Phase transitions in nuclear matter at finite temperatures

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A second-order virial equation of state for a symmetric system of nucleons \((N = Z)\) interacting through a deuteronlike force is established. The dependence of the virial coefficient on temperature and the square-well parameters is discussed. The isotherms are analyzed, and it is shown that the gas-liquid phase transition takes place at a much lower density than that commonly assumed to be the characteristic density of nuclear matter.

I. INTRODUCTION

Recently, an interesting problem has been posed by several investigators.\(^1\) It is concerned with the state of nuclear matter in thermodynamical equilibrium. Ordinary theories of infinite nuclear matter rest on the supposition of a gaseous phase\(^5\) or a Fermi liquid\(^6\) and there may be evidence supporting the idea that it could also exist as a crystal.\(^4\) Neutron star matter provides an excellent field of research on crystalline ordering of nucleons, since it is well known that solidification occurs at the crust of neutron stars where the density ranges between \(10^{4}\) and \(2 \times 10^{10} \text{ g cm}^{-3}\).\(^7\) A great deal of effort also has been devoted to ascertaining whether neutron star cores exhibit crystalline behavior at superhigh densities\(^7\) (i.e., those which exceed by one or two orders of magnitude that observed at the center of finite nuclei, \(\rho_0 \approx 2.8 \times 10^{14} \text{ g cm}^{-3} = 0.17 \text{ nucleon fm}^{-3}\)) and it is presently agreed that realistic forces do not lead to crystallization.

The importance of a clear understanding of the thermodynamics of nuclear matter runs far beyond establishing its equilibrium characteristics as an extended system. Two or three decades ago, attempts to explain the observed data concerning relative abundance of elements,\(^8\) binding energies, and nuclear stability properties were traced to the problem of the origin of atomic species.\(^9\)\(^10\) The whole machinery of thermodynamics and statistical mechanics proved to be highly successful in yielding both qualitative and quantitative explanations of the distribution of elements.\(^11\) Although there still exists a serious polemic on the merits of either equilibrium or nonequilibrium theories,\(^9\)\(^10\)\(^12\) these pioneering works\(^9\)\(^10\) encourage further application of current statistical methods to extended systems of nucleons.

The aim of the present work is to develop a simplified model of nuclear matter in an earlier stage of its thermodynamical evolution. If we assume that actual nuclear matter is frozen at \(T = 0 \text{ K}\), it is possible to conceive that it has reached that situation through a "cooling" process during which it could have experienced at least one phase transition. It would then be interesting to have at our disposal some criterion to analyze the kind of phase transition involved and the order of magnitude of the thermodynamical variables at the critical point. To this purpose, we derive an equation of state for an extended system of nucleons with total isospin zero (i.e., \(N = Z\)) which interacts through a deuteronlike force. Such a procedure is within the spirit of statistical-equilibrium approaches to the description of nuclear-stability properties,\(^9\)\(^10\)\(^11\) where nuclear forces are dealt with by recourse to a mass formula.\(^11\)

We follow the general prescriptions of Lee and Yang\(^13\) to get an expression for the second virial coefficient in the usual cluster expansion of the grand-partition function.\(^14\) The equation of state is then analyzed and it is shown that the system exhibits a gas-liquid phase transition. The critical temperature that arises from this equation of state exceeds by one order of magnitude the clustering temperature found in Ref. 11. Furthermore, the critical specific volume is almost two orders of magnitude larger than that corresponding to nuclear matter density \(\rho_0\).

In spite of the limitations of the model and of the approximations involved, it provides another line of evidence, now based on thermodynamical considerations, to support the idea that nuclear matter in equilibrium is not an interacting Fermi gas. In addition, the standard procedure employed in this work might be checked against the complicated many-body techniques that are usually present in nuclear matter calculations, out of which a similar result concerning the critical volume can be extracted.\(^14\)

In Sec. II we sketch the model and the formalism employed. The calculations are displayed in Sec. III and the final conclusions are presented in Sec. IV.
II. THE MODEL

From the fundamental equations given in Lee and Yang's work\textsuperscript{13} we first derive an expression for the second cluster coefficient for an interacting Fermi gas. Secondly, the particular choice of the interaction and the magnitudes involved will be explained.

Our main task is to eliminate the fugacity $z = e^{\beta \mu}$, from the pair of equations

\begin{equation}
\beta p = \sum_{i=0} b_i e^{\beta \mu},
\end{equation}

\begin{equation}
\frac{1}{v} = \sum_{i=0} b_i e^{\beta \mu},
\end{equation}

with

\begin{equation}
\beta = 1/kT,
\end{equation}

where $\mu$, $k$, and $T$ are the chemical potential, the Boltzmann constant, and the absolute temperature, respectively. The $b_i$'s are the cluster coefficients\textsuperscript{13,15,16} for an infinite volume.

Details of the calculation of $b_i$ are thoroughly discussed in the literature.\textsuperscript{13,15,16} We form a virial expansion of the pressure $p$ with respect to the particle density $1/v$, eliminating $z$ between (2) and (3), and truncate at the second-order term in $1/v$. The validity of this approximation, equivalent to the hypothesis of a weakly interacting gas, will be checked \textit{a posteriori}. The result is

\begin{equation}
p = \left(\frac{kT}{v}\right) [1 + B(T)/v],
\end{equation}

where

\begin{equation}
B(T) = -b_2/b_1^2.
\end{equation}

We easily find

\begin{equation}
b_1 = 4/\lambda^3,
\end{equation}

where the factor 4 takes into account the spin-isospin degeneracy. As for $b_2$, questions of antisymmetrization are avoided\textsuperscript{13} if we evaluate the difference $b_2 - b_2'$, the superscript zero corresponding to a Fermi gas of free nucleons.

Let us define the thermal wavelength associated with the reduced mass particle,

\begin{equation}
\lambda = \sqrt{\frac{2\hbar^2}{mkT}},
\end{equation}

If we introduce $g(k)$, the density of states around the relative wave number $k$ (wave-vector modulus) in the center-of-mass system of a particle pair, we find\textsuperscript{13,16}

\begin{equation}
\begin{split}
b_2 - b_2' = \frac{32/3}{\lambda^3} \left\{ \sum_B \exp(-\beta E_B) + \sum \int \exp \left( \frac{-k^2 \lambda^2}{2\pi} \right) \frac{\partial^2}{\partial k^2} g(k) dk \right\}.
\end{split}
\end{equation}

The usual formulas\textsuperscript{13,16} have been properly corrected to include the spin-isospin degeneracy. The subscript $B$ denotes bound states while $k, l, m$ are the quantum numbers that label the continuum wave functions for the reduced mass particle.

A simplification arises in (9) from the fact that the exponential factor under the integral sign limits the range of integration to that of low energies. One is then left with an $S$-wave approximation.\textsuperscript{13} The density of states $g(k)$ is easily related to the phase shift of the perturbed wave function $\psi_{k00}(r)$,\textsuperscript{16} and Eq. (9) finally gives

\begin{equation}
\begin{split}
b_2 - b_2' = \frac{32/3}{\lambda^3} \left\{ \sum_B \exp(-\beta E_B) \\
+ \frac{1}{\pi} \int \exp \left( \frac{-k^2 \lambda^2}{2\pi} \right) \frac{\partial^2}{\partial k^2} g(k) dk \right\}.
\end{split}
\end{equation}

We then need a model for the system, from which we can decide what $E_2$ and $b_2'$ are going to be. The present choice consists of an infinite many-nucleon gas with $N = Z$, interacting through a deuteronlike force as shown in Fig. 1. The well parameters are chosen so as to produce only one $S$-bound state.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{square_well_potential}
\caption{Square-well potential with hard core at $r = c$. Only one bound state is found at energy $E_B$.}
\end{figure}
which may provide a basis for further clustering into more massive structures (α-clusters, etc). The presence of pairs of particles bound together by a charge-independent force lies within the spirit of independent-pair-model descriptions of nuclear matter. In addition, as the assumed force does not depend on spin or isospin, we can choose the corresponding factor in the two-body wave function so as to guarantee antisymmetrization.

As it is well-known, the S-wave phase shift is

$$\delta_\theta = -k b + \arctan \left( \frac{k'}{k} \right) \tan k'(b - c), \quad (11)$$

where

$$k'^2 = k^2 + 2mV_0/k^2. \quad (12)$$

In order to make possible an analytic approximation to the integral in (10) we take advantage again of the presence of the exponential factor and consider

$$k'^2 \lambda^2 = 2mV_0 \lambda^2/k^2 + k^2 \lambda^2 - 2mV_0 \lambda^2/k^2, \quad (13)$$

if

$$2mV_0 \lambda^2/k^2 \gg 1. \quad (14)$$

The leading parameter is then $V_0/kT$ and it is easy to verify that over a wide range of temperature, up to $kT \sim 100$ MeV, condition (14) is satisfied if $V_0$ is not much less than 100 MeV. We then define

$$\eta = \frac{1}{k'} \tan k'(b - c) \sim \left[ \frac{k}{(2mV_0)^{1/2}} \right] \tan \left[ \frac{(2mV_0)^{1/2}}{k} \right] (b - c), \quad (15)$$

and Eq. (10) reads

$$b_2 = b_2^a + \frac{32\sqrt{2}}{\lambda^3} \exp(-\beta E_\alpha) + \frac{32\sqrt{2}}{\pi \lambda^3} \times \int \left( -b + \frac{\eta}{1 + \frac{k}{k'}} \right) \exp \left( -\frac{k^2 \lambda^2}{2\pi} \right) db. \quad (16)$$

The second term under the integral sign can be evaluated through the following steps: (i) A Fourier representation of the exponential factor; (ii) an interchange of the order of integrations; and (iii) a contour integration over the complex plane. The calculation yields

$$b_2 = b_2^a + \frac{32\sqrt{2}}{\lambda^3} \exp(-\beta E_\alpha) - \frac{16\sqrt{2}}{\pi \lambda^3} \exp \left( \frac{\lambda^2}{2\pi^2} \right) - \frac{32b}{\lambda^3}, \quad (17)$$

and according to (6) the virial coefficient is

$$B(T) = \left( \sqrt{2}/4 \right) \lambda^3 - 2\sqrt{2} \exp(-\beta E_\alpha) \lambda^3 + 2b \lambda^2 - \sqrt{2} \lambda^3 \exp(\lambda^2/2\pi \eta). \quad (18)$$

III. CALCULATIONS

The system under consideration will experience a phase transition for a given $T$ at the volume and pressure for which

$$\frac{\partial V}{\partial V} = 0. \quad (19)$$

Furthermore, if in addition,

$$\frac{\partial V}{\partial V} = 0, \quad (20)$$

we are in the presence of the critical point. Examination of Eq. (5) reveals that conditions (19) and (20) are only consistent with $B(T) = 0$, which yields zero critical volume and infinite critical pressure.

We see from Eq. (18) that $B(T)$ is parametrized by $b$, $E_\alpha$, and $\eta$. The last two of these can be determined if we fix $b$ and $V_0$ by the usual procedure for solving a square-well potential in quantum mechanics (see, for example, Ref. 17). Then for a given well the virial coefficient can be plotted as a function of $T$ (Figs. 2, 3) and the temperature $T_\sigma$ for which $\delta = 0$ can also be drawn as a function of any force parameter, say $\eta$, for a given $b$. Here
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and in what follows we replace $kT$ by $T$, i.e., we measure $T$ in MeV. The value of $c$ is 0.4 fm everywhere (standard hard-core radius in nuclear matter).

Having established a set of values for the force it is seen that for any temperature larger than or equal to $T$, the system does not exhibit any phase transition (Fig. 4). When $T < T_B$, $B(T)$ being negative causes $p$ to be zero for $v = |B(T)|$, i.e., it goes asymptotically to $-\infty$ in a logarithmic scale. The maximum for any isotherm occurs at a volume $v_o = 2|B(T)|$ and a pressure $p_o = T/4|B(T)|$. These values define the transition point. For volumes smaller than $v_o$, the isotherm loses sense, and it becomes evident that for such a compressed system the gaseous phase is no longer a possible physical situation.

In Fig. 4, the square well has been designed so as to fit the binding energy and the root-mean-square radius of the deuteron. For this well, $b = 1.34$ fm and $\eta = -2.8$ fm. A test of consistency of the procedure employed may arise from Fig. 5. Here we have plotted $v_o/\lambda^3$ as a function of $T$. We observe that for a wide range of temperature, even beyond 100 MeV, $v_o/\lambda^3$ may be larger than unity. Since the gas exists only for volumes larger than $v_o$, it is concluded that the virial approximation (cf. Sec. II) is justified. We stress this condition, due to the fact that we are specially interested in temperatures from 1 to 10 MeV, approximately, which are the values appearing in earlier calculations on equilibrium descriptions of the relative abundance of elements (Refs. 8–11). It is seen from Fig. 5 that for these temperatures, which are low when compared with $T_B$, the growth of the thermal wavelength is overcome by the exponential factors in $v_o$ and the validity of the second-order virial expansion is guaranteed. Indeed, for $1 \leq T \leq 10$ MeV, $v_o/\lambda^3$ is large enough to consider that the gas does not, in fact, exhibit quantal effects.

Finally, we wish to examine to what extent the typical parameters of the $p-v$ isotherms may reproduce any well established property of nuclear matter. In Fig. 6 we show the density $\rho_o = 1/v_o$.
FIG. 6. The density \( \rho_e \) at the transition point as a function of \( T \) for \( \eta = 2.8 \) fm.

as a function of the temperature. We first notice that for the range of interest of \( T \) values, the density remains up to 2 or 3 orders of magnitude smaller than the commonly accepted figure for nuclear matter, \( \rho_0 = 0.17 \) nucleon fm\(^{-3} \). This number would correspond to a temperature about 200 MeV. Now, although we include temperatures as high as 600 MeV in our drawings in order to make our description as complete as possible, at least formally, it should be borne in mind that several considerations included in the model collapse along the main part of the whole interval [S-wave approximation in Eq. (9), neglect of Coulomb forces, condition (14), etc.]. If we remain with temperatures about or below 10 MeV, for which the model is valid, we find that a nuclear-matter-like system cannot be found along our gaseous isotherms.

IV. CONCLUSIONS

From the results presented in the preceding section we can summarize as follows. We have seen that a nuclear like force, weakly attractive, able to bind only one state, might be responsible for two-particle clustering in a Fermi gas. Such a gas would be almost nondegenerate; in consequence, a second-order virial equation of state would be a satisfactory approximation to the "true" equation of state. It would then provide a reasonable clue that allows us to identify a gas-liquid phase transition. The main feature of this transition might be the fact that for any temperature lower than 10 MeV, the density of the gas remains much higher (i.e., two or three orders of magnitude) than the nuclear matter value \( \rho_0 \). Temperatures between 1 and 10 MeV are those expected to fit nuclear-stability properties such as distribution of elements and masses.\(^{11} \) Accordingly, for these temperatures, a nondegenerate gaseous phase described in a second-order virial approximation does not yield the "correct" nuclear matter density. This result agrees qualitatively with that obtained by de Llano and Tolmachev.\(^{14} \) These authors proved, by recourse to a particle-hole Green's-function technique, that condensation of a nucleon gas occurs at a density approximately equal to 0.03\( \rho_0 \). The fact that our simple model has provided a conclusion comparable with that arising from a much more sophisticated treatment would then imply that two-particle neutron-proton clusters play a relevant role in the condensation of nuclear matter.

Refinements of the calculations here presented (i.e., extending the model so as to include a more realistic force) are needed in order to decide whether it is convenient to abandon the virial approximation and look for a more sophisticated equation of state. Calculations are in progress and will be given in a forthcoming paper. The author believes that in view of these results, it is reasonable to attempt a thermodynamical description of nuclear matter as a clue for understanding its actual equilibrium properties.

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