Nuclear liquid-gas phase transition within the lattice gas model

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Abstract

We study the nuclear liquid-gas phase transition on the basis of a two-component lattice gas model. A Metropolis type of sampling method is used to generate microscopic states in the canonical ensemble. The effective equation of state and fragment mass distributions are evaluated in a wide range of temperatures and densities. A definition of the phase coexistence region appropriate for mesoscopic systems is proposed. The caloric curve resulting from different types of freeze-out conditions are presented.

It is commonly believed that nuclear matter undergoes a liquid-gas phase transition at lower densities and temperatures. In the early 1980s it was suggested\cite{1} that this phase transition might be probed in heavy-ion collisions at intermediate energies by observing the disintegration of colliding nuclei into many fragments of different sizes, a phenomenon commonly known as \textit{multifragmentation}.

A wide variety of models has been proposed for nuclear multifragmentation, ranging from statistical to dynamical ones (see e.g.\cite{2} for a review). In principle, most of these models yield an equation of state of nuclear matter. The evaluation of the equation
of state is, however, in general rather difficult and has only been done in some simple cases \[3\]. In this paper we focus on the relationship between the fragmentation of a nuclear system and the corresponding equation of state, calculated on the basis of a two-component lattice gas model. In particular, we will discuss the nuclear caloric curve (temperature versus excitation energy) resulting from different types of freeze-out conditions. The details of the model and the numerical simulations will be further discussed in a forthcoming article \[4\]. Here, we only present some main features and results of the model.

Common for all types of lattice gas models is the use of a spatial lattice, with a certain dimension, number of sites, \( N_V \), and a certain Bravais-structure, such that each lattice point has a fixed number of neighbours \( \gamma \). For simplicity and for comparison with earlier works we consider here a simple cubic (\( s.c. \)) lattice with \( \gamma = 6 \). The lattice spacing \( a_0 \) is chosen such that the density of a fully occupied lattice equals the nuclear ground state density \( \rho_0 = 0.16 \text{ fm}^{-3} \), i.e. \( a_0^3 = 1 / \rho_0 \). The effective nucleon-nucleon (\( NN \))-interaction is represented by a nearest-neighbour square well potential \( V \) with a repulsive hard core. In terms of the discretized lattice distance \( r \) between the nucleons \( (r = 0, a_0, \sqrt{2}a_0, \ldots) \) the potential is given as,

\[
V_{ij}(r) = \begin{cases} 
\infty & \text{for } r = 0 \\
\epsilon_{t_3it_3j} & \text{for } r = a_0 \\
0 & \text{for } r > a_0
\end{cases}
\]

Here, \( t_3i \) denotes isospin of nucleon \( i \) and \( \epsilon_{t_3it_3j} \) are the interaction strength parameters. In fact we only allow for two such parameters, \( \epsilon_s \) for \( pp \) and \( nn \) interacting pairs and \( \epsilon_d \) for \( pn \) pairs. According to the dynamical potentials and previous works on lattice models \[5\] \( \epsilon_d \) is chosen slightly repulsive, \( \epsilon_d = 1 \text{ MeV} \). The other parameter, \( \epsilon_s \), is chosen such that the nuclear binding energies are reproduced, \( \epsilon_s = -5 \text{ MeV} \).

If \( \vec{p}_i, \vec{r}_i \) denote respectively the momentum and position of nucleon \( i \), the Hamiltonian of the system of \( A \) nucleons can be written as,

\[
\mathcal{H} = \mathcal{T} + \mathcal{V} = \sum_{i} \frac{p_i^2}{2m} + \sum_{i<j} V_{ij}(\vec{r}_{ij}),
\]

(1)
where $m$ is the nucleon mass. It can be shown that the interaction Hamiltonian $V$ is homomorphic to the spin-1 Ising model, which is well-known in solid state physics. If $\epsilon_s$ is put equal to $\epsilon_d$ the model reduces to the standard lattice gas model which is isomorphic to the spin-1/2 Ising model. This model was first considered in context of nuclear fragmentation in [6] and later used by S. Das Gupta and J. Pan [6, 8] and X. Campi and H. Krivine [9]. The two-component lattice gas model has also been used in [8, 9].

In the following we will for simplicity treat the model in a canonical ensemble. This implies, that the temperature $T$, the volume $V$, the number of particles $A$ and the asymmetry of the system, $y = Z/A$, are the control variables. In this paper we only consider symmetric matter, $y = 0.5$.

The states $f$ of the nuclear system can be classified by the positions, momenta and isospins of all the nucleons, $f = \{(\vec{r}_i, \vec{p}_i, t_3_i) | i = 1, .., A\}$. Due to the classical nature of the model the canonical partition function, $Z$, can be factorized into two parts coming respectively from the momentum space and the configuration space. The first part is proportional to the partition function of an ideal gas. The contribution of the momenta of the nucleons to the various thermodynamical quantities can therefore be calculated in a straightforward way.

The partition function and thus the Helmholtz free energy, $F$, of the configuration space is far less trivial to obtain. In this work it is done numerically by performing a Monte Carlo type of sampling. The realization of this sampling method consists of three parts: the initialization, the equilibration of the system and the calculation of ensemble averages.

The initialization of the system is done by putting the particles one by one in the lattice. At each step the spatial probability distribution is changed with a Boltzmann factor, $e^{-\epsilon_{ij}/T}$, in the neighbourhood of the first particle. This method of initializing the system is identical to the one used in [6].

The equilibration of the system is performed by constructing a random walk of microscopic states $\{f_\nu\}$ through the configuration space via a Markov process, starting

\footnote{A sequence of states each of which depends only on the preceding one}
from the initial state, \( f_{\nu=0} \). The Markov process is defined by specifying a general transition probability matrix, \( p(f \to f') \) from the state \( f \) to the state \( f' \). The choice of the transition matrix is dictated by the detailed balance condition. In the present work it is defined as,

\[
p(f \to f') = \begin{cases} 
  e^{-\beta \Delta V} & \text{if } \Delta V > 0 \\
  1 & \text{otherwise}
\end{cases}
\]  

Here, the test function, \( f' \), is obtained from \( f \) either by changing the position of a randomly chosen nucleon or by interchanging a randomly chosen proton-neutron pair. In case of acceptance, the trial function \( f' \) will be the new state of the system \( f_{\nu+1} = f' \). Otherwise, the system remains in the same state, \( f_{\nu+1} = f_{\nu} \). It can be proven formally \[10\] that the above choice of \( p \) leads to the desired convergence property, i.e. the equilibrated probability distribution of microscopic states will correspond to a macroscopic state of minimum free energy. This algorithm is similar to the one introduced by Metropolis et. al \[11\].

When equilibrium has been reached, the ensemble average \(< Q >\) of any quantity \( Q \) can be calculated by repeating the same procedure a certain number of times and recording the value of the quantity, \( Q_{\nu} \), at each time step \( \nu \).

By a systematic variation of the density \( \rho = A/V \) and the temperature \( T \) the algorithm one can eventually probe all the different points of the phase diagram including the coexistence region. \[4\] The density is varied by varying the number of particles in the lattice for a fixed volume. The volume is put to \( N_V = 6^3 \) which approximately corresponds to the maximum fragment mass, \( A_{\text{max}} = 190 \), observed in heavy ion experiments. The boundaries of this lattice are chosen to be open to mimic the effect of the vacuum surrounding the real nuclear system. The results for periodic boundary conditions will be presented elsewhere \[4\].

The quantities, \( Q \), of interest are the ensemble average \( E(T, \rho) = < V > \) of the potential energy \( V \), and the distributions of cluster sizes, i.e. the mean number of fragments, or the yield \( Y(A) \) as a function of the mass number \( A \). Contrary to most

\[2\]This is an important difference to the grand canonical ensemble which only allows the system to be in a single phase.
statistical models of nuclear fragmentation (see i.e. [2] and references herein), clusters are not explicitly defined in the lattice gas model. In our simulations we implement a definition based on pairwise binding. Two neighbouring nucleons are thus prescribed to the same cluster if their relative kinetic energy is not sufficient to overcome the attractive bond:
\[ \vec{q}^2 / 4m + \epsilon_{i_3i_3} < 0, \]
where \( \vec{q} = \vec{p}_1 - \vec{p}_2 \) is the relative momentum between the two particles. This definition was originally proposed by Hill [12] and has also been used by S. Das Gupta et. al [5].

By applying the standard laws of thermodynamics all other quantities can be derived from the internal energy \( E \) of the system in the different points, \( \rho, T, \) of the phase diagram. One of the most interesting applications is the study of the liquid-gas phase transition in a finite system. The first order phase transition is signalled by the presence of the phase co-existence region. In a finite system the definition of this region is somewhat ambiguous. In the calculations below such regions are identified by the existence of two distinct densities, \( \rho_g < \rho_l \), for which the following conditions are fulfilled,

\[ \mu_l(\rho_l, T) = \mu_g(\rho_g, T) = \mu, \quad F(\rho_l, T)/V = \mu(\rho_l - \rho_g) + F(\rho_g, T)/V \quad (3) \]

The points \((\rho_g, T)\) and \((\rho_l, T)\) belong to respectively the gas branch and the liquid branch of the co-existence curve. Geometrically, the above criteria correspond to the requirement that the points \((\rho_g, f_g)\) and \((\rho_l, f_l)\) belong to a common tangent of the free energy density, \( f = F/V \). For a macroscopic system the free energy density would follow a straight line in the region \( \rho_g \leq \rho \leq \rho_l \). For a mesoscopic system the free energy density is slightly larger in this region due to the presence of an interface between the two phases.

The equation of state for the system with volume \( N_V = 6^3 \) is depicted in Fig. 1 with the pressure \( P \) as a function of density \( \rho/\rho_0 \) and temperature \( T \). The thick solid line is the co-existence curve calculated according to the definition (3). The two branches of the curve terminate at the critical point \((\rho/\rho_0, T, p)_{cr} \approx (0.39, 4.8 \text{ MeV}, 0.15 \text{ MeV/fm}^3)\). For comparison, the critical point in the macroscopic limit is found to be \((\rho/\rho_0, T, P)_{cr} \approx (0.58, 6.7 \text{ MeV}, 0.36 \text{ MeV/fm}^3)\) [4]. In the co-existence region for a fixed temperature the pressure as a function of the density is almost a constant.
One should bear in mind that in experiment one observes only a final state of the system where the fragments cease to interact (freeze-out configuration). It is not clear a priori which thermodynamical conditions correspond to these configurations. Below we consider two possibilities corresponding to constant pressure and constant density at freeze-out. The two lines across the co-existence region are defined by $p = 0.10$ MeV/fm$^3$ and $\rho/\rho_0 = 0.3$, respectively. The letters $A - E$ along the isobar are chosen with a fixed step in densities $\Delta \rho/\rho_0 = -0.15$ starting from $\rho/\rho_0 = 0.75$. The letters along the isochor are chosen at the temperatures $T = (2.4, 3.5, 4.3, 4.9, 6.5)$ MeV (points $c$ and $D$ coincide).

The cluster size distribution corresponding to these points of the phase diagram are shown in fig. 2a and 2b for the isobar $p = 0.10$ MeV/fm$^3$ and the isochor $\rho/\rho_0 = 0.3$ respectively. At point $A$ the system essentially consists of a compound nucleus surrounded by nucleons and small clusters. Point $A$ belongs to the borderline of the co-existence region. At point $B$ the compound nucleus starts to break-up producing some intermediate mass fragments (IMFs: $4 \leq A \leq 20$). At point $C$ and $D$ fragments of all different sizes are present, whereas at point $E$ the size distribution is exponentially decreasing indicating that only the gas phase is present. Thus the appearance of IMFs is a clear manifestation of the first-order liquid-gas phase transition.

The evolution of the size distribution is observed to be smoother along the isochor. Point $a$ belongs to a transition region for which the pressure increases rather abruptly. At even lower temperatures the system essentially consists of one compound nucleus surrounded by vacuum (not shown). The sudden increase of the pressure results from the break-up of this nucleus. As can be seen in the plot this produces some IMFs. The distribution at point $d$ still contains a significant contribution of IMFs although it does not belong to the co-existence region, according to definition of eq. (3). Thus, the cluster size distribution alone can not give a unique relation between multifragmentation and liquid-gas phase transition. At point $e$ the distribution is closer to the exponential one.

Figures 2a and 2b indicate that cluster size distributions are widest at the vicinity of the critical point. If the cluster size distribution is approximated by a power law $Y(A) \sim A^{-\gamma}$, one finds that a good fit can be achieved for a wide range of temperatures and densities around the critical point. The range of fragment masses used for the power
law fit was chosen to $1 \leq A \leq 20$, but the conclusions are not very sensitive to this choice. Typical values of $\chi^2$ per degree of freedom are in the range of $0.03 - 0.13$. Our analysis shows that for each isochor, $\tau$ has a minimum at the binodal line. Furthermore, $\tau$ has a global minimum point in the vicinity of the critical point, where $\tau \approx 2.2$. This is in accordance with the value of the Fisher exponent for the Ising model, $\tau = 2.21$.

From the yield of clusters $Y(A)$ it is not easy to distinguish between the two types of freeze-out conditions. The difference reveals itself more clearly in the associated caloric curves, showing the variation of the temperature with respect to the excitation energy $E^*$ per nucleon. Here, the excitation energy is defined as

$$E^*(A, T) = 3/2 \cdot T \cdot (\langle M \rangle - 1) + E(A, T) - E(A, T = 0),$$

where $\langle M \rangle = \sum_A Y(A)$ is the total multiplicity of the system. Note, that we identify the kinetic part of the excitation energy with the total kinetic energies of the clusters rather than the total kinetic energy $T$ of the individual constituents. The caloric curves for $p = 0.1$ MeV/fm$^3$ and for $\rho/\rho_0 = 0.3$ are shown in Fig. 3. It is seen that the pronounced plateau in the caloric curve appears only in case of the fixed pressure condition. In both cases the caloric curve approaches a straight line for high temperatures. At low temperatures the model predictions are not accurate, since quantal effects cannot be neglected in this region. Qualitatively, the caloric curve at constant pressure looks very similar to the one predicted by the Statistical Multifragmentation Model [13] and recently observed in the ALADIN experiment [14].

To each of curves on the phase diagram, which correspond to a specific change of the system state in a reversible process, a particular heat capacity $C$ can be attributed. Our analysis shows, that the specific heat capacity for fixed pressure, $C_p$, in fact has a singularity along subcritical isobars. This infinity is related to the latent heat of the transition. On the other hand, due to finite size effects the specific heat capacity for fixed number of particles and volume, $C_V$, is finite in all points of the phase diagram. We will elaborate further on these points in a forthcoming publication [14].

In conclusion, our results demonstrate the close connection between the nuclear liquid-gas phase transition and the nuclear multifragmentation. The calculations have
been made on the basis of a two-component lattice gas model. A sampling method has been presented by which both the effective equation of state and the fragment mass distributions have been evaluated in a consistent way. The method has an advantage compared to other statistical approaches to nuclear multifragmentation, where the link between the cluster observables and the corresponding thermodynamical properties of the nuclear system is less transparent.

We have proposed a definition of the phase transition, more relevant for finite systems, which is based on the identification of an interphase between the two phases. The relevance of this definition is supported by the critical exponent analysis and the singular behaviour of the specific heat capacity, $C_p$, along subcritical isobars. We have examined the caloric curve resulting from two different freeze-out conditions. It was demonstrated that the occurrence of a plateau in the caloric curve seems to be consistent with the condition of constant and subcritical pressure in the freeze-out configurations.

There are of course some obvious deficiencies of the model. First, the true Fermi-statistical nature of the nucleons can not be neglected for lower excitation energies. Secondly, the idea of a thermal bath is certainly an idealization and it is necessary to perform a real microcanonical sampling in the Monte Carlo algorithm. Third, for larger systems it is necessary to include the Coulomb repulsion and determine the corresponding change of the phase diagram. Finally, the prescription of clusters in the model is still not unambiguous. The clusters defined by the pairwise binding are generally excited and should undergo de-excitation at later stages (see [15]). In the future, we plan to improve the model in various respects to take these deficiencies into account.

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Figure captions

**Fig. 1.** Pressure $P$ as a function of density $\rho/\rho_0$ and temperature $T$ for a lattice with $N_V = 6^3$ sites. The thick solid line is the co-existence curve. The line with capital letters is the isobar $p = 0.1 \text{ MeV/fm}^3$. The line with small letters is the isochor $\rho/\rho_0 = 0.3$.

**Fig. 2.** The yields $Y(A)$ as functions of the fragment mass $A$ corresponding to different points of the phase diagram: a) The points $(A - E)$ belong to the isobar $p = 0.10 \text{ MeV/fm}^3$, b) the points $(a - e)$ belong to the isochor $\rho/\rho_0 = 0.3$. Note the different scales on the x-axis.

**Fig. 3.** The temperature $T$ as a function of the specific excitation energy $E^*/A$ for two different freeze-out conditions. The solid line corresponds to the fixed pressure condition, $p = 0.1 \text{ MeV/fm}^3$, and the dotted line corresponds to the fixed density condition, $\rho/\rho_0 = 0.3$. The letters along the lines refer to fig. 1.
Figure 3