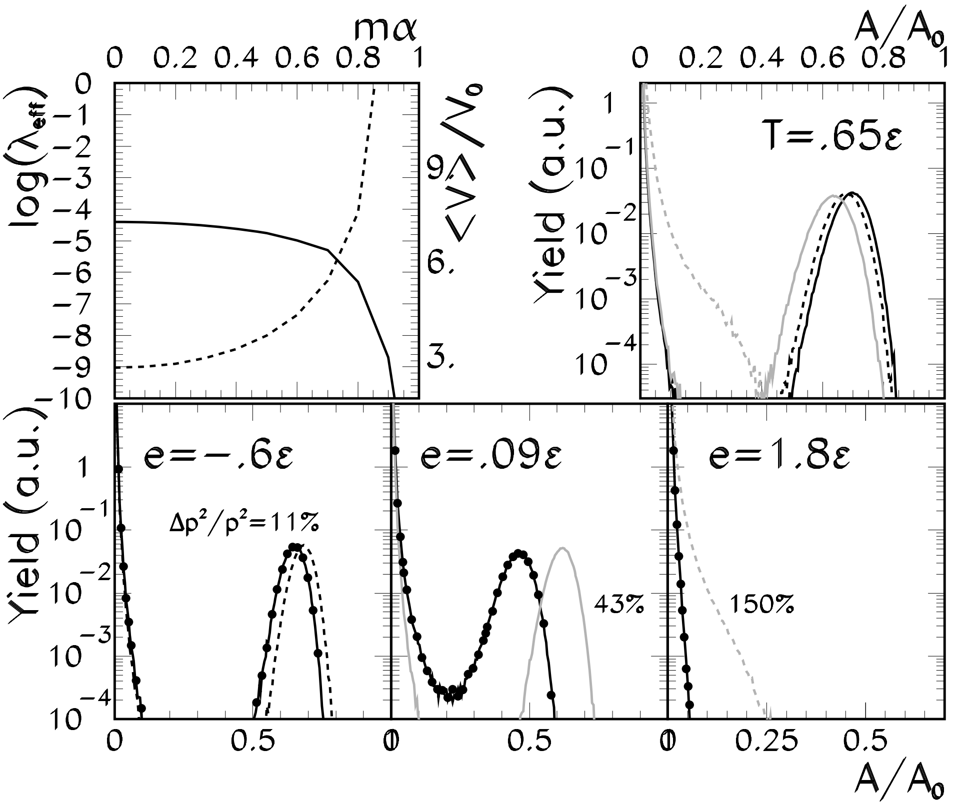

FIG. 2: *Fragment size distributions in the Lattice Gas model with 216 particles. Upper (lower) part: canonical (microcanonical) calculations. Full lines: isotropic momentum distributions. Dashed, dotted and dashed-dotted lines: different degrees of transparency (see text).*

From this illustrative example we can clearly see that partitions are affected by a collective longitudinal component and a higher degree of fragmentation does not necessarily imply higher temperatures but can also be consistent with an increased degree of transparency of the collision. To quantify this statement, the lower part of figure 1 compares the clusters size distributions of the IMRE for different $\Delta p^2/p^2$ with the standard microcanonical ensemble (fixed energy, spherical momentum distribution) at the same total energy. It is clear that thermal agitation is much more effective than transparency to break up the system: at $e = .78\epsilon$ where the microcanonical ensemble predicts a complete vaporization of the system, a residue persists if the non relaxed momentum component is as large as the relaxed one ($\Delta p^2/p^2 = 100\%$).

### *2. The dynamics of the expansion*

An interesting example of a nuclear observable which is not related to a constant of the motion is the collective (radial or elliptic) flow that is observed in high energy heavy ion collisions. We can describe this dynamical situation as an equilibrium with non random directions for velocities which are preferentially oriented in the radial direction. In the information theory formulation this corresponds to the independent observation of the average energy $< E >$ and the average local radial momentum $< p_r(r) >$ . The partition sum reads

$$Z_{\beta,\gamma} = Tr \; e^{\left(-\beta\hat{H}-\sum_{i=1}^{N}\gamma r_i \hat{\vec{p}}\cdot\vec{u}_{r_i}\right)} \tag{24}$$

where $\beta$ the inverse canonical temperature and $\gamma\,(r)$ a local Lagrange multiplier. Imposing in the local equation of state $< p_r >= \partial logZ/\partial\gamma$ that the observed velocity is self-similar $< p_r(r) >= m\alpha r$ we obtain $\gamma(r) = -\beta\alpha r$ which gives for the argument of the exponential in the probability (24)

$$-\beta\sum_{i=1}^{N}\frac{< \left(\hat{\vec{p}}_i - \vec{p}_0(r_i) >\right)^2 >}{2m} + \beta\frac{\alpha^2 m}{2}\sum_{i=1}^{N} < \hat{r}_i^2 > -\beta < \hat{U} > \tag{25}$$

with the local radial momentum $\vec{p}_0(r) = m\alpha r\vec{u}_r$. In the expanding ensemble the total average kinetic energy is the sum of the thermal energy $< e_{th} >= 3/(2\beta)$ and the radial flow $< e_{fl} >= m\alpha^2/2 < R^2 >$. The situation is equivalent to a standard Gibbs equilibrium in the local expanding frame. This scenario is often invoked in the literature to justify the treatment of flow as a collective radial velocity superimposed on thermal motion; however eq.(25)contains also an additional term $\propto r^2$ which corresponds to an outgoing pressure. The probability under flow being the exponential of eq.(25), it diverges at infinity reflecting the trivial dynamical fact that asymptotically particles flow away. This divergence should be cured by introducing an external confining pressure which is not a mathematical artifact but has to be interpreted as a Lagrange multiplier imposing a finite freeze out volume[1]. Eq.(25) has then to be augmented by a term $-\lambda\sum_i r_i^2$ with $\lambda \geq m\alpha^2/2T$ leading to a positive pressure coefficient $\lambda_{eff} = \lambda - m\beta\alpha^2/2$.

We can see that there is a close connection between the two constraints of radial flow and mean square radius.

This can be understood from the general fact that as soon as one of the constraining observables $\hat{A}_\ell$ is not a constant of the motion, the statistical ensemble (3) is not stationary.

In the case of a finite unbound system in the vacuum, as it is the case for a nucleus excited above the particle emission threshold, it is clear that a part of the information has to contain its finite spatial extension. In order to get analytical results, let us consider the simple case of a system of $n = 1, \ldots, N$ free particles in spherical symmetry. Then the minimum bias density matrix associateds to a definite value for the mean square radius $< \hat{\vec{R}}^2 >= \sum_n < \hat{\vec{r}}_n^2 >$ :

$$\hat{D}_{\beta\lambda_0} = \frac{1}{Z_{\beta\lambda_0}}\exp -\beta\sum_{n=1}^{N}\left(\frac{\hat{\vec{p}}_n^2}{2m} + \frac{\lambda_0}{\beta}\hat{\vec{r}}_n^2\right) \tag{26}$$

is not a stationary solution of the dynamics. The Liouville Von Neumann equation for the density matrix

$$\partial_t\hat{D} = \frac{1}{i\hbar}\left[\hat{H},\hat{D}\right] \tag{27}$$

in this specific very simple case can be analytically solved with eq.(26) as initial condition giving

$$\hat{D}_{\beta,\lambda_0}(t) = \frac{1}{Z_{\beta,\lambda_0}}\exp\sum_n -\beta_{eff}\,(t)\,\frac{\hat{\vec{p}}_n^2}{2m} - \lambda_0\hat{\vec{r}}_n^2 + \frac{\nu_0\,(t)}{2}\left(\hat{\vec{p}}_n\cdot\hat{\vec{r}}_n + \hat{\vec{r}}_n\cdot\hat{\vec{p}}_n\right), \tag{28}$$

with

$$\beta_{eff}(t) = \beta + 2\lambda_0 (t - t_0)^2 / m \;\; ; \;\; \nu_0(t) = 2\lambda_0 (t - t_0)/m. \tag{29}$$

which is nothing but the statistical ensemble with radial flow. This remarkable result stems from the fact that the observables $\hat{\vec{r}}^2$, $\hat{\vec{p}}^2$, $\hat{\vec{r}} \cdot \hat{\vec{p}} + \hat{\vec{p}} \cdot \hat{\vec{r}}$. form a closed Lie algebra, implying that the exact evolution of (28) preserves it algebraic structure[12].

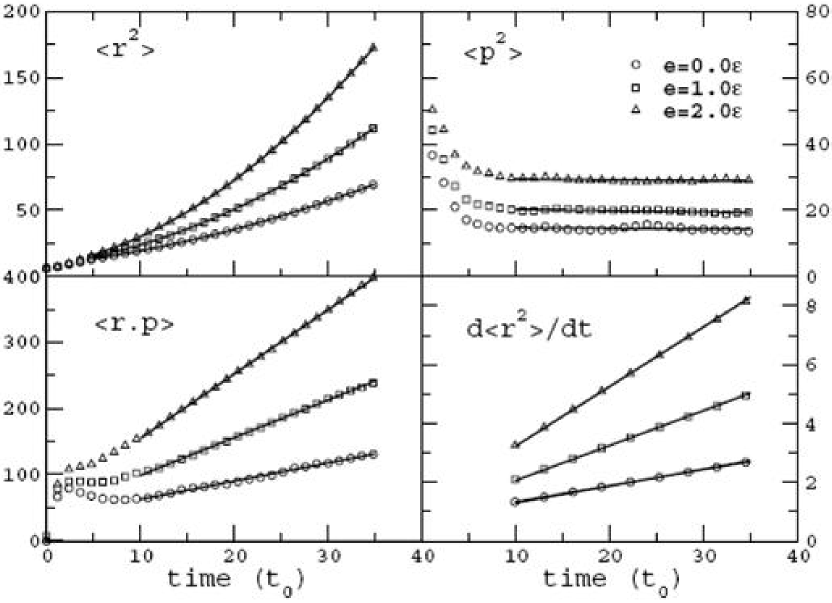

FIG. 3: Time evolution of $< R^2 >$, $< P^2 >$ and $< R \cdot P >$ for an initially constrained Lennard Jones system of 147 particles freely expanding in the vacuum, at different total energies. Lower right: expansion dynamics (symbols) compared to the prediction of eq.(28) (lines). Figure taken from ref.[13].

An illustration of the predictive power of the collective flow statistical ensemble is given in Figure 3[13] in the framework of classical molecular dynamics. A Lennard Jones system is initially confined in a small volume and successively freely expanding in the vacuum. We can see that after a first phase of the order of $\approx 10$ Lennard Jones time units, where interparticle interactions cannot be neglected, the time evolution predicted by eq.(28) is remarkably fulfilled for all total energies. This result is due to the fact that the system's size and dynamics are dominated by the free particles.

### *3. Heterogeneous energy components and frustration*

Even if the Hamiltonian is a very pertinent operator in the study of any physical system, it is perfectly conceivable to construct an equilibrium theory which does not contain this operator as a constraint, that is where the concept itself of temperature (the Lagrange conjugate of energy) is ill-defined.

An interesting application concerns systems subject to interactions depending on different couplings. We have already mentioned the study of quantum phase transitions in the framework of the IBM model, where the variable strength of the different couplings is supposed to reflect the variation of the effective interaction along the isotopic chains. A general

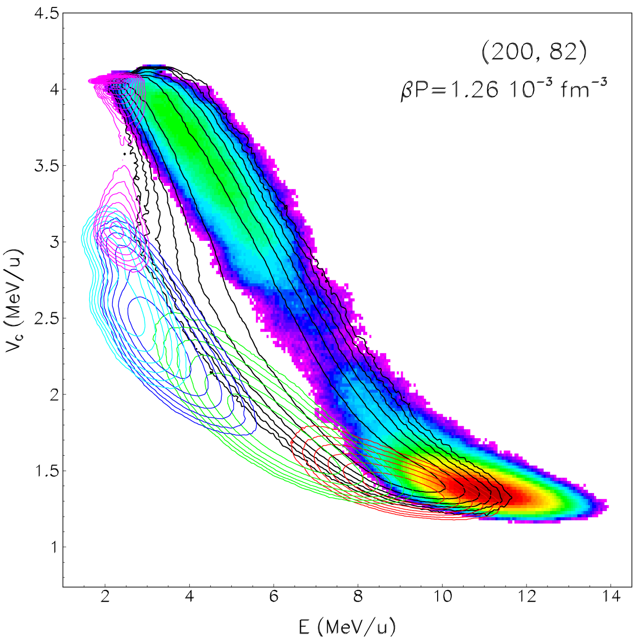

FIG. 4: *Event distribution of the SMM model in the Coulomb energy versus total energy plane for a finite nucleus of atomic number $Z = 82$ in the multi-canonical ensemble. Contour plots: uncharged system $\beta_C = 0$; contour lines: charged system $\beta_C = \beta_N$ with different values of $\beta_N$. Figure taken from ref.[16].*

formalization of this idea concerns the study of frustration. Frustration occurs in condensed matter physics whenever interactions with opposite signs act on a comparable lenght scales; applications range from magnetic systems to liquid crystals, from spin glasses to protein folding[14]. Applications of frustration in nuclear physics are given by the multifragmentation observed in violent ion collisions, and by the emergence of complex dishomogeneous phases in high density neutron star matter[15].

The statistical tool to deal with frustrated systems is given by the multi-canonical ensemble[16]. Writing $\hat{H} = \hat{H}_N + \hat{H}_C$, the two energy components $E_N =< \hat{H}_N >$,$E_C =< \hat{H}_C >$ are treated as two independent observables associated to two Lagrange multipliers $\beta_N, \beta_C$. A generalized canonical potential is defined by

$$Z_{\beta_N,\beta_C,\alpha,\vec{N}} = Tr_{<\vec{N}>} e^{\left(-\beta_N \hat{H}_N - \beta_C \hat{H}_C\right)}. \tag{30}$$

If $E_C$ represents the Coulomb energy and $E_N$ the nuclear term, the choice $\beta_C = \beta_N$ gives the usual (grand)canonical thermodynamics for charged systems, $\beta_C = 0$ leads to the uncharged thermodynamics, while all intermediate values $0 < \beta_C < \beta_N$ correspond to interpolating ensembles, or equivalently to physical systems with an effective charge $(q_{eff}/q_0)^2 = \beta_C/\beta_N$. The multi(grand)canonical ensemble allows one to construct a single unified phase diagram for neutral and charged matter, and is therefore an ideal statistical tool to make some connections between the idealized nuclear matter model and physical charged system, as finite nuclei or stellar matter.

As an example let us consider the phenomenon of multifragmentation as modelized in the Statistical Multifragmentation Model[16]. The event distribution in the multi-canonical ensemble eq.(30) is represented in Figure 4 for a value $\beta_N$ corresponding to the transition temperature for the uncharged case. As we will better formalize in the next section, the first order phase transition gives rise to a two peaked distribution in the (multi)canonical ensemble, representing the two coexisting phases. The direction separating the two peaks can be taken as a definition of the order parameter of the transition, and the zone between the two peaks can be identified to the spinodal region. From Fig.4 we can see that when the Coulomb effect becomes important, the spinodal region pertinent to the neutral matter liquid-gas phase transition is not explored by the charged system and the phase transition becomes a cross-over.

## III. PHASE TRANSITIONS IN FINITE NUCLEI

The study of phase transitions in the laboratory opens the important challenge of the definition of a phase transition in a finite system.

### A. Transition rounding

We have seen in the previous chapter that a phase transition can be recognized from a non-analyticity of the partition sum. In the case of commuting operators this latter is defined as

$$Z_{\vec{\alpha},\vec{B}} = \sum_n \delta\left(\vec{B}^{(n)} - \vec{B}\right) e^{-\sum_l \alpha_l A_l^{(n)}} \tag{31}$$

where the sum runs over microstates and $A_l^{(n)} =< \psi^{(n)}|\hat{A}_l|\psi^{(n)} >$, $B_j^{(n)} =< \psi^{(n)}|\hat{B}_j|\psi^{(n)} >$. If the number of microstates is finite, as in a finite closed system, the partition sum is thus a sum of exponentials, that is a continuous infinitely differentiable function which does not present any non-analyticity. Such non-analyticities can only develop in the bulk limit, when because of the infinite number of microstates the finite sum is transformed into a series. Because of that, it is generally stated in the literature[6] that phase transitions are only defined at the bulk limit.

We have seen in the previous chapter that exceptions to this general statement exist. The first situation concerns the case where one of the constraining Lagrange diverges, $\lambda_l \to \infty$. In this case $\ln Z$ diverges but the thermodynamic potential $\lim_{\lambda_l\to\infty} \frac{1}{\lambda_l} \ln Z_{\vec{\alpha},\vec{B}}$ is still defined. We have explicitly worked out the case of quantum phase transitions and shown that in this case, because of the $T \to 0$ limit, the thermodynamic potential may develop discontinuous derivatives even for systems with only two possible microstates. This means that quantum phase transitions do not need the bulk limit to be defined. This reasoning is however restricted to first order phase transitions, characterized by a jump in the order parameter. A second order phase transition associated to a critical point is defined by divergent fluctuations of the order parameter, see eq.(12) or spatial correlations over infinite length scales, see eq.(14), while these quantities in a finite system will necessarily stay finite and the concern about the thermodynamic limit will persist.

In the domain of thermal phase transitions, where all constraints are finite, the occurrence of non-analyticities requires eq.(31) to be an infinite series. In principle this can perfectly occur within a finite system if this latter is an open system. This is generally the case of all systems presenting a continuum spectrum, and nuclei are no exception. However the presence of a continuum spectrum is not sufficient to allow the appearence of non-analyticities, as we now show. A continuum spectrum in quantum physics is associated to high energies, and if the energy is high enough the classical limit may be employed. The canonical partition sum of a system of $N$ classical particles reads

$$Z_{\beta,N} = \int d\vec{r}_1 \dots d\vec{r}_N d\vec{p}_1 \dots d\vec{p}_N \exp -\beta \left( \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j} v(|\vec{r}_i - \vec{r}_j|) \right) \tag{32}$$

The integrals in configuration space are limited by the finite range of the interaction, but the same is not true for the kinetic term, meaning that the number of microstates is indeed infinite even in a finite system. However in the absence of momentum dependent interactions, position and momentum space are completely decoupled giving

$$-T \ln Z_{\beta,N} = -T \left( \int d\vec{p} \exp -\beta \frac{p^2}{2m} \right) - T \ln Z_{\beta,N}^{conf} \tag{33}$$

where $Z_{\beta,N}^{conf}$ contains all the information about the interparticle interactions. The first term in eq.(33) coincides with the thermodynamic potential of an ideal Boltzmann gas, meaning that the possible occurrence of a phase transition should be only ascribed to $Z_{\beta,N}^{conf}$, which can develop non-analyticities only in the $N \to \infty$ limit.

This demonstration shows that in physical situations one should expect that the thermodynamic definition of phase transitions and critical phenomena will not apply in finite systems.

An example is given in Fig.5, which gives the measured energy and heat capacity of a finite $Na$ cluster as a function of the temperature, compared to the bulk expectation of a solid to liquid phase transition for $Na$[17]. We can see that not only the transition point is shifted due to finite size effects, but that the bulk discontinuity is replaced by a smooth behavior which makes the phenomenon difficult to distinguish from a cross-over. This phenomenon is called *transition rounding.*

The extra complication in nuclear physics applications is that, contrary to condensed matter physics, the bulk behavior is not directly accessible. This means that it appears very important to develop a formal framework to describe phase transitions in finite systems.

### B. Yang-Lee zeroes

The definition of phase transitions in finite systems may be achieved using a fundation theorem in statistical mechanics, the Yang-Lee theorem[18]. This theorem relates the occurrence of phase transitions to the presence of zeroes in the partition sum at the thermodynamic limit.

Let us consider a phase transition concerning a single scalar real order parameter $A =< \hat{A} >$ and its associated Lagrange $\alpha$. For simplicity we will omit the dependence on the other observables and write as a shorthand notation for the partition sum of the finite system composed of $N =< \hat{N} >$ particles $Z(\alpha)$. We will refer to this partition sum as to the *canonical ensemble*, though $\alpha$ does not necessarily represent an inverse temperature.

As we have discussed in the previous section, the canonical partition sum of a finite system must be positive and finite for any value of $\alpha$. Indeed a divergence or a zero of $Z(\alpha)$ would imply a divergence of the thermodynamic potential, which cannot occur in a finite system (within the exceptions discussed above). However it is clear that if we consider an analytic continuation of $Z(\alpha)$ in the complex plane, this function, though still finite, can have zeroes anywhere out of the real axis.

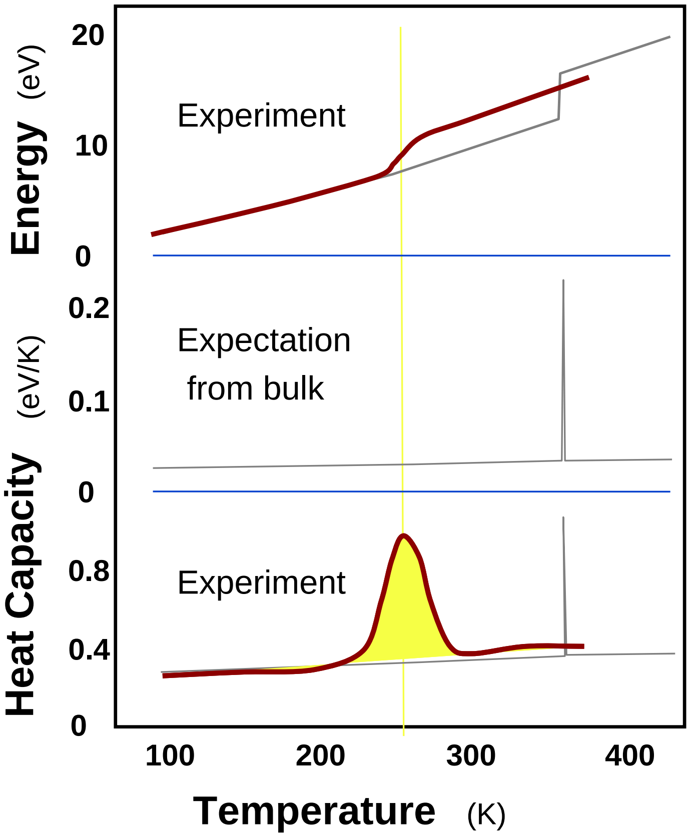

FIG. 5: *Energy (upper part) and heat capcity (lower part) as a function of the temperature, measured from the melting of a Na cluster composed of 139 atoms, in comparison with the expactation from the melting transition. Figure adapted from ref.[17].*

The Yang-Lee theorem[18] states that a phase transition occurs when a complex zero in the finite system partition sum falls onto the real axis in the thermodynamic limit. Specifically, a first order phase transition corresponds to a distribution of zeroes for the partition sum of the finite system of size $N$, that asymptotically forms a line parallel to the imaginary axis and cuts across the real axis with a density increasing with the number of particles of the system, leading to a vanishing imaginary part for $N \to \infty$ (and consequently to a non-analyticity at a definite real value of $\alpha$). This theorem has been extended to transitions of arbitrary orders by P.Borrmann et al[19].

Introducing a complex Lagrange as $\gamma = \alpha + i\lambda$, the partition function can be expanded in terms of zeroes using the Weierstrass theorem:

$$Z(\gamma) = C \prod_i \left(1 - \frac{\gamma}{\gamma_i}\right)\left(1 - \frac{\gamma}{\gamma_i^*}\right) \tag{34}$$

The zeroes in the partition function will appear as poles in thermodynamic variables; for instance the order parameter eq.(6) reads

$$A(\gamma) = \sum_i \left(\frac{1}{\gamma_i - \alpha} + \frac{1}{\gamma_i^* - \alpha}\right) \tag{35}$$

while the susceptibility eq.(11) results

$$\chi(\gamma) = \sum_i \left( \frac{1}{(\gamma_i - \alpha)^2} + \frac{1}{(\gamma_i^* - \alpha)^2} \right), \tag{36}$$

and more generally we have $d^k(\ln Z)/d\alpha^k \approx \sum_i (\gamma_i^* - \alpha)^{-k}$. The classification of phase transitions can thus be extended to a finite system by considering how the branch of zeroes approach the real axis. By labeling the zeroes starting from the closest one to real axis, the crossing angle can be given as

$$\nu = arctan \frac{\alpha_2 - \alpha_1}{\lambda_2 - \lambda_1}. \tag{37}$$

An exponent $a$ giving the speed at which the real axis is reached is defined by $|\gamma_{i+1} - \gamma_i| \approx \lambda_i^{-a}$. The first order phase transition corresponds to a vertical uniform approach of poles $\nu = 0, a = 0$. $0 < a < 1$ is associated to second order phase transitions while the transition is of higher order if $a > 1$.

This classification scheme has been recently used to analyze the pairing transition in nuclear physics[20]. A simplified pairing Hamiltonian is introduced as

$$\hat{H} = 2 \sum_i \epsilon_i \hat{n}_i + \sum_{i,j} G_{ij} \hat{p}_i^+ \hat{p}_j \tag{38}$$

where $\hat{p}^+$ is a pair creation operator, $\hat{n}$ is a number operator, the summation runs over pair-orbitals, $\epsilon_i$ are single-particle energies and $G_{ij}$ determines the strength of pair scattering.

The resulting phase diagram as a function of temperature and constant pairing strength $G$ is shown in Figure 6 for a half occupied 12 level ladder system constituted of $N = 12$ particles and corresponding to a maximal occupancy of 24. Though the order parameter, given by the fraction of paired particles, is a continuously varying function of the intensive constraints, the performed analysis through Yang Lee zeroes allows one to localize a second order phase transition for sufficiently high pairing interaction. This study confirms that the pairing transition is the finite system counterpart of superfluid-normal fluid transition as described by the BCS theory.

### C. Bimodality

The distribution of zeroes in the complex Lagrange parameter plane presented in the last section is a very powerful tool to identify and characterize phase transitions in finite systems, but the fact that by definition such analysis can only be applied to a model is a very important drawback of the method. Indeed, the possibility of associating a phase transition to a given phenomenology is dependent on the model used to describe the phenomenon and cannot be directly inferred from experimental data.

A step forward can be achieved in the case of first order phase transitions, that is transitions presenting a discontinuity of the order parameter at the transition point. In this case, it is possible to demonstrate[21] that the specific distribution of complex zeroes associated to first order transitions is connected to a measurable property of the system, namely the probability distribution of the order parameter. Specifically, equidistant zeroes on the imaginary axis are equivalent to a bimodal distribution of the order parameter.

To simplify notations, we will consider as in the previous section a single intensive observable $\alpha$ conjugated to the order parameter $< \hat{A} >$. It is then easy to see that a two-peaked probability distribution for the order parameter corresponds to a partition sum fulfilling the Yang-Lee theorem in the thermodynamic limit, as we now show.

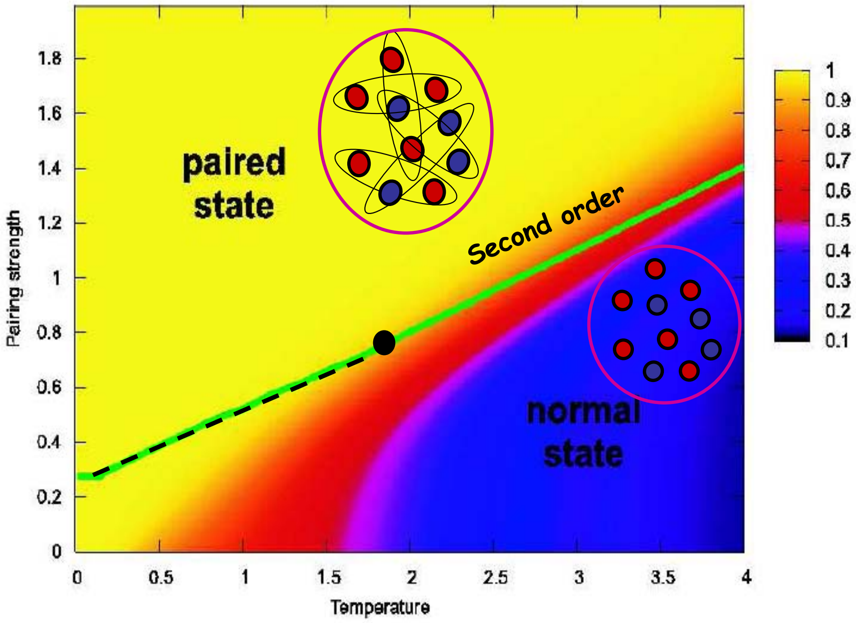

FIG. 6: *Fraction of paired particles (color code) in the plane given by temperature and pairing strength for a half occupied 12 level ladder system evaluated from an exact solution of the pairing Hamiltonian. The line gives the position of the phase transition as deduced from the analysis of Yang-Lee zeroes. Figure adapted from ref.[20].*

It is always possible to express the partition sum as an integral

$$Z_\alpha = \sum_n \exp -\alpha A^{(n)} = \int dA W(A) \exp -\beta A \tag{39}$$

where $A \equiv < \hat{A} >$ and we have introduced the density of states $W(A) = \sum_n \delta(A - A^{(n)})$ The distribution of the order parameter reads

$$P_\alpha(A) = \frac{1}{Z_\alpha} \int dA W(A) \exp -\beta A \tag{40}$$

We can thus see that the partition sum for a complex parameter $\gamma = \alpha + i\lambda$ is nothing but the Laplace transformation of the probability distribution $P_{\alpha_0}(A)$ for any arbitrary parameter $\alpha_0$

$$Z_\gamma = \int dA Z_{\alpha_0} P_{\alpha_0}(A) \exp - (\gamma - \alpha_0) A = \int dA p_\alpha(A) \exp -i\lambda A \tag{41}$$

where we have defined a non normalized distribution $p_\alpha = Z_\alpha P_\alpha$. In order to study the thermodynamic limit, if $p_\alpha$ is a standard distribution presenting a single maximum we can use a saddle point approximation around the maximum $\overline{A}$ giving $Z_\gamma = \exp \phi_\gamma \left(\overline{A}\right)$, with

$$\phi_\gamma(A) = \ln p_\alpha(A) - i\lambda A + \frac{1}{2}\eta^2\sigma^2(A) + \frac{1}{2}\ln\left(2\pi\sigma^2(A)\right) \tag{42}$$

where $1/\sigma^2 = -\partial_A^2 \ln p_\alpha(A)$. This equation does not admit any zeroes, showing that a normal distribution for the order parameter is not compatible with a phase transition, whatever its order.

The interesting case corresponds to a density of states which is not everywhere concave. Then it exists a range of $\alpha$ for which the equation $\partial_A \ln P_{\alpha_t}(A) - (\alpha - \alpha_t) = 0$ has three solutions, $A_1, A_2$ and $A_3$. Two of these extrema are maxima so that we can use a double saddle point approximation

$$Z_\gamma = \exp\phi_\gamma(A_1) + \exp\phi_\gamma(A_3) = 2\exp\phi_\gamma^+ cosh\left(\phi_\gamma^-\right) \tag{43}$$

where $2\phi_\gamma^+ = \phi_\gamma(A_1) + \phi_\gamma(A_3)$ and $2\phi_\gamma^- = \phi_\gamma(A_1) - \phi_\gamma(A_3)$. The zeroes of $Z_\gamma$ then correspond to $2\phi_\gamma^- = i(2n+1)\pi$. The imaginary part is given by $\lambda = (2n+1)\pi/(A_3 - A_1)$ while for the real part we should solve the equation $\Re\left(\phi_\gamma^-\right) = 0$. In particular, close to the real axis this equation defines a value of $\alpha = \alpha_t$ which can be taken as the transition point. If the order parameter scales with the number of particles $A \propto N$, then the loci of zeroes corresponds to a line perpendicular to the real axis with a uniform distribution, as expected for a first order phase transition. It is also possible[21] to demonstrate the necessary condition showing that a uniform distribution of zeroes perpendicular to the real axis with the density linearly increasing with the number of particles implies within the same hypotheses a bimodal probability distribution.

This demonstration implies that first order phase transitions in finite systems can be inferred directly from experimental data without any model calculation. Indeed any variable which is collective enough to fulfill an asymptotic scaling with the total number of particles, and which exhibits a two-hamped distribution can be recognized as an order parameter following the Yang-Lee theorem at the thermodynamic limit.

We have already given a theoretical example of the bimodal behavior of the order parameter distribution in a finite system in the calculation displayed in Fig.4. A spectacular confirmation of this theory has been observed[22] for the metallic cluster melting. A measurement of the energy distribution after thermalization with an helium bath has revealed a bimodal shape at the temperature corresponding to the solid-liquid transition (see Figure 5 ) rounded by finite size effects.

### D. Multidimensional order parameters

In the previous section we have considered a single order parameter $A$ together with its associated Lagrange $\alpha$. The prototype of such a situation is the canonical ensemble. Then, the phase transition can be univocally recognized studying the curvature properties of the density of states[23]. Indeed from eq.(40) we can immediately see that a bimodality in the canonical energy distribution is exactly equivalent to a convex intruder in the microcanonical entropy $S = \log W$, which leads to the well known microcanonical negative heat capacity[23, 24].

Let us now consider the case of a second observable $B = \langle\hat{B}\rangle$. If both $A$ and $B$ are order parameters, and the transition is first order, the two-dimensional probability distribution $p(A, B)$ should be bimodal in both the $A$ and the $B$ direction within the ensemble where the observables are fixed by the conjugated Lagrange multipliers $\alpha, \beta$ :

$$p_{\alpha,\beta}(A, B) = W(A, B)\exp(-\alpha A - \beta B)Z_{\alpha,\beta}^{-1} \tag{44}$$

All conservation laws on other variables are implicitly accounted in the definition of the density of states $W$. The search for bimodalities can only be done in this extended canonical ensemble, and is exactly equivalent to the study of the curvature matrix of the entropy in the two-dimensional observable space

$$C = \begin{pmatrix} \partial^2 S/\partial A^2 & \partial^2 S/\partial A \partial B \\ \partial^2 S/\partial B \partial A & \partial^2 S/\partial B^2 \end{pmatrix} \tag{45}$$

If this curvature matrix has two positive eigen-values, this means that and $A$ and $B$ are associated to two independent order parameters. In the case of a one-dimensional order parameter, only one eigen-value is positive, and the associated eigen-vector can be taken as the "'best"' order parameter. It is the linear combination of the $A$ and $B$ observables, which gives the best separation of the two phases in the two-dimensional space.

Concerning nuclear physics applications, several works have reported bimodal behaviors of different observables in the energy regime corresponding to multifragmentation[25]. The order parameter of fragmentation transitions is typically the size of the heaviest cluster (or its atomic number $Z$), and in principle any observable correlated with it may play the role of an order parameter. However for these nuclear collision data an extra complication arises. Indeed it is experimentally well established that $Z$ is strongly correlated with the deposited energy $E$, meaning that if $Z$ is an order parameter, energy will be an order parameter too, or in other words the transition will have a latent heat. This means that a study of bimodality should be done in the ensemble defined by eq.(44), that is it would require to dispose of a nuclear sample in canonical equilibrium ($\beta$ and $\alpha$ fixed). Concerning the constraint $\alpha$ on $Z$, there is no reason to believe that the collision dynamics or the data treatment induces a specific constraint on the size of the largest cluster, other than the total mass and charge conservation, which are already implemented in the definition of the state density. This means that we can consider $\alpha = 0$. Conversely the distribution of the deposited energy in a nuclear collision crucially depends on the entrance channel dynamics and data selection criteria and it cannot be considered as canonical.

In the case of quasi-projectile events selected in heavy ion collisions, the energy distribution is very large, and is determined by the impact parameter geometry and dissipation dynamics. If events are sorted in centrality bins, the distribution is centered on a well defined value given by the average dissipation at the considered impact parameter, but the distribution has a finite width that depends in a non-controlled way on the selection criteria. The statistical ensemble describing multi-fragmentation data is thus neither canonical nor microcanonical, and should rather be described in terms of the gaussian ensemble[26], which gives a continuous interpolation between canonical and microcanonical. Because of the correlation between $E$ and $Z$ $W(E,Z) \neq W_E(E) W_Z(Z)$, and the distribution of energy will affect also the distribution of $Z$, meaning that the concavity of the $Z$ distribution will not be univocally linked to the concavity of the entropy, and the presence (or absence) of the bimodality signal may depend on the experimental sorting conditions.

It is however important to note that if the energy distribution cannot be experimentally controlled, it can be - at least approximately - a-posteriori measured. This means that it is possible to unfold from the experimental distribution the contribution of the entropy, giving the phase properties of the system, and the contribution of the energy distribution, which depends on the collision dynamics. Indeed, as long as no explicit bias acts on the $Z$ variable, the experimental distribution can be calculated from the canonical one eq.(44) by a simple reweighting of the probabilities associated to each deposited energy

$$p_{exp}(E,Z) = p_\beta(E,Z) \frac{p_{exp}(E)}{p_\beta(E)} \tag{46}$$

where $p_{exp}(E)$ is the measured energy distribution. This reiweighting method has been successsfully applied to multifragmentation data in refs.[27, 28] as shown in Figure 7. A clear indication of bimodality in the decay pattern is observed. This behavior appears to be

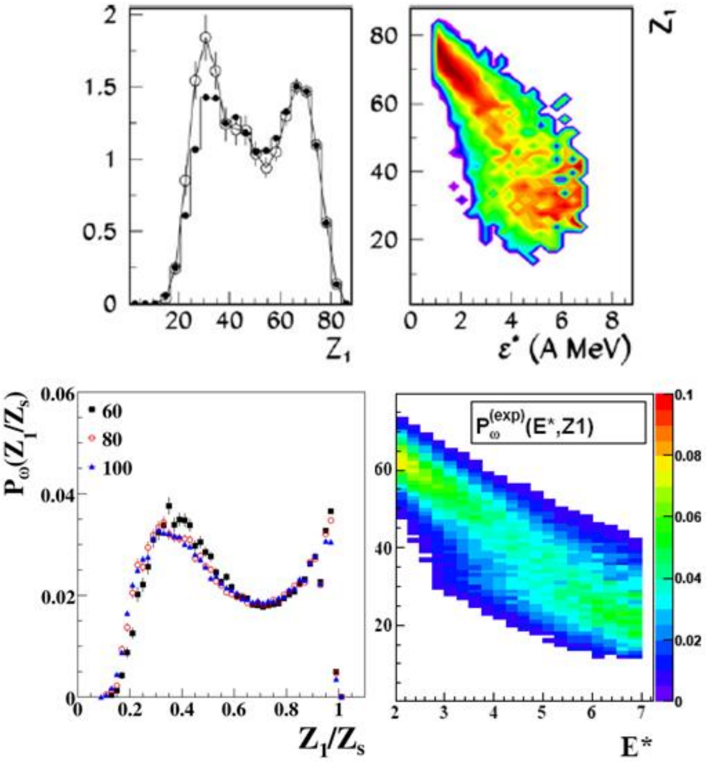

FIG. 7: *Left side: distribution of the atomic number of the largest fragment detected in the decay of a Au source produced in Au+Au collisions, normalized to the charge of the source. Right side: correlation between the largest fragment charge and the deposited energy. Upper panels: MULTICS data at 32 A.MeV from ref.[27]. Lower panels: INDRA data at 60,80 and 100 A.MeV from ref.[28]. All distributions have been normalized to have the same statistics in each excitation energy bin.*

robust against the selection method, the entrance channel dynamics and the estimator of the deposited excitation energy. These analyses support the interpretation of the discontinuity already observed in the decay pattern[25] as the finite system counterpart of a first order phase transition with finite latent heat.

### E. Ensemble Inequivalence

An interesting consequence of the results presented in the previous sections is that the different ensembles do not lead to the same thermodynamics in finite systems subject to a first order phase transition, that is thermal properties are not intrinsic properties of the systems but depend on the applied constraints, or in other words on their information content.

To illustrate this, let us take the textbook example of the relation between the canonical and microcanonical ensemble. The associated partition sums read

$$\begin{aligned} Z_\beta &= Tr \exp -\beta \hat{H} = \int dE W(E) \exp -\beta E; \quad (47) \\ Z_E &= Tr\{E^{(n)} = E\}\hat{I} = W(E) \quad (48) \end{aligned}$$

We can see that the relation between the two ensemble is an integral Laplace transform. If $S(E) \equiv \ln W$ is a concave function, at the thermodynamic limit all observables scale with the particle number $E(N) = Ne, S(N,E) = Ns(e)$ and the integrand function $f(e,N) \equiv \exp N(s - \beta e) \to \delta(e - e_0)$ where $e_0$ is defined by $\beta = ds/de|_{e_0}$. This means that the Laplace transform can be approximated with a linear Legendre transform

$$\ln z_\beta \approx s(e_0) - \beta e_0 \quad (49)$$

As a consequence, the relation between energy and temperature in the canonical ensemble eq.(7)

$$\beta = \frac{ds_\beta}{de_0} \quad (50)$$

is the same as in the microcanonical one at the energy $e_0$

$$\frac{1}{T} = \frac{ds}{de}|_{e=e_0}. \quad (51)$$

On the other hand, a bimodal energy distribution in the canonical ensemble

$$P_\beta(E) = Z_\beta^{-1} W(E) \exp -\beta E \quad (52)$$

implies a convexity in the underlying microcanonical entropy $S = \ln W$. Because of that, the approximation (49) is not adequate and ensemble inequivalence arises. In particular the microcanonical heat capacity from eq.(51) $c = T^{-2} d^2 s/de^2$ is negative in the convexity region, while the same quantity in the canonical ensemble is linked to the energy fluctuation $\sigma^2(e)$ by

$$c_\beta = \beta^2 \frac{d^2 \ln z_\beta}{d\beta^2} = \beta^2 \sigma^2(e) \quad (53)$$

that is, it is a positively definite quantity. This remarkable property of ensemble inequivalence in first order phase transitions of finite systems, with the associated abnormal thermodynamics including negative heat capacity, has suscitated a great interest in the literature[22–25, 29, 30]. Unfortunately a direct verification in nuclear physics requires the availability of experimental samples in thermal equilibrium, which is very difficult to prove experimentally[31] as well as a very precise evaluation of fluctuations. This is why the observation of negative heat capacity in nuclear multifragmentation[29] relies on different hypothesis in the data analysis procedure. For the moment, though many circumstantial evidences of the phenomenon have been proposed, it has not be possible to prove the actual measurement of negative heat capacity in a model independent way.

## IV. APPLICATIONS TO STAR MATTER

From the phenomenological point of view, nuclear systems at the thermodynamic limit (that is, *nuclear matter*) can be found in supernova explosions as well as in neutron stars. The possible presence of phase transitions in these astrophysical objects is of importance in understanding their structure and properties. Different phases and phase transitions are expected in stellar matter, depending on the regime of density and temperature[15]. Triggered by the recent unexpected observations of excessively massive neutron stars[32], the phase structure and composition of these compact objects has become the subject of an intense interest in the last few years.

Nuclear matter, that is the bulk limit of a nuclear system with the electromagnetic interaction artificially switched off, is the object of theoretical studies since the beginning of nuclear physics. However these studies are not completely adapted to the description of baryonic matter in the stellar environnement. The qualitative difference respect to the standard treatment of nuclear matter is that in stellar matter charge neutrality is achieved by the screening effect of delocalized electrons. This means that short range (nuclear) as well as long range(electromagnetic) interactions are at play, which makes the statistical properties very different from the ones of normal fluids. In particular, similar to the case of finite systems discussed in the previous chapter, it is possible to show that ensembles are not equivalent in these systems.

## A. The crust-core transition in neutron stars

As we have developed in the last chapter, the issue of ensemble in-equivalence, namely the possible dependence of the observed physics on the externally applied constraints, has been widely studied theoretically in the case of the thermodynamics of finite systems[23] and has also given rise to different experimental applications in nuclear and cluster physics [22, 29, 30]. In these specific examples 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 [10, 33, 34] but phenomenological applications are scarce. In this section 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$^{-3}$ 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 [35]. 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 [36]. 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 [15, 37]. This specific situation of stellar matter respect to ordinary nuclear matter is due to Coulomb frustration which quenches the first order phase transition [38].

Let us consider the dense matter in neutron-star crusts and supernova cores formed of electrons ($e$), neutrons ($n$) and protons ($p$). The microscopic Hamiltonian reads

$$\hat{H} = \hat{H}_{np} + \hat{K}_e + \hat{V}_{ee} + \hat{V}_{pp} + \hat{V}_{ep} \ , \tag{54}$$

where $\hat{H}_{np}$ is the nuclear strong interaction including the nucleon kinetic energy, $\hat{K}_e$ is the electron kinetic term and $\hat{V}_{ii'}$ is the Coulomb interaction between different types of particles

$(i \in \{e,p\})$ :

$$\hat{V}_{ii'} = \frac{\alpha q_i q_{i'}}{1+\delta_{ii'}} \int \frac{\rho_i(\vec{r})\rho_{i'}(\vec{r}')}{|\vec{r}-\vec{r}'|} \mathrm{d}\vec{r}\mathrm{d}\vec{r}' \ , \tag{55}$$

where $\alpha$ is the fine-structure constant and $\rho_i(\vec{r})$ is the local density of the particle of type $i$ and charge $q_i = \pm 1$.

Since the Coulomb field is a long-range interaction, the existence of a thermodynamics, i.e. the convergence of a thermodynamic limit and the equivalence between statistical ensembles, is not guaranteed [6]. Let us consider the canonical ensemble with densities $\rho_i = N_i/\Omega$, where $\Omega$ is the volume containing a number $N_i$ of particles $i = n$, $p$ or $e$. If the net charge density $\rho_c = \rho_p - \rho_e$ is not strictly zero at the thermodynamic limit, the Coulomb energy per unit volume $\langle V_c \rangle / \Omega \propto \rho_c^2 \Omega^{2/3}$ diverges. The important consequence of this charge-neutrality constraint is that the canonical free-energy density $f$ is defined only for $\rho_c = 0$. Hence $f\,(T, \rho_n, \rho_p, \rho_e) = f\,(T, \rho_n, \rho)$ with $\rho = (\rho_p + \rho_e)/2$ and the chemical potential associated with $\rho_c$ can not be defined since the free energy is not differentiable in the total-charge direction.

This suppression of one degree of freedom arises from the thermodynamic limit and should not be confused with an additional constraint, such as constant particle fraction or chemical ($\beta$) equilibrium. These conditions may or may not be realized in the supernova evolution; they are restrictions of the accessible states and do not affect the thermodynamical properties, which are state functions. Conversely, charge neutrality has to be fulfilled for each (macroscopic) physical state. This changes the the number of degrees of freedom of the thermodynamic potentials, which directly affects the thermodynamics.

In particular, phase coexistence can occur only between two neutral phases leading to the quenching of the nuclear matter phase transition in stellar matter. Indeed, because of the charge neutrality constraint over macroscopic distances, a biphase density solution given by a linear combination of a high density homogeneous region and a low density dilute region would imply an infinite repulsive interaction energy due to the electron density discontinuity at the (macroscopic) interface.

This argument requires electrons to be completely incompressible. Since the electron incompressibility, while high, is not infinite, it could be argued that a slightly modified coexistence region could be observed, where the liquid fraction would be constituted by large but still mesoscopic clusters, such that the interface energy would not diverge and the thermodynamics would not be affected.

An actual calculation of the thermodynamics of star matter demonstrates that this is not true: the presence of microscopic, instead than macroscopic, fluctuations, qualitatively change both the thermodynamics and the composition of matter. This is illustrated in Figure 8 which presents the functional relation between the different thermodynamic variables in the grancanonical and in the canonical ensemble within a simple exactly solvable model of star matter[39].

The grancanonical calculation (left side) shows a first order phase transition with density as an order parameter, very similar to the well-known phenomenology of ordinary neutral nuclear matter. At variance with nuclear matter which is homogeneous by definition, the low density phase is essentially constituted of nucleons and light clusters. As the density increases towards the values typical for the outer crust of neutron star above $10^{-6}$ fm$^{-3}$, intermediate mass fragments organized in a Coulomb lattice appear. Such structures are however metastable in the grancanonical ensemble, since a linear combination of the nucleon gas with ordinary liquid nuclear matter at saturation density maximizes the thermodynamical potential (dashed line). This leads to the Gibbs construction characteristic of first order phase transitions. As discussed above, in the physical system this phase coexistence is hindered by the Coulomb field. This is demonstrated in the right part of the figure, where the partition sum is calculated under the constraint of a given baryonic density.

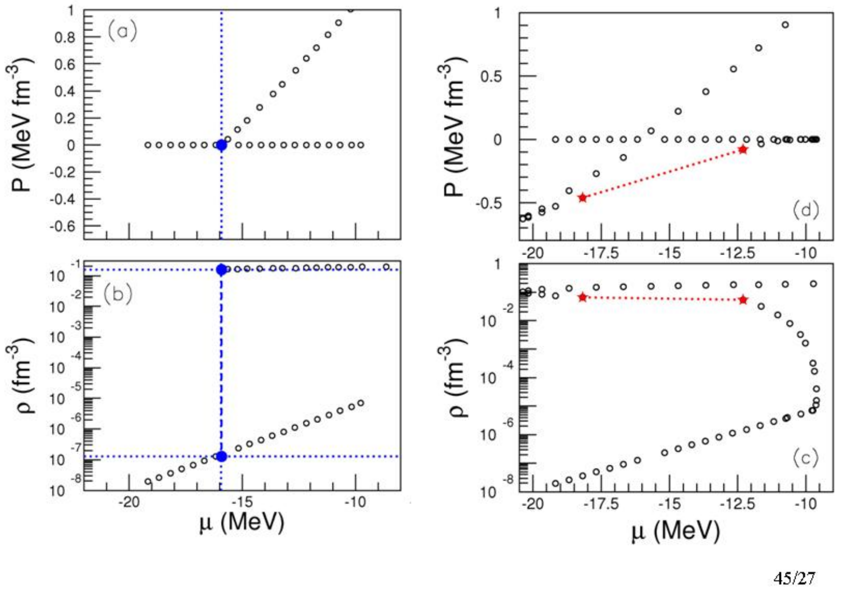

FIG. 8: Baryonic chemical potential as a function of the baryonic pressure (upper panels) and baryonic density (lower panels) in the grandcanonical (left) and canonical(right) ensemble at $T$=1.6 MeV in a phenomenological model of statistical equilibrium between homogeneous matter, clusters and electrons[39]. Dashed line: Gibbs construction corresponding to a first order phase transition. The low density branch in panels a,b at chemical potentials above the phase transition are metastable.

We can see that the canonical calculation allows one to interpolate between the dense and diluted 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 [10]. 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 [23].

From the observables point of view, the inequivalence region is characterized by the emergence of clusters (see figure 9) with an average size continuously increasing with the density, and the temperature jump is associated to the melting of clusters inside the homogeneous dense medium.

## B. Phenomenological consequences of ensemble in-equivalence

Besides the relevance of the issue of ensemble in-equivalence from the statistical physics viewpoint, it is interesting to remark that the assumption of ensemble equivalence 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. 9, which

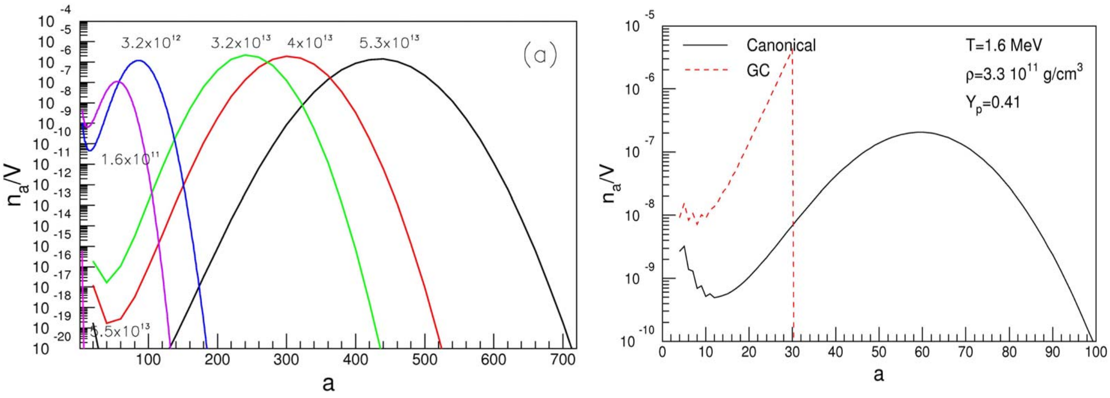

FIG. 9: Left: cluster distributions as a function of the density in the ensemble in-equivalence region; right: comparison between canonical (full line) and grandcanonical (dashed line) predictions for the cluster distribution in a specific thermodynamic condition relevant for supernova dynamics. From ref.[39].

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shows the cluster distribution for a chosen thermodynamic condition which is typical for the dynamics of supernova matter after the bounce and before the propagation of the shock wave [35]. 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 [40]. 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) [41], 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. [42], is shown by the dashed line in Fig. 9. It is clear that such approach completely misses the correct cluster distribution. Alternatively, hybrid canonical-grandcanonical formulations are routinely used in the astrophysical community [43]. Such approaches do not share the drawback of grandcanonical NSE calculations, but, because of the implicit hypothesis of ensemble equivalence, 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 modelized by a single representative nucleus. It is clear from Fig. 9 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.

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