Heated nuclear matter, condensation phenomena and the hadronic equation of state

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Abstract

The thermodynamic properties of heated nuclear matter are explored using an exactly solvable canonical ensemble model. This model reduces to the results of an ideal Fermi gas at low temperatures. At higher temperatures, the fragmentation of the nuclear matter into clusters of nucleons leads to features that resemble a Bose gas. Some parallels of this model with the phenomena of Bose condensation and with percolation phenomena are discussed. A simple expression for the hadronic equation of state is obtained from the model.

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Properties of heated nuclear matter are of current interest, with heavy-ion collisions used to obtain information about nuclear matter away from the typical nuclear matter density and temperature. Theoretical concerns have centered around the nuclear equation of state, the specific heat, the behavior of the entropy per particle, and other thermodynamic issues [1–3]. The notion that nuclear matter undergoes a phase transition has gained special attention [4]. Most treatments of the equation of state have treated heated nuclear matter as a homogeneous system. Statistical [5–23] and percolation [24–26] models have been used by many groups to study nuclear multifragmentation and the role of clusters on nuclear properties. This paper explores various thermodynamic properties using an exactly solvable canonical ensemble model that allows for clusterization and leads to simple analytic expressions for thermodynamic quantities such as the equation of state. This canonical ensemble approach has properties that are similar in many ways to those obtained from models used in other areas, such as Bose condensation, Feynman’s approach to the $\lambda$ transition in liquid helium [27] and in polymer physics [28]. For example, the cycle class decomposition of the symmetric group which appears in the symmetry of the bosonic system in Feynman’s approach is isomorphic to the cluster structure of a heated nuclear system. The cost function of moving a helium atom from one location to another is the same as internally exciting a cluster.

The canonical ensemble partition function given below is obtained from the following simple picture. At $T = 0$, a system of $A$ nucleons is in its ground state, which is treated as a degenerate Fermi gas. As $T$ increases, the Fermi gas is excited into low lying excited states whose level density grows as $\rho(E) \sim \exp(2\sqrt{aE})$. Particles and clusters can also be emitted with increasing $T$. The formation of clusters is an expression of the attractive nature of the nucleon-nucleon interaction. The repulsive nature of this interaction will be treated here in terms of a density dependent Skyrme approach [29,30]. At high density an excluded volume correction is needed to avoid some unphysical consequences of the model. At very large $T$ clusterization is unlikely, and the nucleons behave essentially as a dilute Maxwell-Boltzmann gas.
Considered as a statistical system, this model exhibits a phase transition in the fixed density but infinite $A$ limit, at which the specific heat per nucleon is maximal. An infinite cluster suddenly appears at this point in a manner similar to the infinite cluster of percolation theory. Real nuclear systems are far from infinite collections of nucleons, but the evidence of such phase transitions can be obtained from a finite scaling analysis in the region of the phase transition [24-4].

In earlier papers [20-23] the question of the thermodynamics of a fragmenting system was raised. There, it was assumed that the thermodynamic variables were contained in a single parameter $x$ such that the weight of a particular cluster partition was proportional to $x^m$, where $m$ is the total number of clusters in that partition. Specifically, the partition function of the system was a polynomial in the variable $x$ of degree $A$, where $A$ is the number of particles in the system. This $x$ contains physical quantities as discussed below in Eq. (6). The computation of various thermodynamic quantities could then be reduced to functions of $x$ and various moments of the number of clusters. Here the slightly more general case where there are two thermodynamic parameters $x, y$ with the probability of a particular fragmentation outcome proportional to $x^m y^{A-m}$ is analyzed. This choice reduces to the early models by noting $x^m y^{A-m} = y^A (x/y)^m$ where $x/y$ can be identified with the tuning parameter $x$ used earlier and $y^A$ is an overall factor which has no effect on cluster yields. However, this more general case is necessary for an evaluation of some thermodynamic properties.

We begin by assuming that each fragmentation outcome happens with a probability proportional to

$$W(\vec{n}) = \prod_{k \geq 1} \frac{x^{n_k}}{n_k!} = \prod_{k \geq 1} \frac{1}{n_k!} \left(\frac{xy^{k-1}}{\beta_k}\right)^{n_k},$$

where $x$ and $y$ are functions of the thermodynamic variables $V, T$, $\beta_k$ is the cluster size dependence of the weight discussed below, and $\vec{n} = (n_1, n_2, \ldots)$ is the fragmentation vector, with $n_k$ the number of fragments with $k$ nucleons such that $\sum_k k n_k = A$. The free energy for such a canonical system is given by $F_A(V, T) = -k_B T \ln Z_A$ with
\[ Z_A = \sum_{\vec{n} \in \Pi_A} W(\vec{n}) = \sum_{m=0}^{A} Z_A^{(m)}(\vec{\beta}) x^m y^{A-m}, \tag{2} \]

where \( \Pi_A \) is the set of all partitions of \( A \) and \( Z_A^{(m)} \) is a function only of the vector \( \vec{\beta} \), not of the thermodynamic variables.

It is fairly straightforward to derive relations between logarithmic derivatives of the partition functions and moments of the multiplicity \( m = \sum_k n_k \), e.g.

\[ x \frac{\partial}{\partial x} \ln Z_A = \langle m \rangle, \quad \left(x \frac{\partial}{\partial x}\right)^2 \ln Z_A = \langle m \rangle_2, \tag{3} \]

where \( \langle m \rangle_k = \langle (m - \langle m \rangle)^k \rangle \) is the \( k \)th central moment. In general, \( (x \frac{\partial}{\partial x})^k \ln Z_A(x) \) is the \( k \)’th cumulant moment of \( m \). The relations for derivatives with respect to \( y \) are similar.

Given these formulae, the determination of thermodynamic quantities can be reduced to a computation of the cumulant moments of the fragmentation multiplicity \( m \), since only logarithmic derivatives of the partition function (such as those given above) are used in the determination of the energy, pressure, specific heat, etc. Applying the usual relations between the thermodynamic functions and the partition function, the result for the specific heat and pressure is

\[
\frac{C_V}{k_B} = \langle m \rangle \left( \frac{2T}{x} \frac{\partial x}{\partial T} - \left( \frac{T}{x} \frac{\partial x}{\partial T} \right)^2 + \frac{T^2}{x} \frac{\partial^2 x}{\partial T^2} \right) \\
+ (A - \langle m \rangle) \left( \frac{2T}{y} \frac{\partial y}{\partial T} - \left( \frac{T}{y} \frac{\partial y}{\partial T} \right)^2 + \frac{T^2}{y} \frac{\partial^2 y}{\partial T^2} \right) \\
+ (\langle m^2 \rangle - \langle m \rangle^2) \left( \frac{T}{x} \frac{\partial x}{\partial T} - \frac{T}{y} \frac{\partial y}{\partial T} \right)^2
\]

\[
\frac{PV}{k_B T} = \langle m \rangle \frac{V}{x} \frac{\partial x}{\partial V} + (A - \langle m \rangle) \frac{V}{y} \frac{\partial y}{\partial V}, \tag{4}
\]

where the last equation is the equation of state. The calculation of the cumulant moments of \( m \) can be done by applying Eq. (3) and using a recursive evaluation of the coefficients of the partition function \( Z_A^{(m)} \), namely \[ Z_A^{(m)} = \frac{1}{m} \sum_{k=1}^{A} \frac{1}{\beta_k} Z_A^{(m-1)}, \tag{5} \]
where $Z_A^{(1)} = 1/\beta_A$. The whole recursive procedure is easy to implement as a computer program.

The choice of $x$, $y$ and $\beta_k$ is determined by the physics of the situation. The term $x^m$ comes from phase space factors and translational partition function considerations, namely $x = V/\lambda^d$, with $\lambda$ the thermal wavelength of a nucleon and $d$ the dimensionality of the system (with $d = 3$ appropriate for nuclear fragmentation). This $x$, with $\beta_k = k^{1+d/2}$ in Eq. (1) is essentially the weight given to Bose condensation problems in $d$ dimensions.

In this case, $n_k$ is the number of cycles of length $k$ in a cycle class decomposition of the permutation associated with a particular Bose gas state. For a nuclear system, the term $y$ is due to cluster binding and internal excitations. In a simplified view of binding energy considerations, each fragment of size $k$ has a binding energy of $a_V(k - 1)$, so a total binding energy of $E_B \sim a_V(A - \langle m \rangle)$ suggests a Boltzmann weight of $y = \exp(a_V/k_B T)$. It is appropriate to also include in this factor a Fermi gas level density term arising from internal excitations, leading to the result,

$$x = V \left( \frac{2\pi m k_B T}{\hbar^2} \right)^{d/2},$$

$$y = \exp \left\{ \frac{a_V}{k_B T} + \frac{k_B T}{\varepsilon_0} \frac{T_0}{T + T_0} \right\},$$

where $a_V$ is the binding energy per nucleon, $\varepsilon_0$ is the level spacing parameter for excited states, and $T_0$ is a temperature cutoff factor for internal excitations. The expression $x/y$ is the tuning parameter in previous papers [20, 23].

In general the parameters $a_V$ and $\varepsilon_0$ are density dependent. In the Skyrme approach, $a_V(\rho)$ is given by

$$a_V(\rho) = a_D \left( \frac{\rho}{\rho_0} \right)^{2/3} - a_0 \left( \frac{\rho}{\rho_0} \right) + a_3 \left( \frac{\rho}{\rho_0} \right)^{1+\sigma},$$

and for a Fermi gas, $\varepsilon_0(\rho) = (4/\pi^2)\varepsilon_F(\rho)$ with $\varepsilon_F(\rho) \sim \rho^{2/3}$ the Fermi energy, $a_D = 3\varepsilon_F(\rho_0)/5$ and $a_0, a_3$ are Skyrme parameters, which can be determined by requiring the binding energy/nucleon to be a maximum at $\rho = \rho_0$ with the value of 8.0 MeV. It should be noted that the factor $\exp(k_B T/\varepsilon_0)$ can be rewritten as $\exp(a(m d^2/2\hbar^2) k_B T)$. Using the above relation
between Fermi energy and the density of states, \( a \) is a numerical constant close to 1 and \( a^3 = V/A \). This factor with \( a = 1 \) is the cost function of moving a Helium atom from one location to another in Feynman’s approach to the \( \lambda \) transition in liquid Helium [27].

The only remaining parameter to set in this model is \( \beta_k \). If the weight \( W(\vec{n}) \) from Eq. 1 was for a Bose gas, then [33]

\[
x_k = \frac{x}{k^\tau} + \frac{1}{k},
\]

with \( \tau = 1 + d/2 \). The \( 1/k \) term arises from the zero momentum states of the Bose condensate. This additional term is irrelevant at high temperatures, but of some importance below the critical point. Since the low temperature behavior we want is essentially Fermi gas like, we can ignore the zero momentum term, which suggests we use \( \beta_k = k^\tau \). Here \( \tau \) is the critical parameter \( \tau \) discussed in Fisher [31], Finn, et. al. [32] and Gilkes, et. al. [4]. We choose \( \tau = 5/2 \) to match the exponent of a Bose gas in three dimensions, but data from [4] suggests a somewhat lower \( \tau \approx 2.2 \). Although in a Bose gas \( \tau \) is fixed by the dimension of the system, this nuclear fragmentation model is not so constrained, and a different \( \tau \) can be used.

Applying the above choice of parameters to Eq. (4) gives

\[
\frac{C_V}{k_B} = \langle m \rangle \frac{d}{2} + (A - \langle m \rangle) \frac{2k_BT}{\varepsilon_0} \left( \frac{T_0}{T + T_0} \right)^3 + \langle m \rangle^2 \left( \frac{d}{2} + \frac{k_BT}{k_B} - \frac{\varepsilon_0}{\varepsilon_0} \left( \frac{T_0}{T + T_0} \right)^2 \right)^2
\]

\[
PV = \langle m \rangle k_B T + (A - \langle m \rangle) \times \left( \frac{2}{5} \varepsilon_F(\rho) \left( 1 + \frac{5\pi^2}{12} \left( \frac{k_BT}{\varepsilon_F(\rho)} \right)^2 \left( \frac{T_0}{T + T_0} \right) \right) - a_0 \left( \frac{\rho}{\rho_0} \right) + a_3 (1 + \sigma) \left( \frac{\rho}{\rho_0} \right)^{1+\sigma} \right).
\]

Note that the equation of state is particularly simple. The first term is the ideal gas law, while the second term contains the low temperature degeneracy pressure and interaction terms from the Skyrme potential.
The specific heat and equation of state given by the above expression are plotted in Fig. 1. For low $T$, $C_V \propto T$ and is that of a heated nucleus of nucleons treated as a nearly degenerate Fermi gas. At higher $T$, nucleons and clusters are emitted from this nucleus, increasing the number of degrees of freedom and the specific heat. At a relatively low temperature this effect causes a transition from a degenerate Fermi gas to a Bose gas-like state. This change in $C_V$ shows up in the figure as a shoulder. At very high $T$ the nucleus of $A$ nucleons dissolves into $A$ independent nucleons and $C_V = \frac{4}{3} k_B A$. The “cusp” like behavior of $C_V$ can be understood as a critical point in the infinite $A$ limit as discussed in the next paragraph. A rounded peak is seen instead of the cusp because of the finite size of the system. Figure 1(b) illustrates the behavior of $P$ with $V/A$ in the transition region. In this region, the equation of state behaves in many ways like a van de Waals gas.

The thermodynamic limit $A, V \to \infty$ with $\rho = A/V$ finite is of interest since it specifies the critical point behavior and the nature of any phase transitions. In this case, we can work in the grand canonical limit and consider the question of behavior of the largest cluster. A specific concern is whether this theory has the same characteristic as the infinite cluster in percolation theory [34], i.e. for $p > p_c$ the infinite cluster exists while for $p < p_c$ it does not exist. In the grand canonical limit $\langle n_k \rangle$ is given by

\[ \langle n_k \rangle = \frac{x e^{ik/k_B T}}{k^\tau} = \frac{x z^k}{y k^\tau} \tag{10} \]

which implies the mass constraint

\[ \frac{A}{x/y} = \sum_k z^k k^{1-\tau} \tag{11} \]

Here $A/(x/y)$ is finite in the thermodynamic limit since $x \propto V$ and $y = y(\rho, T)$. For $z \leq 1$, the sum is always less than or equal to the case $z = 1$, for which the sum gives $\zeta(\tau - 1)$, i.e. the Riemann zeta function. When $z > 1$ the sum diverges and therefore the constraint cannot hold. Now $A/(x/y)$ is a function of $A/V, T$ which are fixed, so $z$ is the only parameter we can adjust. If $(x/y)/A \leq 1/\zeta(\tau - 1)$ then we can find a $z \leq 1$ such that the mass constraint is satisfied. However, if $(x/y)/A > 1/\zeta(\tau - 1)$ then the constraint can’t
be met. The sum must be truncated, which implies that the expectation of certain large clusters must be identically zero. In other words, when \((x/y)/A > 1/\zeta(\tau - 1)\), there can be no infinite cluster, and \((x/y)_c/A = 1/\zeta(\tau - 1)\) defines a critical point for this system, which is identical to the critical point of a Bose gas if \(y = 1\). Since \(\zeta(\tau - 1) < \infty\) only if \(\tau > 2\), this also implies that the infinite cluster can not exist if \(\tau \leq 2\).

Universality implies the model near the critical point is specified uniquely by two critical exponents. We already mentioned the critical exponent \(\tau\), but another exponent is needed to determine the critical behavior. By the above discussion, the fraction of mass not in the infinite cluster, \(m_x = \lim_{A \to \infty} \sum_{k=1}^{A-1} k\langle n_k \rangle/A\) satisfies \(m_x < 1\) for \(T \leq T_C\) and \(m_x = 1\) for \(T > T_C\). Thus \(\langle n_\infty \rangle = 1 - m_x\) is zero for \(T > T_C\). Near \(T = T_C\), \(\langle n_\infty \rangle \sim (T - T_C)/T_C\).

The analog of \(m_x\) in the Bose system is the fraction of Bose particles in excited states, while \(\langle n_\infty \rangle\) is the fraction in the condensed ground state. For the Bose system the order parameter is taken as the square root of the number of Bosons in the ground state, and in analogy \(\sqrt{\langle n_\infty \rangle} \propto (T - T_C)^{1/2}\), which gives the second critical exponent \(\beta = 1/2\).

In summary, this paper introduced a simplified model for nuclear systems which attempts to be valid across a wide range of temperatures and densities. Building on a model developed earlier [20, 23] with simple expressions for cluster yields, fluctuations and correlations useful in the analysis of inclusive and exclusive data, the thermodynamic properties of the model have been made explicit and the corresponding thermodynamic functions such as the pressure and specific heat were shown to be simple analytic functions of the density, temperature and cumulant moments of the multiplicity. At typical nuclear matter densities and very low temperatures the model is equivalent to a nearly degenerate Fermi gas. At very high temperatures and low densities it reduces to an ideal Maxwell-Boltzmann gas of nucleons. In intermediate regions, the nucleus will break up into clusters of various sizes and the system has some features similar to that of a Bose gas. More importantly, this model exhibits a phase transition in the infinite \(A\) but finite density limit with critical parameters similar to other models of nuclear fragmentation. As in percolation theory, the infinite cluster appears suddenly at the critical point. As in a Bose gas or Feynman’s model of the
\( \lambda \) transition in liquid helium, the specific heat has a maximum at the critical point with a discontinuous derivative. The “cusp” in this model however is smoothed out by the finite size of the system.

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FIGURES

FIG. 1. The specific heat (a) and equation of state (b). The specific heat is Bose-like except at low temperatures, where it transitions to Fermi gas like behavior. In this region, the equation of state shows the characteristic van de Waals behavior.
