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Liquid-gas coexistence and critical behavior in boxed neutral, isosymmetric pseudo-Fermi matter

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A schematic model is presented that allows one to study the behavior of interacting neutral isosymmetric pseudo-Fermi matter, locked in a thermostatic box. As a function of the box volume and temperature, the matter is seen to show all of the familiar characteristics of a van der Waals gas, which include the coexistence of two phases under certain circumstances and the presence of a critical point.

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I. INTRODUCTION

The possibility that a liquid-gas phase transition in finite nuclei may manifest itself via copious production of intermediate-mass fragments in energetic heavy-ion reactions has driven both, theoretical and experimental studies of nuclear multifragmentation over more than a decade. A prominent role in theoretical considerations is played by the concept of a freezeout configuration [1,2]. This concept implies the existence of a definite volume, within which the system reaches a state close to thermal equilibrium. While the existence of an effective freezeout volume may be debatable, the concept itself is useful for understanding the possible behavior of nuclear matter under various conditions. With such a didactic strategy in mind, and as an extension of earlier studies modeling the behavior of finite Fermi systems [3–5], the present study considers neutral, isosymmetric pseudo-Fermi matter confined to a box of definite volume. It evaluates the isothermal behavior of such matter and its dependence on box volume and temperature. The utmost simplicity of the formalism allows one to gain insight into physical phenomena that may be obscured in more rigorous approaches.

While the present formalism can be readily extended to include isoasymmetric matter, inclusion of a Coulomb interaction would require a number of qualitative changes, all resulting from the long range of the Coulomb interaction. Notably, the presence of a Coulomb interaction renders crucial extensive thermodynamic quantities nonadditive. For example, the Helmholtz free energy of a charged two-phase system is no longer equal to the sum of free energies of its separated gaseous and liquid parts. Furthermore, neither the pressure nor the density of charged matter is constant over the volume of any single phase, depending not only on the geometrical configuration assumed by this phase, but also on that of the coexisting phase. The above, highly nonlinear features make it very difficult in the present formalism to include the Coulomb interaction in a satisfactory manner. In common practice, this interaction is also disregarded in more rigorous approaches to the liquid-gas coexistence (see, e.g., Ref. [6], and references therein).

II. THEORETICAL FORMALISM

The present study considers a scenario of neutral, isosymmetric pseudo-Fermi matter of mass number A, locked in a spherical box of a volume V, and kept at constant temperature T. In the proposed formalism, thermostatic properties of the matter are modeled by two equations, the isochoric caloric equation of state and the zero-temperature equation of state. The equilibrium state of the system is then found as a function of V and T, based on the requirement that the free energy of the system is minimal.

First, we consider homogeneous systems with constant density throughout their volume, i.e., systems in states where only one phase is present. The isochoric caloric equation of state for such a system is taken in a simple form adequate for low-temperature Fermi gases

$$E^*_{therm} = aT^2, \tag{1}$$

where E^*_{therm} is the thermal energy and a is the level density parameter. The latter parameter is assumed to depend on matter density as

$$a = a_o\left(\frac{\rho}{\rho_o}\right)^{-2/3}, \tag{2}$$

in accordance with the low-temperature Fermi gas model.

It is worthwhile keeping in mind that, for Fermi gases, Eq. (1) is a good approximation only for temperatures that are small compared to the Fermi energy, i.e., for $T \ll E_{Fermi}$. Notably, for diluted or very hot Fermi systems, with a matter density approaching zero, $\rho \to 0$, or for high temperatures, $T \to \infty$, the isochoric caloric equation of state approaches asymptotically that of a classical gas:

$$E^*_{therm} = \frac{3}{2}AT. \tag{3}$$

For the sake of simplicity and without loss of generality, the present study uses Eq. (1) over the full range of matter densities and temperatures considered. The term ''pseudo-Fermi'' matter is used to distinguish the matter considered here from true Fermi matter. Note that for a noninteracting Fermi gas, the Fermi energy scales with the density as $E_{Fermi} \approx 39(\rho/\rho_o)^{2/3}$ MeV. For interacting Fermi gases, this energy is even higher, as it scales with the inverse of the effective nucleonic mass. Accordingly, the present concept of pseudo-Fermi matter provides a reasonably good approximation of true Fermi matter, in the most interesting domains of the plots discussed in Sec. III, notably, in the vicinity of the critical point ($T_c \approx 10$ MeV$< E_{Fermi,c} \approx 22$ MeV).

The second defining equation, the zero-temperature equation of state, expresses the compressional (potential) energy of the system as a function of the system volume or as a function of matter density. The present study adopts a harmonic approximation in the form used in the expanding emitting source model [7]. Here, the in-medium nucleonic (potential) energy changes quadratically with the relative deviation of the actual matter density from the ground-state density by an amount

$$\epsilon_{compr}=\epsilon_B\left(1-\frac{\rho}{\rho_o}\right)^2. \tag{4}$$

In Eq. (4), ϵ_{compr} and ϵ_B are compressional and ground-state binding energies per nucleon, respectively, and ρ and ρ_o are the actual and the ground-state matter densities, respectively. Equation (4) implies an effective ground-state incompressibility constant of $K_o=18\epsilon_B$. Assuming $\epsilon_B=8$ MeV, the effective incompressibility, including the effects of surface tension, equals $K_o=144$ MeV. Note that, for infinite nuclear matter characterized by $\epsilon_B\approx 16$ MeV, the incompressibility constant turns out to be equal to $K_o\approx 288$ MeV, in this harmonic approximation. The latter value places the present harmonic approximation ''neutrally'' between the currently considered limits of ''soft'' and ''hard'' equations of state for nuclear matter.

While the two defining equations (1) and (4) may be considered rather crude approximations, they do contain the essential physics responsible for first-order phase transitions and critical phenomena. Given these two equations, one can write expressions for all thermodynamic quantities characterizing the system, including the Helmholtz free energy F. The state of the system can then be found by minimizing the free energy, for any box volume V and temperature T.

Based on Eq. (1), one can write for the entropy S of a homogeneous system

$$S=\int_0^{E^*}\frac{1}{T}d\epsilon=2\sqrt{aE^*_{therm}}. \tag{5}$$

The free energy F for a homogeneous, single-phase system is given by

$$F=E^*_{total}-ST=E^*_{compr}+E^*_{therm}-2aT^2=E^*_{compr}-aT^2. \tag{6}$$

For the sake of simplicity, the free energy is expressed in Eq. (6) relative to a constant ground-state energy of the system. Furthermore, using Eqs. (2) and (4), the free energy [Eq. (6)] can be rewritten in a form revealing explicitly the important dependence on the matter density ρ, i.e.,

$$F=E_B\left(1-\frac{\rho}{\rho_o}\right)^2-a_o\left(\frac{\rho}{\rho_o}\right)^{-2/3}T^2. \tag{7}$$

Equation (7) allows one to write expressions for the system pressure p and the chemical potential μ as functions of volume (matter density) and temperature.

The pressure p can be expressed generally as the negative partial derivative of the free energy F with respect to volume V, at fixed number of nucleons A and fixed temperature T, i.e.,

$$p=-\left(\frac{\partial F}{\partial V}\right)_{A,T}=\frac{1}{A}\rho^2\left(\frac{\partial F}{\partial \rho}\right)_{A,T}. \tag{8}$$

Thus, for the case of pseudo-Fermi matter considered here, one obtains, based on Eqs. (7) and (8),

$$p=-2\epsilon_B\rho_o\left(1-\frac{\rho}{\rho_o}\right)\left(\frac{\rho}{\rho_o}\right)^2+\frac{2}{3}\alpha_o\rho_o\left(\frac{\rho}{\rho_o}\right)^{1/3}T^2, \tag{9}$$

where ϵ_B and α_o are the binding energy per nucleon and the level-density parameter per nucleon, respectively.

The chemical potential μ can be expressed generally as the partial derivative of the free energy F with respect to the number of nucleons A, taken at fixed volume V and fixed temperature T, i.e.,

$$\mu=\left(\frac{\partial F}{\partial A}\right)_{V,T}. \tag{10}$$

Using Eqs. (7) and (10) and noting further that $\rho=A/V$, $E_B=A\epsilon_B$ and $a_o=A\alpha_o$, one obtains for the chemical potential

$$\mu=\epsilon_B\left[1-4\frac{\rho}{\rho_o}+3\left(\frac{\rho}{\rho_o}\right)^2\right]-\frac{1}{3}\alpha_o\left(\frac{\rho}{\rho_o}\right)^{-2/3}T^2. \tag{11}$$

It is worth noting in Eq. (11) that, as a result of the requirement that V is a constant, the magnitude of the chemical potential differs significantly from the value of the free energy per nucleon. For example, the contribution of thermal excitation to the chemical potential is only one-third of what constitutes the thermal part of the free energy per nucleon.

III. LIQUID-GAS COEXISTENCE

Confined to a thermostatic box, matter will eventually fill the available volume V entirely such that the free energy of the system is minimized. For noninteracting matter, the minimum free energy always corresponds to a uniform density distribution. This is generally not true for an interacting system. In particular, for interacting pseudo-Fermi matter at the minimum free energy, low-density and high-density phases coexist.

For a two-phase system of A nucleons at temperature T confined to a volume V, the free energy can be written as a function of two variables, e.g., in terms of the volume of the gaseous phase V_{gas} and the number of nucleons contained in this phase, A_{gas},

$$F=F_{gas}+F_{liquid}. \tag{12}$$

Inserting for F_{gas} and F_{liquid} the expressions given by Eq. (7) for the corresponding numbers of nucleons, A_{gas} and A_{liquid}, respectively, one obtains

$$F_{gas}=A_{gas}\epsilon_B\left(1-\frac{A_{gas}}{V_{gas}\rho_o}\right)^2-A_{gas}\alpha_o\left(\frac{A_{gas}}{V_{gas}\rho_o}\right)^{-2/3}T^2 \tag{13}$$

and

$$F_{liquid}=(A-A_{gas})\epsilon_B\left[1-\frac{A-A_{gas}}{(V-V_{gas})\rho_o}\right]^2-(A-A_{gas})\alpha_o\left[\frac{A-A_{gas}}{(V-V_{gas})\rho_o}\right]^{-2/3}T^2. \tag{14}$$

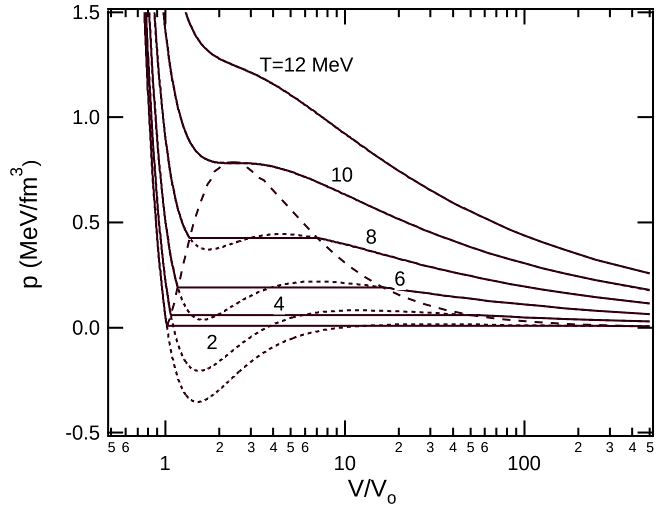

FIG. 1. Isotherms calculated for an ^{197}Au-like system. Dotted lines illustrate isotherms for hypothetical single-phase matter, while the dashed line visualizes the boundary of the liquid-gas coexistence domain.

The condition for the minimum free energy can be expressed in form of two equations, reflecting requirements of dynamical and chemical equilibrium, respectively,

$$\left(\frac{\partial F}{\partial V_{gas}}\right)_{T,A_{gas}}=\left(\frac{\partial F_{gas}}{\partial V_{gas}}\right)_{T,A_{gas}}-\left(\frac{\partial F_{liquid}}{\partial V_{liquid}}\right)_{T,A_{liquid}}$$
$$=p_{gas}-p_{liquid}=0 \tag{15}$$

and

$$\left(\frac{\partial F}{\partial A_{gas}}\right)_{T,V_{gas}}=\left(\frac{\partial F_{gas}}{\partial A_{gas}}\right)_{T,V_{gas}}-\left(\frac{\partial F_{liquid}}{\partial A_{liquid}}\right)_{T,V_{liquid}}$$
$$=\mu_{gas}-\mu_{liquid}=0. \tag{16}$$

Results of a numerical minimization of the free energy of a two-phase system are shown in Figs. 1–4. Figure 1 presents system isotherms, as predicted by the present formalism, in a representation of system pressure p versus system volume V. Note that Eqs. (13) and (14) represent single-phase states as special cases. A pure liquid/gas state is thus among the possible outcomes of the calculations with $A_{gas/liquid}=0$. As seen in Fig. 1, the isotherms feature segments representing pure liquid, pure gas, or, notably, a liquid-gas coexistence "plateau." The presence of such coexistence plateaus does not come as a surprise, since the harmonic interaction term of Eq. (4) has the salient characteristics of a van der Waals interaction.

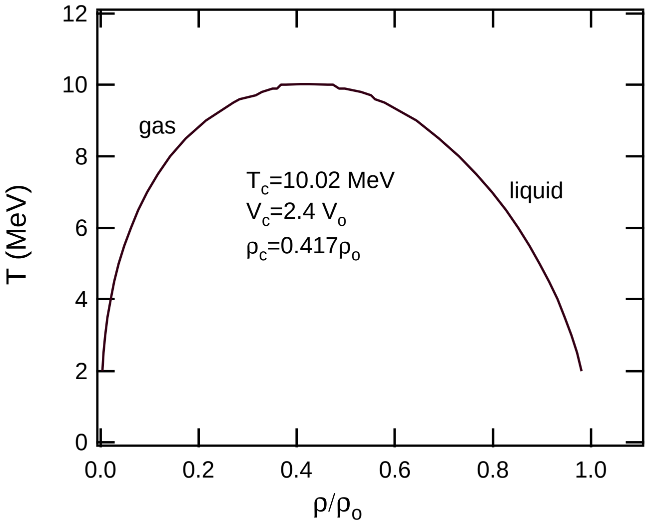

FIG. 2. Liquid-gas coexistence line in the temperature versus matter density representation, as predicted by the present formalism.

It is worth noting that the coexistence plateaus in this calculation result naturally from the actual minimization of the free energy and are not obtained via the well-known phenomenological Maxwell construct. Isotherms for hypothetical single-phase states are shown as dotted lines. These latter isotherms feature domains of spinodal instability characterized by negative compressibility. The dashed curve in Fig. 1 illustrates the boundary of the liquid-gas coexistence domain. The "summit" point of this curve represents the critical point for the system and corresponds to a critical temperature of $T_c\approx 10.0$ MeV. At temperatures higher than T_c, the system can reside only in a single-phase, vapor state.

A different representation of the liquid-gas coexistence line is illustrated in Fig. 2. In this case, the temperature T is plotted versus the matter density, for points along the boundary of the liquid-gas coexistence line (dashed line in Fig. 1). In the domain below this curve, the system is in a two-phase state. In this coexistence domain, the densities of gaseous and liquid phases at a given temperature are defined by the intersection points of the coexistence curve with the horizontal line for $T=$const. On the left shoulder of the curve and in the domain further left to it, the system is in a pure gaseous state, while on the right shoulder and in the domain further right to it, the system is in a pure liquid state. The difference

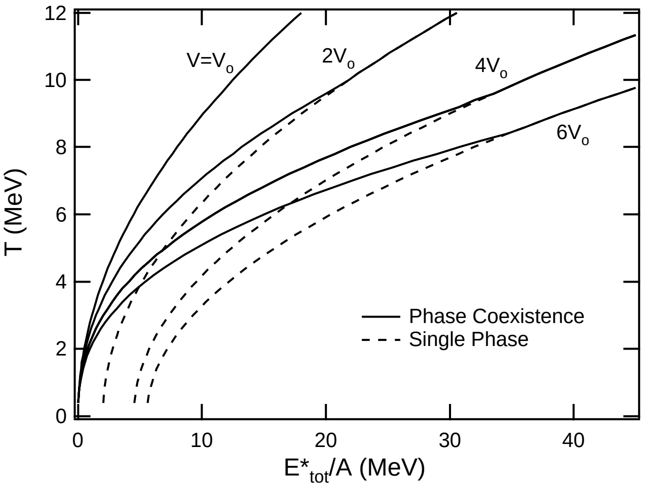

FIG. 3. Isochoric caloric curves for boxed pseudo-Fermi matter, calculated for different volumes of the confining box, as indicated by labels.

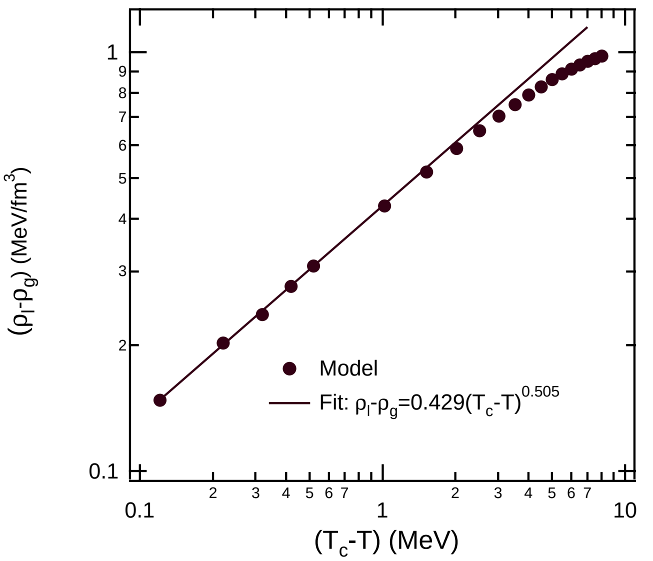

FIG. 4. Critical behavior of densities of coexisting liquid and gaseous phases at temperatures close to (and below) the critical temperature T_c.

between liquid and gaseous phases vanishes for temperatures above $T = T_c = 10.0$ MeV.

The search for the minimum free energy for a given temperature T and a given volume V yields the total excitation energy E^*_{total} of the boxed matter, along with the corresponding volumes $V_{gas/liquid}$ and densities $\rho_{gas/liquid}$ of gaseous and liquid phases. This allows one to construct isochoric caloric curves for the modeled system at different volumes of the confining box. A set of such caloric curves is illustrated in Fig. 3. As expected, these curves do not feature plateaus of the kind reported in various experimental studies [8], but show rather inconspicuous kinks at the locations on the boundary of the coexistence domain.

IV. CRITICAL BEHAVIOR

One of the salient features of critical behavior in van der Waals systems is the presence of a singularity at the critical point. When the system temperature T approaches the critical temperature T_c from below, the difference between the densities of coexisting liquid and gaseous phases is predicted to vanish according to a power law

$$\rho_{liquid} - \rho_{gas} = C(T_c - T)^{\beta}. \tag{17}$$

In Eq. (17), C is a constant and β is the critical exponent. The magnitude of the critical exponent can be extracted conveniently by fitting a straight line to a double-logarithmic plot of $(\rho_{liquid} - \rho_{gas})$ versus $(T_c - T)$. Such a plot, obtained in the present calculations, is shown in Fig. 4. The plot features, indeed, an approximately 2-MeV-wide linear domain extending from the critical temperature T_c down to lower temperatures. A linear fit to this domain allows one to extract the ‘‘coordinates’’ of the critical point of $T_c = 10.0$ MeV, and $\rho_c / \rho_o = 0.42$. Furthermore, it yields a value of $\beta = 0.51$ for the critical exponent.

Given the schematic nature of the present formalism, the predicted characteristics of the critical point are well within a reasonable domain that can be inferred from more sophisticated, but less transparent calculations.

V. DISCUSSION

A simple formalism has been presented that allows one to model the behavior of interacting neutral, isosymmetric pseudo-Fermi matter under the conditions of controlled volume and temperature. The formalism is shown to capture the essential physics of a first-order liquid-gas phase transition. The calculation demonstrates the characteristics of a nuclear liquid-gas coexistence in a certain domain of system parameters and the presence of a critical point. While such characteristics are well expected, based on the similarity of the utilized form of the nuclear interaction to that of the van der Waals interaction, the present formalism offers many didactic benefits. For example, due to its simplicity, it offers clear insight into physical phenomena it purports to describe and a relatively strict test bench for possible qualitative or ‘‘handwaving’’ arguments. The results obtained, while almost trivial, may alert one to possible challenges found by more complete models.

The formalism presented here leaves ample room for further refinements, such as a more strict modeling of dilute Fermi matter, or the inclusion of isotopic and, perhaps, Coulomb effects. At any rate, it offers a convenient didactic tool to achieve a better understanding of nuclear thermodynamics.

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