A CLASSICAL MOLECULAR DYNAMICS STUDY OF THERMODYNAMIC VARIABLES FOR FINITE NUCLEAR SYSTEMS

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Abstract

The classical molecular dynamics model is used for a study of the possible nuclear phase transition in heavy ion collisions at intermediate energies. We implemented this model through Monte Carlo techniques. Different kinds of initial configurations are considered, as well as different methods of particles propagation. In order to simulate the canonical ensemble dynamic evolution we investigate two methods of keeping the temperature constant.

We consider a system of 85 nucleons interacting through two-body nucleon-nucleon potential. The calculations are first carried out ignoring Coulomb interaction and then including it. Data on various thermodynamic quantities are obtained and the question of the existence of the phase transition is investigated.

To estimate the effect of a finite particle number on critical parameters we go to a system of 200 nucleons.

Résumé

L'approche de la dynamique moléculaire classique est utilisée pour l'étude de la transition de phase liquide-gaz éssentuelle, dans les collisions d'ions lourds aux énergies intermédiaires. Des techniques Monte Carlo sont utilisées dans l'application de ce modèle. Nous considérons plusieurs types de configurations initiales, ainsi que plusieurs méthodes de propagation des particules. Nous avons également comparé deux méthodes destinées à maintenir la température constante, pour des simulations numériques dans l'ensemble canonique.

Nos calculs concernent tout d'abord des systèmes de 85 nucléons en interaction binaire. Nous étudions l'effet du potentiel de Coulomb. Nous obtenons des résultats sur plusieurs variables thermodynamiques et nous traitons aussi de l'existence de la transition de phase.

Finalement, nous jugeons de l'étendue des effets du nombre fini de particules en allant à un système de 200 nucléons.

Aknowledgments

It is my pleasure to express my deep gratitude to Prof. Charles Gale who advised me through the course of the study and whose kind support, patience and attention inspired me all this time.

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Contents

Chapter 1

Introduction

The description of a nuclear reaction at high energies represents one of the very interesting issues straddling nuclear physics and high energy physics. It has been widely investigated experimentally in heavy-ion collisions at intermediate and high energies. Nevertheless only a small subset of the reaction channels available can be theoretically handled in even an approximate way. Considerable progress during recent years in the experimental research [1, 2, 3] causes further interest in theoretical studies. One of the fundamental problems in studying heavy-ion reactions is how the formed nuclear system will disassemble. Experimental evidence for a universal property of nuclear fragmentation, almost independent of the chosen targets, energies of the bombarding particles and experimental techniques, offers us opportunity of applying and inspecting various models proposed previously for the phenomenon. We are concerned here with one of those approaches.

1.1 Foreword

A heavy ion collision forms a system of a few hundred nucleons. The number of particles participating in a reaction is far from the thermodynamical limit, but still hopefully large enough that the signs of collective behaviour can be clearly observed. On the other hand, a large part of the cross section at intermediate and high energies involves multiple scattering among the many nucleons present in the reaction region. The great number of particles also creates a great number of relevant degrees of freedom. It offers the possibility that statistical effects will dominate.

At the same time, the heavy ion reaction is a highly dynamical process. Both equilibrium and nonequilibrium properties of the matter can be studied. In statistical equilibrium, the thermodynamical observables of the system are described by an equation of state. One of the interesting aspects of the equation of state of a "small"

dynamical system is the phase transition from continuous nuclear liquid into a nuclear vapor of fragments and nucleons, the so-called nuclear liquid-gas phase transition, and its connection to multifragmentation [4]. It is still very much an open and active field of research of intermediate energy heavy ion reactions.

One might consider the nuclear multifragmentation as a multi-step process. In the first step, a highly excited thermalized nuclear source with certain mass, energy and other macroscopic parameters, dependent on the impact parameter b, is formed. Then the so-called transition stage [11, 12] takes place. After this, the system decays into fragments observed as final products of the reaction. The second step is relevant to our understanding of the equation of state at densities smaller than the normal nuclear density $\rho_0 = 0.16\, fm^{-3}$. Figure 1.1 illustrates how knowledge of statistical properties of hot nuclear matter could allow us to predict fragment production in heavy ion collisions.

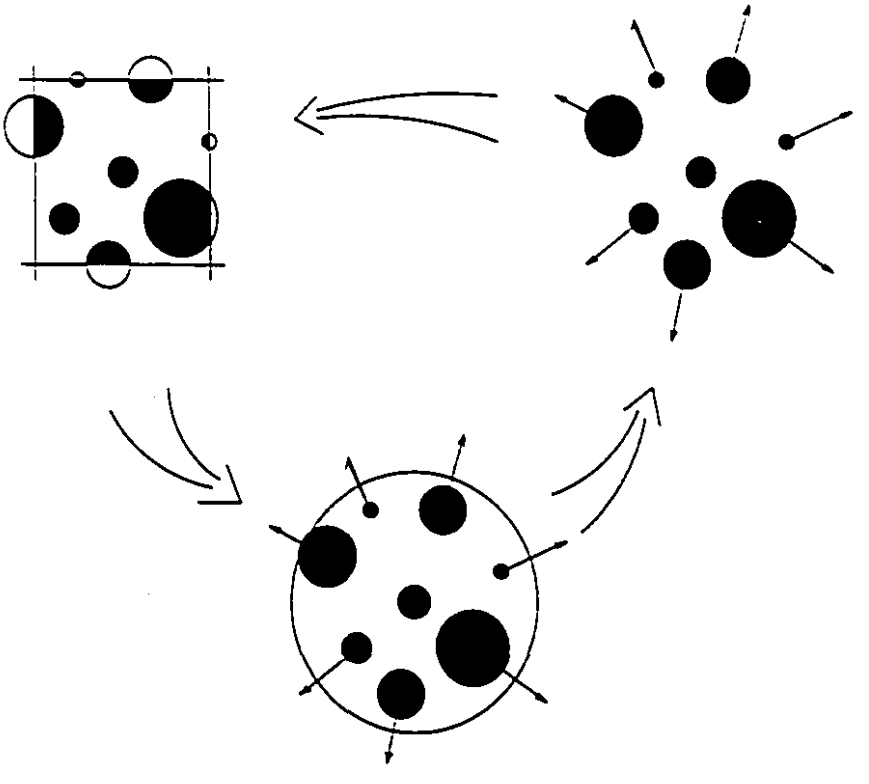

Figure 1.1: Illustration of nuclear multifragmentation. In left upper corner the highly excited nuclear system is formed, at the bottom of the picture the transition state is drawn, and in the right upper corner – the nuclear fragmentation.

There are many models to describe the phenomenon of multifragmentation. Most

common of those are the percolation model [5, 6], the lattice gas model [7, 8], the quantum molecular dynamics model [9], the thermodynamical model [10], the statistical multifragmentation model [11, 12, 13] and the classical molecular dynamics model [14].

The theoretical studies of classical molecular dynamics are interesting in their own right, and we turn to them now.

1.2 General description of the molecular dynamics model

We shall here formulate the model that allows a statistical simulation of nuclear multifragmentation and the extraction of associated thermodynamic quantities, such as the equation of state using the methods of classical molecular dynamics.

We can start considering our molecular dynamics model from the reference to the microcanonical ensemble presentation. Work has been done [11, 12, 13] in the microcanonical simulation of nuclear multifragmentation. In that ensemble the macrostate of the system was defined through a fixed number of particles N, a fixed volume V and a fixed energy E. However, in our study, since we look for a thermodynamic phase transition and try to extract the data on critical parameters, we rather would like to search for an alternative approach to this ensemble theory, an ensemble where the parameters are N, V and T. Such an ensemble is referred to as a canonical ensemble. This choice allows us to calculate easily the value of the specific heat, that, as will be shown in Section 2.2.2, can be used in the critical parameters determination.

We define the interparticle interaction differently for neutron-proton interaction, which is attractive for large separation distances, but has a hard repulsive core for small ones, and for neutron-neutron and proton-proton interactions, which are chosen to be identical and purely repulsive. We postpone a complete description of the potential until page 7. Such a choice of interparticle interaction helps us to obey the basic requirements of nuclear matter structure, simulating partially the Pauli exclusion principle. Coulomb interaction is then added separately, if desired.

The system is initially constructed using a cubic lattice distribution (see page 24) for the particle positions in space and Maxwell-Boltzmann distribution to generate particle velocities. The ensemble is relaxed to thermal equilibrium. Then the temperature is reset to the desired value.

The particles are propagated in phase space satisfying Newton's equation of motion, slightly modified in order to keep the temperature constant (page 13).

Pressure data for canonical ensemble simulation has been obtained by means of a virial expansion on page 16.

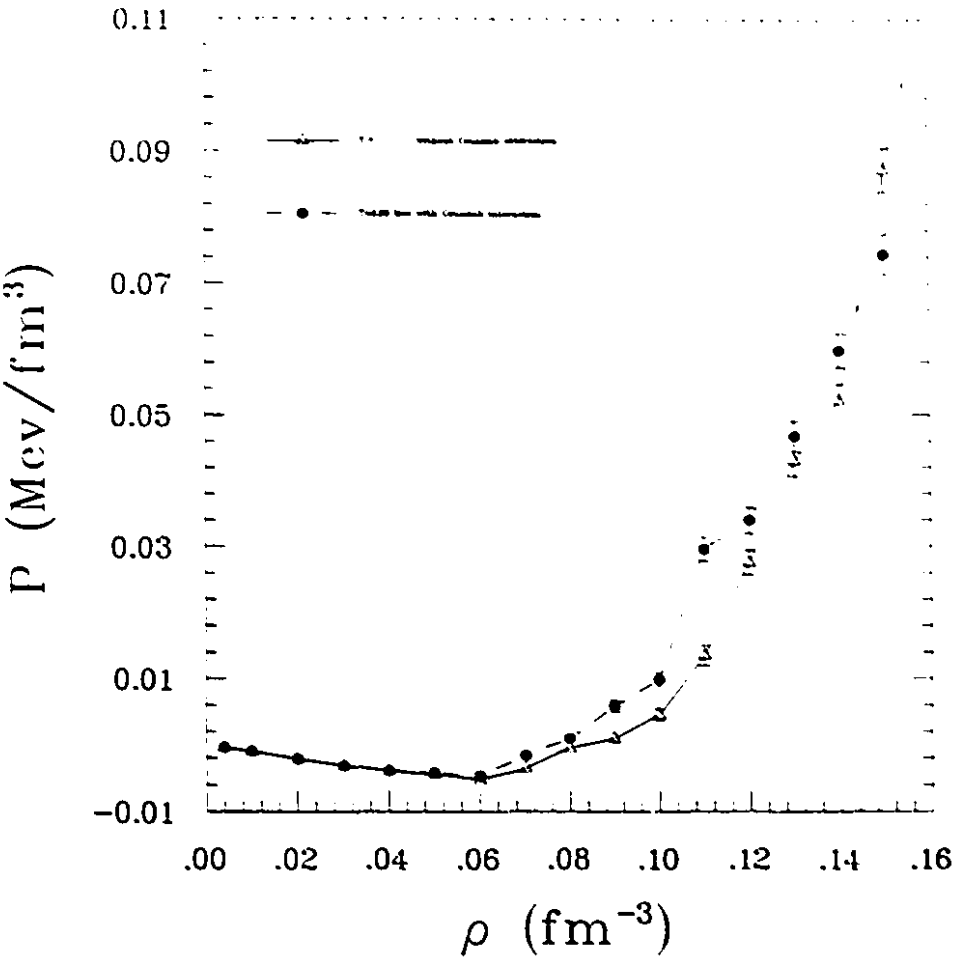

Figure 1.2: Pressure against density for the system of 137 nucleons at temperature $T = 0.3\,MeV$ with (circles) and without (triangles) taken into account Coulomb interaction.

Using the molecular dynamics approach we are trying to find out whether the liquid-gas phase transition takes place, and if so, determine the critical parameters. There are clear evidences of nuclear phase transition obtained in molecular dynamics model. For example for a system of 137 nucleons, 57 protons and 80 neutrons, as can be seen in Figure 1.2, pressure is about constant for a variety of densities for $P - \rho$ isotherm $T = 0.3\,MeV$, this can be considered as an evidence of mixed phase region. The negative slope regions of this graph can not be interpreted literally: they are due to finite-particle number effects [14]. The flattening happens also for the system with the Coulomb interaction turned on. That is why it is important to consider the question of the phase transition existence in presence of the Coulomb field and without it. Going one step further it does look interesting to estimate the effect of the finite number of particles on phase transition appearance.

The thesis is organized according to the course of our calculations. First in Chapter 2 we investigate the appearance of a phase transition in a system of 85 particles interacting through a two-body nucleon-nucleon potential ignoring the Coulomb interaction. Second in Chapter 3 we take into account the Coulomb field and search for its effects on the critical parameters. And at last, we investigate the influence of finite number of particles by comparing the results obtained with those for a system of 200 nucleons.

Chapter 2

Searching for signs of a nuclear phase transition for a system of 85 nucleons

In this chapter we shall investigate the appearance of a phase separation in a canonical ensemble of 85 particles interacting through a two-body nucleon-nucleon potential ignoring the Coulomb interaction. Our choice of a 85 particles system is connected to experimental work [15] that has been done for the system earlier.

2.1 Description of the computer experiment

To simulate the behaviour of the system in time we use the Monte Carlo method of computer simulation. This type of calculation provides what may be considered as essentially exact results for a given interparticle force law, which in our case is combinations of Yukawa interactions [16]:

$$V_{nn}(r < r_c) = V_0 \left[exp(-\mu_0 r)/r - exp(-\mu_0 r_c)/r_c\right] \quad (2.1)$$

$$V_{np}(r < r_c) = V_r \left[exp(-\mu_r r)/r - exp(-\mu_r r_c)/r_c\right] - V_a \left[exp(-\mu_a r)/r - exp(-\mu_a r_c)/r_c\right] \quad (2.2)$$

where $V_0 = 373.118\, MeV \cdot fm$, $V_r = 3088.118\, MeV \cdot fm$, $V_a = 2666.647\, MeV \cdot fm$, $\mu_0 = 1.5\, fm^{-1}$, $\mu_r = 1.7468\, fm^{-1}$, $\mu_a = 1.6\, fm^{-1}$.

We use neutron-proton interaction $V_{np}(r)$ (Equation 2.2) that is attractive at large r and repulsive at small r, while $V_{nn}(r)$ (Equation 2.1) is purely repulsive. Figure 2.1

represents our potentials as functions of distance. This choice allows us to construct a system in such a way that nuclear matter is bound with the correct binding energy per nucleon, while di-neutrons and di-protons can not form. This potential, therefore, generates good nuclear phenomenology.

One may choose a cutoff radius $r_c = 5.4\, fm$ as a result of the practical assumption that

$$V_{nn}(r > r_c) = V_{np}(r > r_c) = 0 \tag{2.3}$$

In fact, for distances greater than the cutoff radius, r_c, the interaction between nucleons is negligibly small and is ignored in order to simplify numerical calculations (see Figure 2.1).

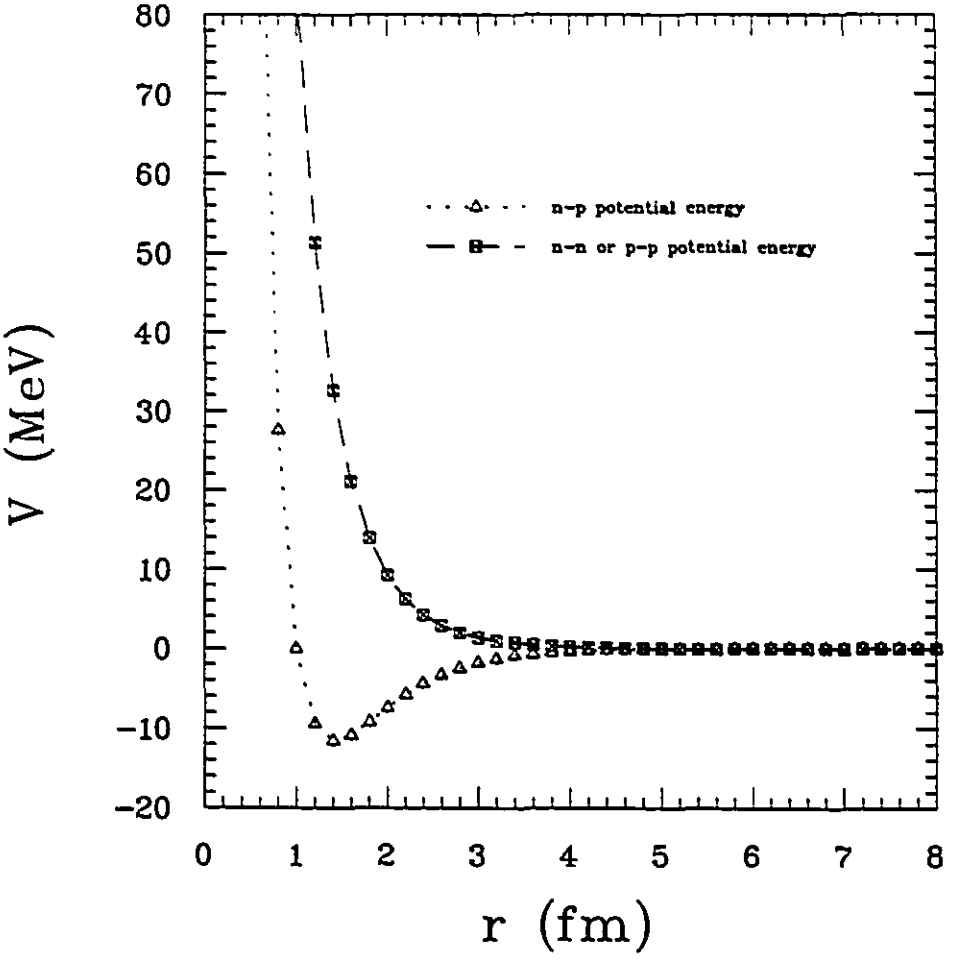

Figure 2.1: Potential energies acting between neutron and proton and between two identical nucleons as a function of distance.

In these studies, the Coulomb interaction is first ignored and the potential V_{nn} is taken to be equal to V_{pp}.

In the Monte Carlo technique it is necessary to define a starting configuration for the first simulation, that then can be relaxed to the structure and velocity distribution appropriate to the system. To assign the initial particle positions in space we used a cubic lattice distribution. We shall postpone the discussion of the cubic lattice distribution until page 24. Let us simply state for the moment that this way of designing a starting configuration helps us to avoid overlaps and infinities in the calculation of the potential since we control the initial distances between particles.

Particle velocities were generated according to the Maxwell-Boltzmann distribution for a specified temperature T:

$$f_{MB}(\mathbf{r},\mathbf{p}) = \frac{\rho(\mathbf{r})}{(2\pi m k_B T)^{3/2}} \exp[-\beta\,|\mathbf{p}|^2/2m)] \tag{2.4}$$

where $\rho(\mathbf{r})$ is defined as

$$\rho(\mathbf{r}) = \int f_{MB}(\mathbf{r},\mathbf{p})\,d\mathbf{p}$$

and m is the mass of a nucleon, k_B is Boltzmann's constant and $\beta = 1/k_B T$ with the probability density normalization for N identical particles:

$$\iint f_{MB}(\mathbf{r},\mathbf{p})\,d\mathbf{r}\,d\mathbf{p} = N.$$

From here on, we set $k_B = 1$ and therefore now we measure the temperature in energy units.

In order to relax the initial lattice to an appropriate configuration of our system one can propagate it in time, rescaling the velocities at each timestep by some factor, until system has come to the thermal equilibrium. From then an instantaneous pressure, potential, kinetic and total energy will be oscillating about average values independent of time, having reached their limiting behaviour. In the calculation, this so-called "cooling" period was chosen to be 100 timesteps that corresponds to $5\cdot10^{-13}$ sec.

Evolution of the parameters mentioned above during equilibration phase are shown in Figure 2.2, 2.3. At the end of the time sufficient for equilibration the temperature is reset to the desired value.

Solution of the classical equations of motion for a system of N particles via computer supposes using one of the finite-difference methods of particle propagation. Let

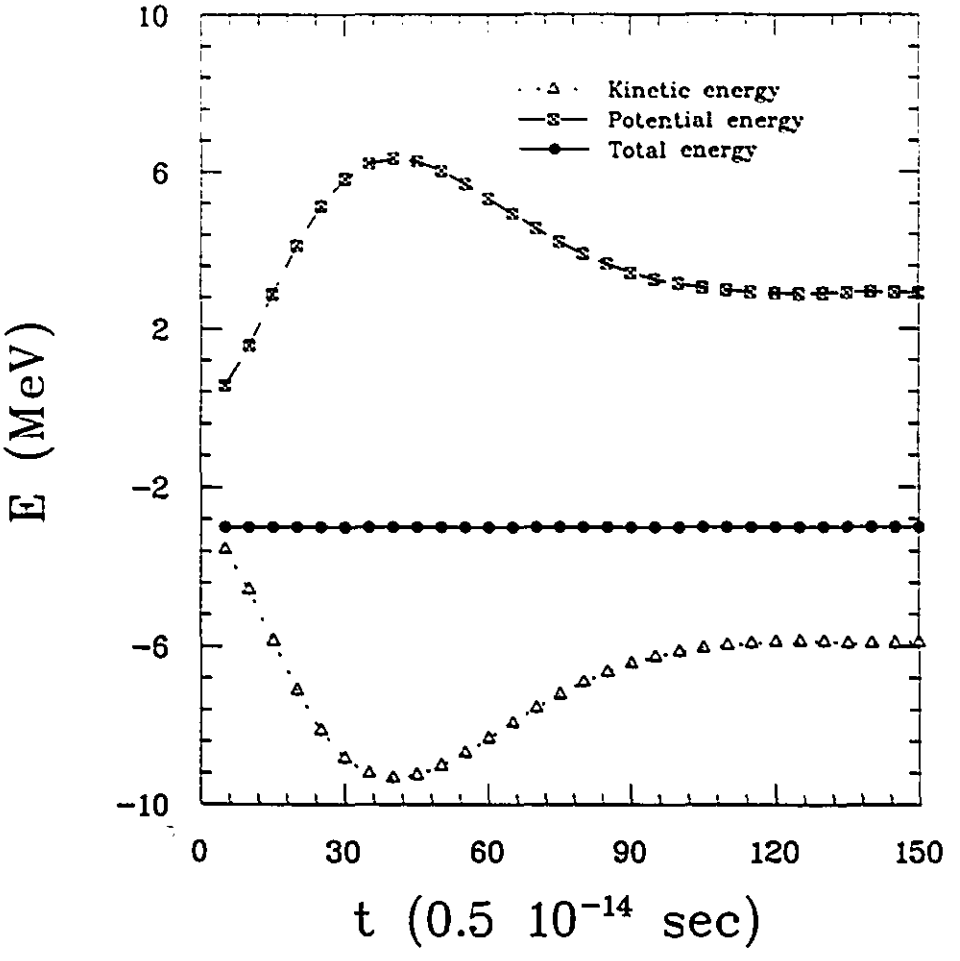

Figure 2.2: Kinetic, Total and Potential energies. Particle propagation is calculated in the "leapfrog" algorithm.

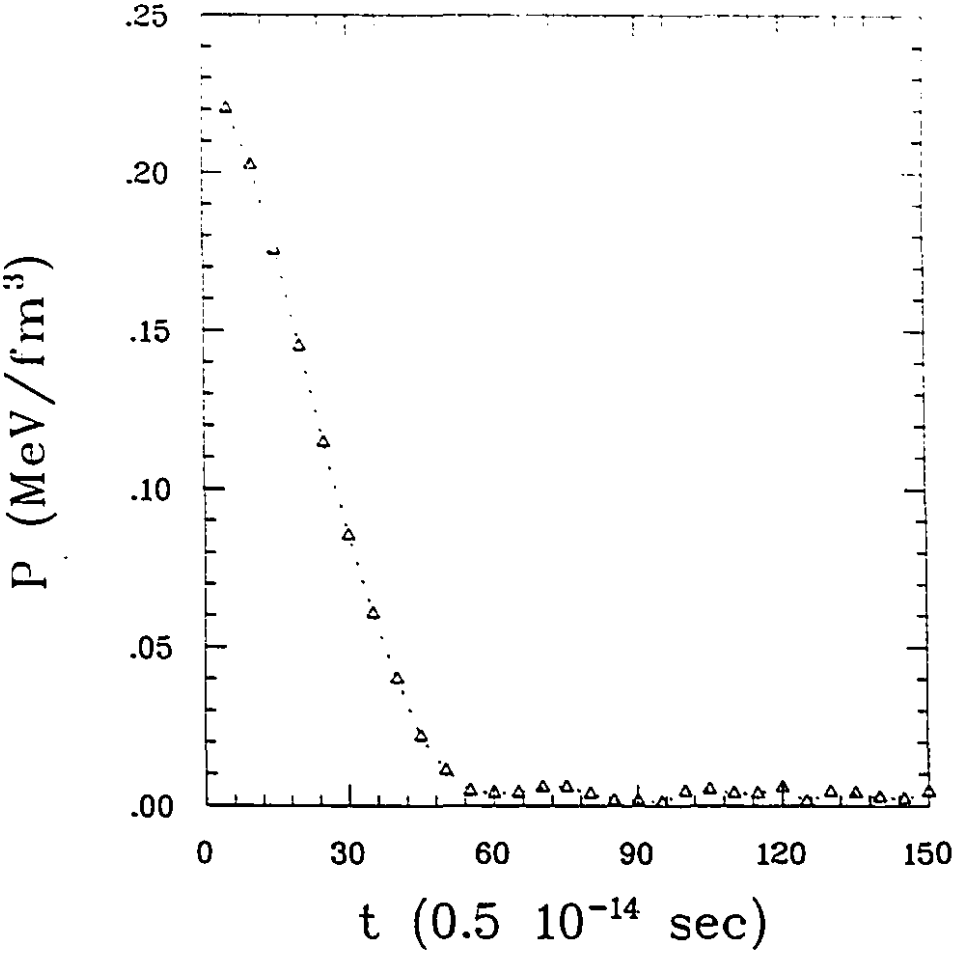

Figure 2.3: Instantaneous Pressure. The value of the pressure in the equilibium limit is small but nonzero. The cooling period, discused on page 9, corresponds here to $t < 60$ timesteps ($3 \cdot 10^{-13}$ sec).

us consider as an example one of the last point approximations, Euler's method, where positions are propagated in time with a step δt as

$$\mathbf{r}(t + \delta t) = \mathbf{r}(t) + \mathbf{v}(t)\,\delta t + \mathbf{a}(t)\,(\delta t)^2 \tag{2.5}$$

and velocities as

$$\mathbf{v}(t + \delta t) = \mathbf{v}(t) + \mathbf{a}(t)\,\delta t \tag{2.6}$$

As a measure of accuracy of the numerical method it is necessary to pay attention to the deviation of numerically calculated energy from its original value. For Euler's algorithm the error in energy is proportional to δt. Results obtained for the system of

85 nucleons interacting through potential in Equations 2.1, 2.2 using Euler's method of time propagation are represented in Figure 2.4.

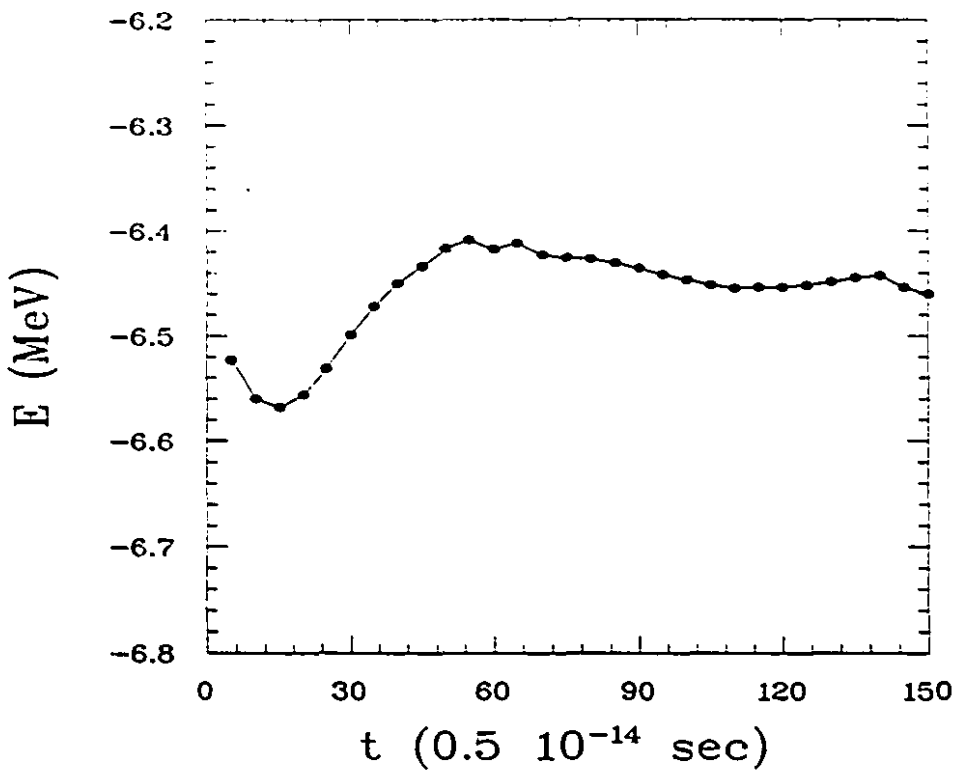

Figure 2.4: Total energy calculated using Euler's method of time propagation against time.

As can be seen the total energy significantly fluctuates over some average value.

A better way to propagate the system in time is a half-step approximation, the so-called "leapfrog" scheme [17, 18]. Current positions and mid-step velocities are calculated as

$$\mathbf{r}(t+\delta t) = \mathbf{r}(t) + \mathbf{v}(t+\frac{1}{2}\delta t)\,\delta t \tag{2.7}$$

$$\mathbf{v}(t+\frac{1}{2}\delta t) = \mathbf{v}(t-\frac{1}{2}\delta t) + \mathbf{a}(t)\,\delta t \tag{2.8}$$

The current velocities may then be evaluated

$$\mathbf{v}(t) = \frac{1}{2}\left[\mathbf{v}(t+\frac{1}{2}\delta t) + \mathbf{v}(t-\frac{1}{2}\delta t)\right] \tag{2.9}$$

In such an algorithm, errors in the total energy are proportional to $(\delta t)^2$. Therefore it has some considerable advantages concerning energy conservation. As can be seen in Figure 2.2 the graph for total energy is essentially a straight line.

Other benefits of the method derive also from the fact that, using "leapfrog" scheme, it is much easier to develop and apply a numerical method keeping temperature constant. It is convenient to define an instantaneous "kinetic" temperature function

$$\mathcal{T} = 2K/3N = \frac{1}{3N}\sum_{i=1}^{N} \mid \mathbf{p}_i \mid^2 /m \tag{2.10}$$

whose average is equal to Θ. K here is a kinetic energy. Then a simple method of fixing the kinetic temperature of a system is to rescale the velocities at each timestep by a factor of $(T/\Theta)^{1/2}$ where Θ is the current kinetic temperature and T is the desired thermodynamic temperature. We shall call it - "rescaling method". It turns out to be a crude method of solving the equations of motion that differs from Newtonian ones. A better way is a constraint method, where constant kinetic temperature dynamics is generated by the equations of motion [19, 20] for individual position and momentum

$$\dot{\mathbf{r}} = \mathbf{p}/m \tag{2.11}$$

$$\dot{\mathbf{p}} = \mathbf{f} - \xi \mathbf{p} \tag{2.12}$$

where $\mathbf{f}$ is a force acting on particle.

The quantity ξ

$$\xi = \sum_{i=1}^{N} \mathbf{p}_i \cdot \mathbf{f}_i / \sum_{i=1}^{N} |\mathbf{p}_i|^2 \tag{2.13}$$

is a "friction coefficient" which varies in time so as to keep Θ constant and, hence, has to be recalculated at each timestep.

In Figure 2.5 both methods of keeping the temperature constant are compared. As one can see constraint method corresponds to a straight line, while temperature defined using rescaling method significantly fluctuates and leads away from the required value.

For the leap-frog algorithm Equation 2.11 takes the form of a modified velocity equation

$$\dot{\mathbf{r}}(t + \frac{1}{2}\delta t) = \dot{\mathbf{r}}(t - \frac{1}{2}\delta t) + [\mathbf{f}/m - \xi \dot{\mathbf{r}}(t)]\, \delta t \tag{2.14}$$

and implemented in [14].

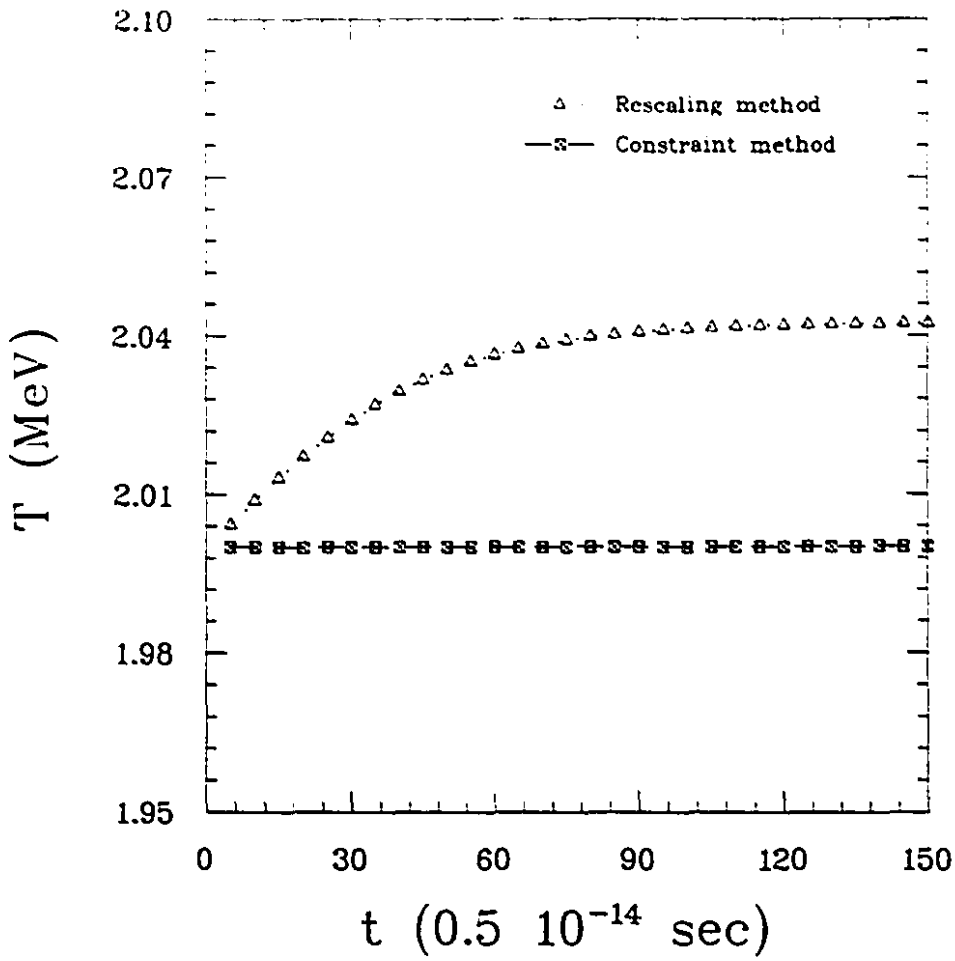

Figure 2.5: Temperature versus time calculated using rescaling and constraint methods of temperature fixing.

This technique gives us a chance to perform constant temperature dynamics calculations by defining the constrained Newtonian trajectories that generate the canonical ensemble.

2.2 Dynamic Evolution and Thermodynamic Quantities

It is instructive to discuss the dynamic evolution of a canonical ensemble of N particles in terms of thermodynamic quantities, such as temperature T, pressure P and density ρ. Our task is to estimate those quantities that would characterize the statistical equilibrium of the system. The problem can be stated as follows: one has to extract definite but unknown values of thermodynamic quantities from knowledge of position and velocity configuration of the particles propagating in time. In this section we describe how to achieve this and the results obtained.

2.2.1 Pressure

Before proceeding to collect pressure data one had better discuss the way we define density. For purposes of the initial configuration simplicity we define our volume V as a volume of the cubic box of a fixed size. The mean density then follows as $\rho = N/V$. We can always choose the size of the box so as to obtain the desired value of density.

A simple method of obtaining the value of the pressure is to calculate the momentum transfer caused by elastic reflections of the particles off the walls and then to take an average over time. Then pressure on a cubic box can be expressed in terms of the acting force per unit area. If δt is a time interval where the change of velocity $2v_i$ takes place, then the force is

$$F_i = m\,a_i = \frac{2m\,v_i}{\delta t} \tag{2.15}$$

Since the total area of the box contains six areas S of the box sides finally we have

$$P_{change} = \left\langle \sum_{i=1}^{N} \frac{F_i}{6\,S} \right\rangle = \left\langle \sum_{i=1}^{N} \frac{m\,v_i}{3\,S\,\delta t} \right\rangle \tag{2.16}$$

where the sum includes N identical particles of mass m.

Another way to get the pressure in the case of a two-body interaction comes from the use of the virial theorem. Pressure in the system of N particles at density ρ is calculated as follows [21]

$$\frac{P_{virial}}{\rho T} = 1 - \frac{1}{6NT} \left\langle \sum_i \sum_{j>i} r_{ij} \frac{\delta V_{ij}}{\delta r_{ij}} \right\rangle - \frac{\rho}{6T} \int_{r_{cut}}^{\infty} r \frac{\delta V}{\delta r}\, g(r) \delta r \tag{2.17}$$

where $g(r)$ is the pair distribution function defined as

$$g(r) = \rho^{-2} \left\langle \sum_i \sum_{j \neq i} \delta(r_i)\, \delta(r_j - r) \right\rangle = \frac{V}{N^2} \left\langle \sum_i \sum_{j \neq i} \delta(r - r_{ij}) \right\rangle \tag{2.18}$$

The first term in Equation 2.17 corresponds to the ideal gas term. The second one is the time average of the virial, where $-\delta V_{ij}/\delta r_{ij}$ is the force acting between particles i and j. The last term is the correction that takes into account the contribution of the tail of the potential V. The size of this tail term in final results can be estimated by considering the cutoff tail as a weak long-range perturbation. In [22] it is shown that the effect on the main term is quite small for our kind of potentials, it is even smaller than the statistical error and can be neglected.

As can be seen in Figure 2.6 the results for the pressure as a function of density at temperature 1.0 MeV obtained using those two methods are identical, up to statistical errors.

To check the consistency of our numerical approach it would be appropriate to compare the results obtained with the results of an approved model of thermodynamics. As a test we can turn off the interaction between particles creating in such a way the system of identical point-like particles that may be treated as an ideal monoatomic gas. In that model we expect the pressure to satisfy the equation of state of N particles at temperature T [21]

$$PV = NT \tag{2.19}$$

We see that, at constant temperature, pressure P is proportional to $1/V$, that is, P is proportional to the density.

The pressure data obtained in such simplification for 85 particles and $T = 2.0$ MeV are drawn on the Figure 2.7. It completely coincides with the theoretical curve of Equation 2.19 for an ideal monoatomic gas.

As a result of the Monte-Carlo calculation carried out for different densities and temperatures we obtained some data for canonical ensemble averages over certain period of time. Pressure versus density for different given temperatures 0.5 MeV, 0.7 MeV and 0.9 MeV are represented in Figure 2.8.

As one can see from the Figure 2.8 for the isotherms T below 0.9 MeV and densities within the range 0.02 and 0.06 fm^{-3} there is a plateau in the pressure that may be considered as a mixed phase region [21] where the nuclear matter liquid is converted into vapour of nuclear fragments as one goes to the lower densities. Analyzing data of pressure dependences on density for a variety of temperatures, we can estimate the critical parameters for a given system. We expect the critical temperature to be below 0.9 MeV, since for this isotherm there is already no apparent inflection point in the

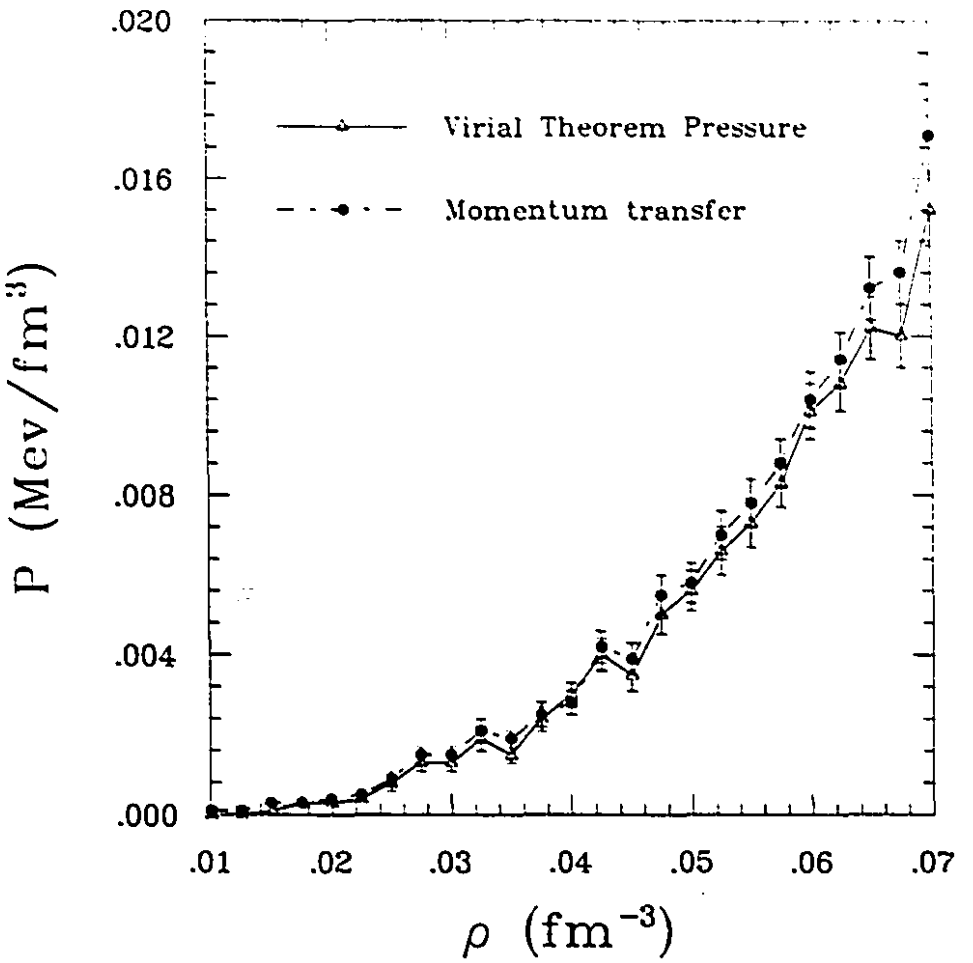

Figure 2.6: Pressure as a function of density at $T = 1.0\,MeV$. The errors are statistical.

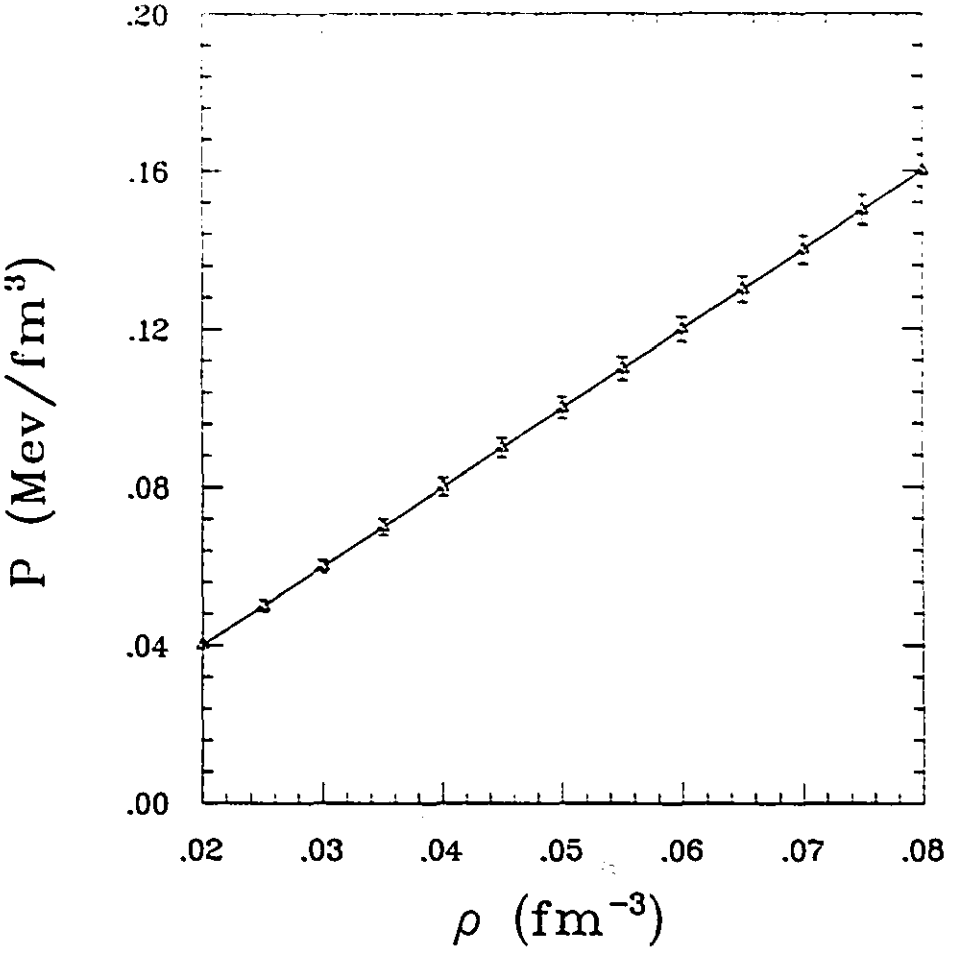

Figure 2.7: Pressure of our noninteracting system (triangles) and pressure of an ideal gas (solid line) versus density for $T = 2.0\,MeV$

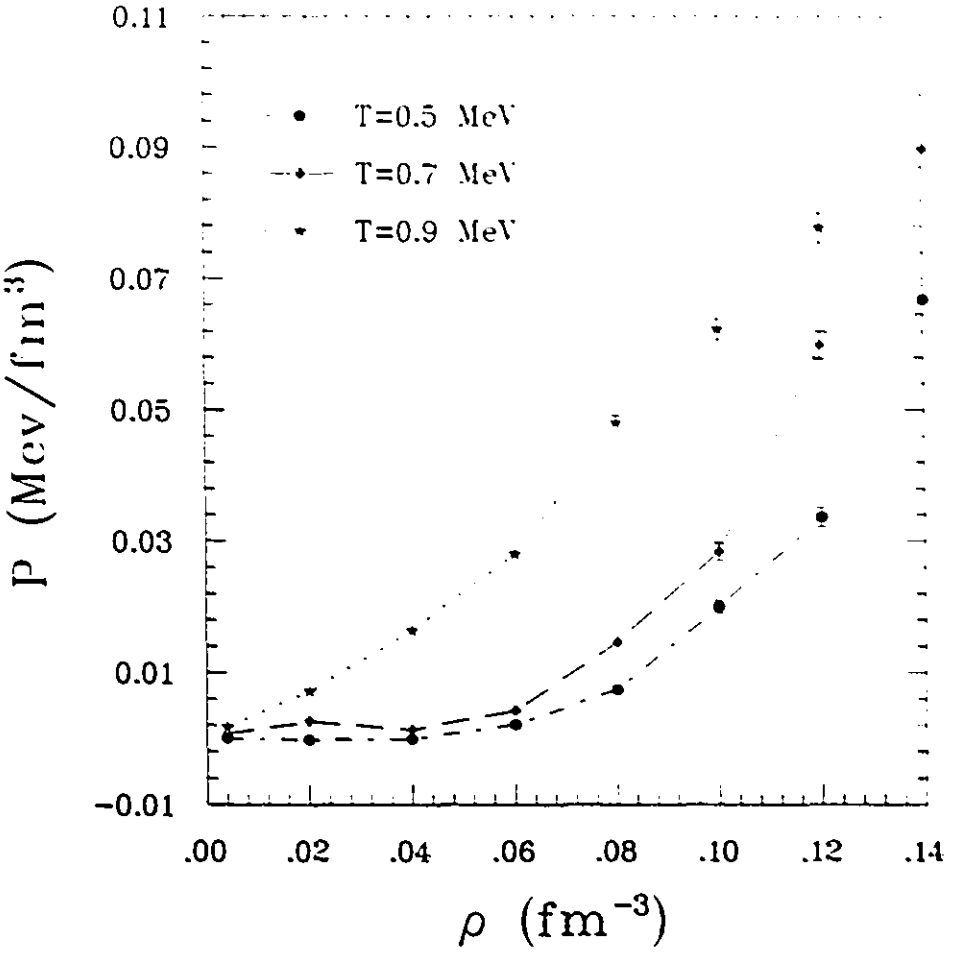

Figure 2.8: Pressure as a function of density for different values of temperature T.

pressure curve, and higher than 0.7 MeV, since for the isotherms below 0.7 MeV there is a wide plateau there. Critical density lays between 0.03 and 0.04 fm^{-3}. That region corresponds to the flattening of pressure over a variation of density. To help us in our estimates, we need some additional information as, for example, data on the specific heat or isothermal compressibility, on potential and total energy.

2.2.2 Specific heat

In order to obtain an expression for specific heat at constant volume characterizing the canonical ensemble we recall that specific heat is defined thermodynamically as a derivative of energy with respect to temperature

$$C_V = \left(\frac{\delta\langle E_N\rangle}{\delta T}\right)_V = \frac{\delta\langle E_N\rangle}{\delta\beta}\frac{\delta\beta}{\delta T} = -\frac{1}{T^2}\frac{\delta\langle E_N\rangle}{\delta\beta} \tag{2.20}$$

where $\beta = 1/T$.

Taking into account the fact that

$$\langle E_N\rangle = \frac{\sum_i E_i\, e^{-\beta E_i}}{\sum_i e^{-\beta E_i}} \tag{2.21}$$

Equation 2.20 can be transformed to

$$C_V = \frac{1}{T^2}\frac{\sum_i E_i^2\, e^{-\beta E_i}}{\sum_i E_i\, e^{-\beta E_i}} - \frac{1}{T^2}\frac{\left(\sum_i E_i^2\, e^{-\beta E_i}\right)^2}{\left(\sum_i E_i\, e^{-\beta E_i}\right)^2} \tag{2.22}$$

that is related to mean-square deviation of the total energy from its average value:

$$C_V = \frac{1}{T^2}[\,\langle E_N^2\rangle - \langle E_N\rangle^2\,] \tag{2.23}$$

The total energy can be separated into kinetic and potential terms $E_N = K_N + V_N$ which are uncorrelated (i.e. $\langle\,\delta K_N\,\delta V_N\,\rangle = 0$). The kinetic part is calculated easily in the case of a system of N particles at constant temperature T. Taking into account the fact that $\langle K_N\rangle^2 = 0$, the answer is

$$\langle K_N^2\rangle = \frac{3N}{2}T^2 \tag{2.24}$$

yielding the ideal part of the heat capacity $C_V^{id} = (3/2)N$.

Then equation 2.23 transforms to

$$C_V = \frac{1}{T^2}[\,\langle V_N^2\rangle - \langle V_N\rangle^2\,] + \frac{3}{2}N \tag{2.25}$$

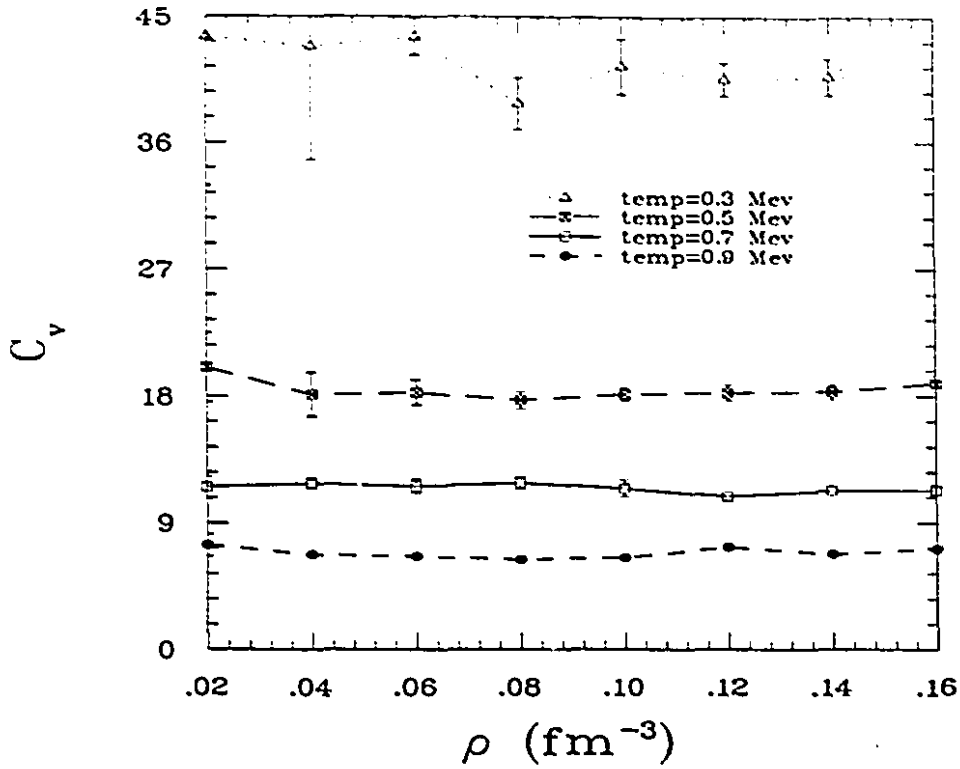

Figure 2.9: Heat Capacity per nucleon as a function of density for different value of temperature T for a system of 85 nucleons. In the system of units, that we use, C_v is dimensionless, since we set the temperature to be measured in units of energy.

Results for *specific* heat capacity (heat capacity per particle) versus density calculated using formula 2.25 are shown in Figure 2.9.

For a density near the critical density, it is known from mean field theory that the specific heat capacity as a function of temperature is expected to have a maximum for $T = T_c$. In our case, since we have an exact model, we can easily go beyond the mean field estimate and obtain the results to all orders of correlations. In Figure 2.8 we have seen that the coexistence region lays below temperature $T = 0.9\,MeV$. From our calculation of specific heat shown in Figure 2.10 we confirm that the upper bound of the critical temperature is $T = 1.0\,MeV$. Comparing this fact with our previous result on lower and upper bounds of critical temperature represented in Figure 2.8, we finally estimate critical temperature to be within the range $0.7\,MeV \leq T_c \leq 0.9\,MeV$ and critical density as $\rho_c = 0.04\,fm^{-3}$.

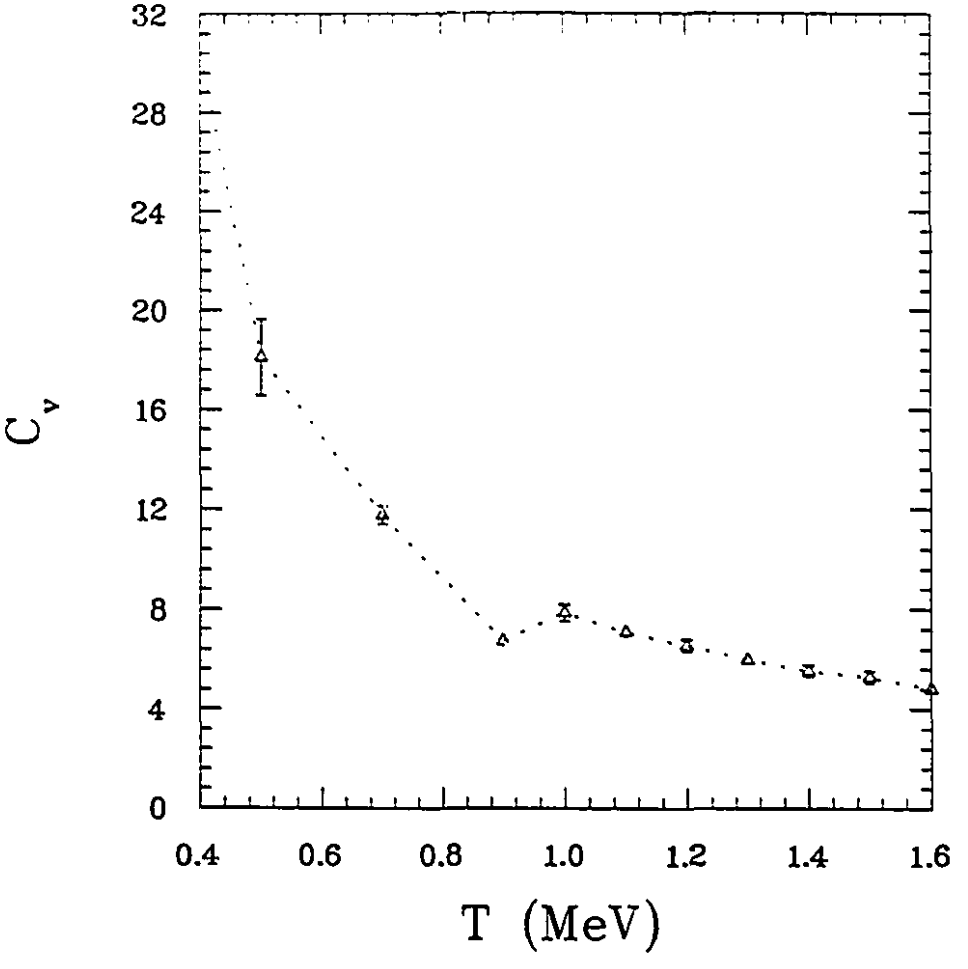

Figure 2.10: Heat capacity versus temperature T for density $\rho = 0.04\, fm^{-3}$ for a system of 85 nucleons.

Chapter 3

Role of Coulomb forces in two-phase separation

To construct a model describing any physical process as close to reality as possible it is necessary to include in a consideration all significant forces acting in system. This chapter is dedicated to the influence of the Coulomb interaction between charged protons interacting through two-body nucleon-nucleon potential on the appearance of the phase transition.

3.1 Implementing Coulomb interaction

To take into account the contribution of Coulomb forces into the interaction between nucleons first we have to introduce the technique to distinguish between protons and neutrons. It is easily achieved by assigning an isotopic spin to each nucleon. Then for each pair of interacting particles, we can definitely determine either this is a proton-proton pair or not. In the case of proton-proton interaction the Coulomb contribution [24]

$$V_{Coulomb}(r) = k\frac{e}{r} \tag{3.1}$$

is added to the repulsive potential $V_{nn} = V_{pp}$ (Eq. 2.1) acting between two identical nucleons. Here e is an elementary charge and k is a proportionality constant. In SI units k is

$$k = 8.988 \times 10^9\, N \cdot m^2/C^2$$

and e has value

$$e = 1.602 \times 10^{-19} C$$

We have used the asymptotic form of the electrostatic interaction potential, since interacting particles rarely overlap in realistic situations, due to the high incompressability of nuclear matter reflected in the nuclear interaction potential.

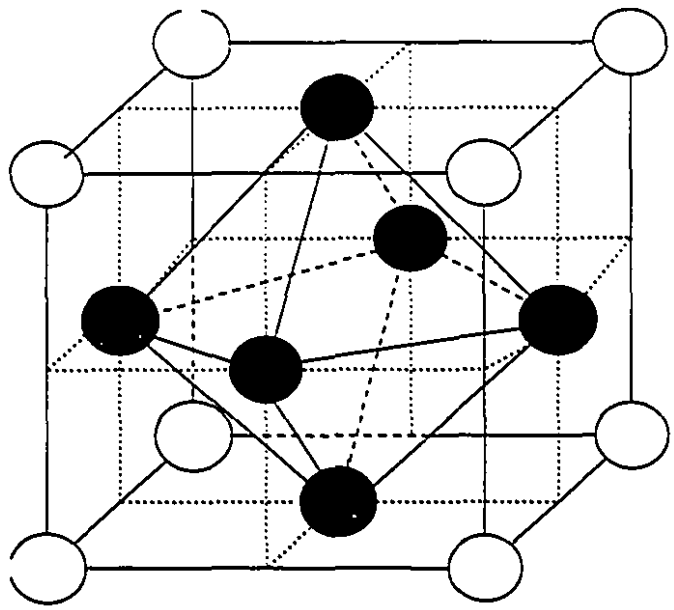

Figure 3.1: Unit cell of the cubic lattice structure. Grey and white spheres are protons and neutrons respectingly.

On the other hand we have to take care about starting configuration of the system. The simplest method of constructing a liquid structure is to place particles randomly inside the tested box. A problem arises from the fact that the configuration constructed in such a way may contain substantial overlaps. For hard-core system, as in our case, it would be totally unphysical, as stated above. Having turned on the Coulomb interaction, increased interparticle potentials and correspondingly large forces can cause difficulties in the solution of the differential equations of motion. Using cubic lattice distribution [14], as we have done, is much more appropriate for our system. Each proton has been placed following the simple rule: nearest neighbours of a proton are to be neutrons and vice versa. The method gives us the opportunity to

construct initial configurations homogeneously keeping protons apart of each other. In Figure 3.1 one can see a sample of a suggested configuration. During the course of the simulation, namely, the cooling time, the lattice structure disappears, replaced by a structure typical of liquids.

To solve the equations of motion taking into account Coulomb interaction we have to add a Coulomb force contribution [24]

$$\mathbf{F}_{Coulomb}(r) = k\frac{e^2}{r^3}\mathbf{r} \tag{3.2}$$

to the corresponding nuclear force for each two protons.

3.2 Influence of the Coulomb interaction on Thermodynamic Quantities

As it is expected the Coulomb interaction plays a remarkable role in behaviour of thermodynamic quantities in a system of 85 nucleon where 41 of those are protons. To understand better the reasons of its significant influence it makes sense in the first place to look how much values of the energies change having turned on the Coulomb interaction.

3.2.1 Energy

The core of the Coulomb potential is similar to the nucleon-nucleon one. The Coulomb potential also plays a considerable role at long distances. In our case of fixed density and, therefore, of volume, since there is no particles outside of it we are always able to limit the range of Coulomb interaction by the size of the box. That is why it is still possible to calculate the Coulomb force contribution for the system of finite number of particles.

In Figure 3.2 we can see that the shortest distance, where potential energy between two charged protons significantly differs from nucleon-nucleon potential, is about $2.5\,fm$. Then for distances between two protons greater than $2.5\,fm$ the Coulomb interaction taken into account will significantly increase repulsion and, therefore, velocities of the particles and, therefore, pressure.

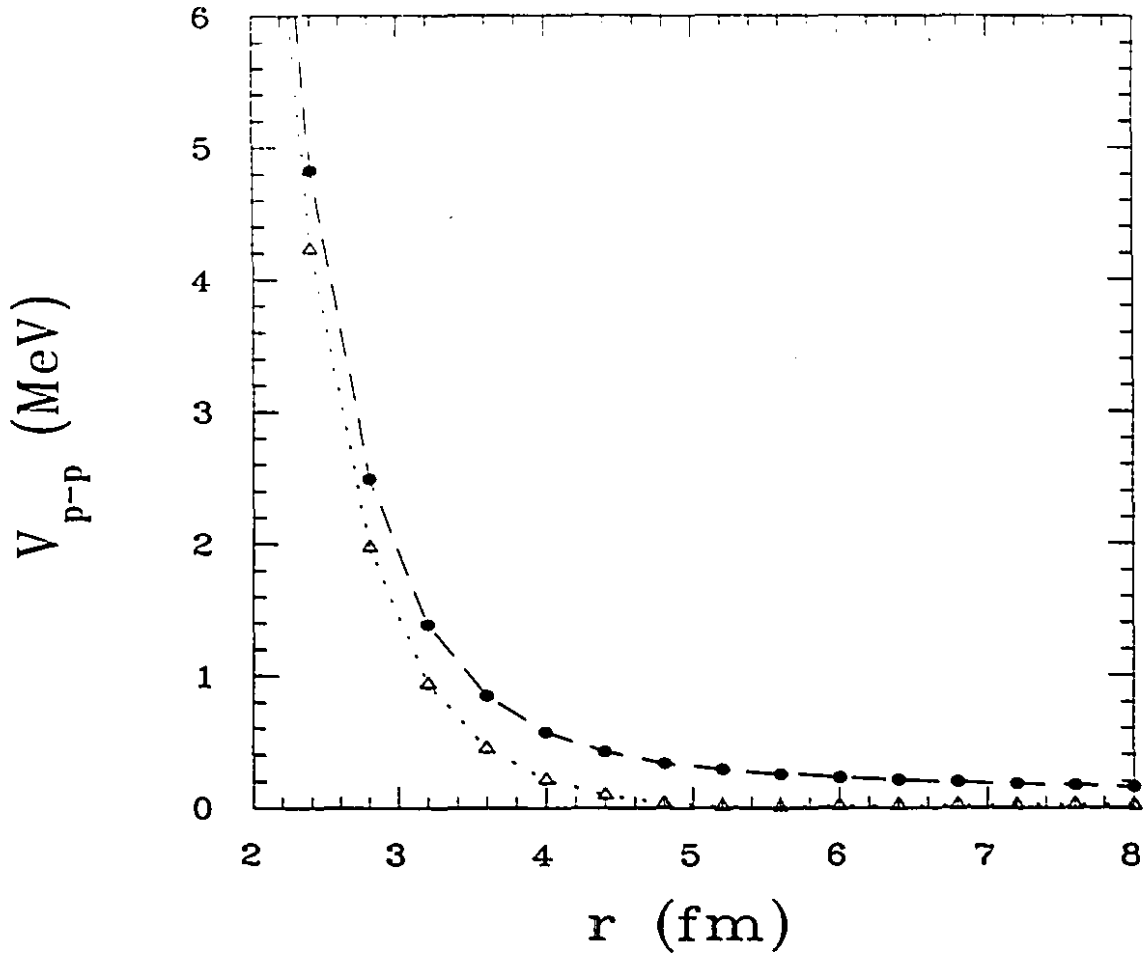

Figure 3.2: Nucleon-nucleon potential energy (triangles) and potential energy including Coulomb repulsion between two protons (circles).

3.2.2 Pressure

We calculate pressure using the virial theorem [21] in complete accordance with our previous calculation (section 2.2.1):

$$P_{virial} = \rho T - \frac{\rho}{6N} \left\langle \sum_i \sum_{j>i} r_{ij} \frac{\delta V_{ij}}{\delta r_{ij}} \right\rangle \tag{3.3}$$

where V_{ij} is a potential energy of the particles i and j. In the case of two protons now we have to take into account Coulomb contribution of Equation 3.1.

As can be seen from the Figure 3.3 the results for the pressure as a function of density at temperature $1.5\,MeV$ with Coulomb interaction are considerably dif-

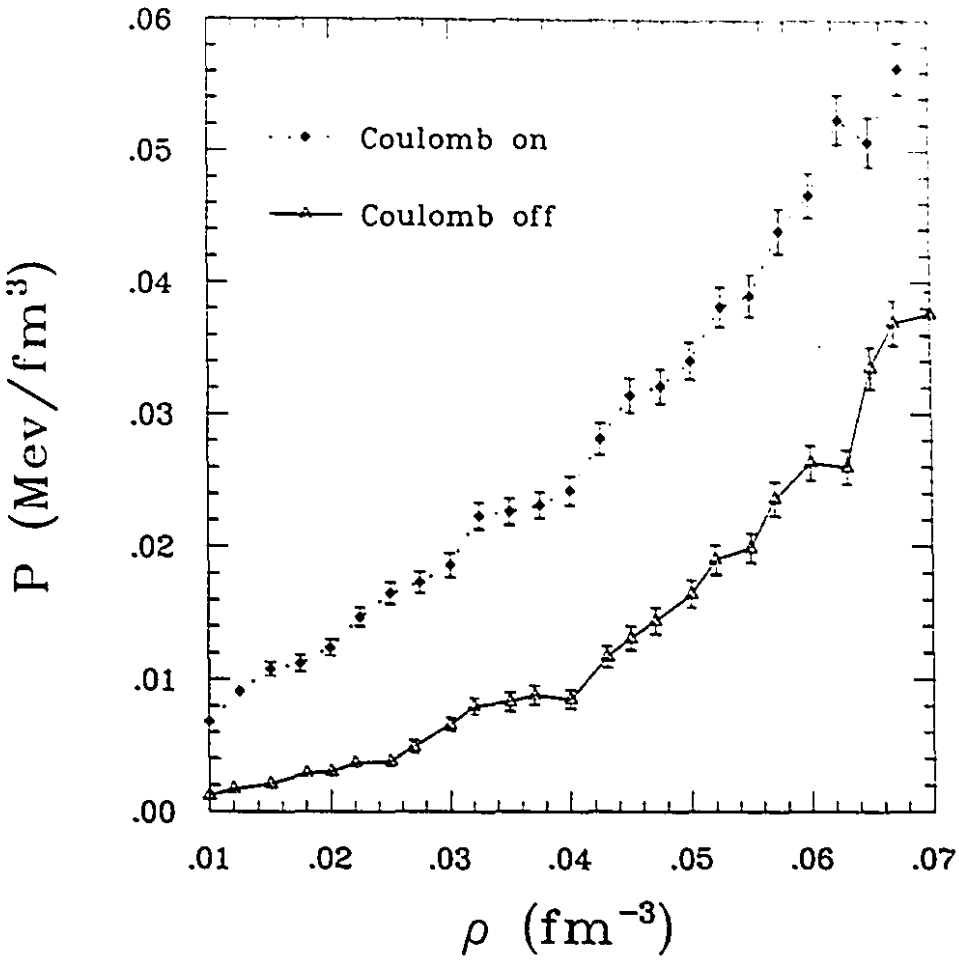

Figure 3.3: Pressure as a function of density obtained with and without taking into account Coulomb interaction at temperature 1.5 MeV

ferent from those obtained without it. As it has been expected, Coulomb repulsion increases velocities of the nucleons forcing pressure to grow. The effect is not that strong as temperature goes down. In Figure 3.4 at temperature 0.3 MeV one can not see such great influence of the Coulomb field as in Figure 3.3 at temperature 1.5 MeV especially at low densities. We understand that by general consideration of energetic balance. As temperature decreases, the kinetic energy decreases also and the contribution of potential energy grows. But we have seen in Figure 3.2 that for the large value of potential energy the Coulomb contribution is less significant.

The pressure curves below the temperature 0.9 MeV are shown in Figure 3.5. One can see that there is still a plateau region for the isotherms below 0.9 MeV and densities within the range 0.02 and 0.06 fm^{-3}.

Due to the statistical errors the problem of the critical parameters determining turns out to be difficult to resolve. However the calculation of specific heat shows that

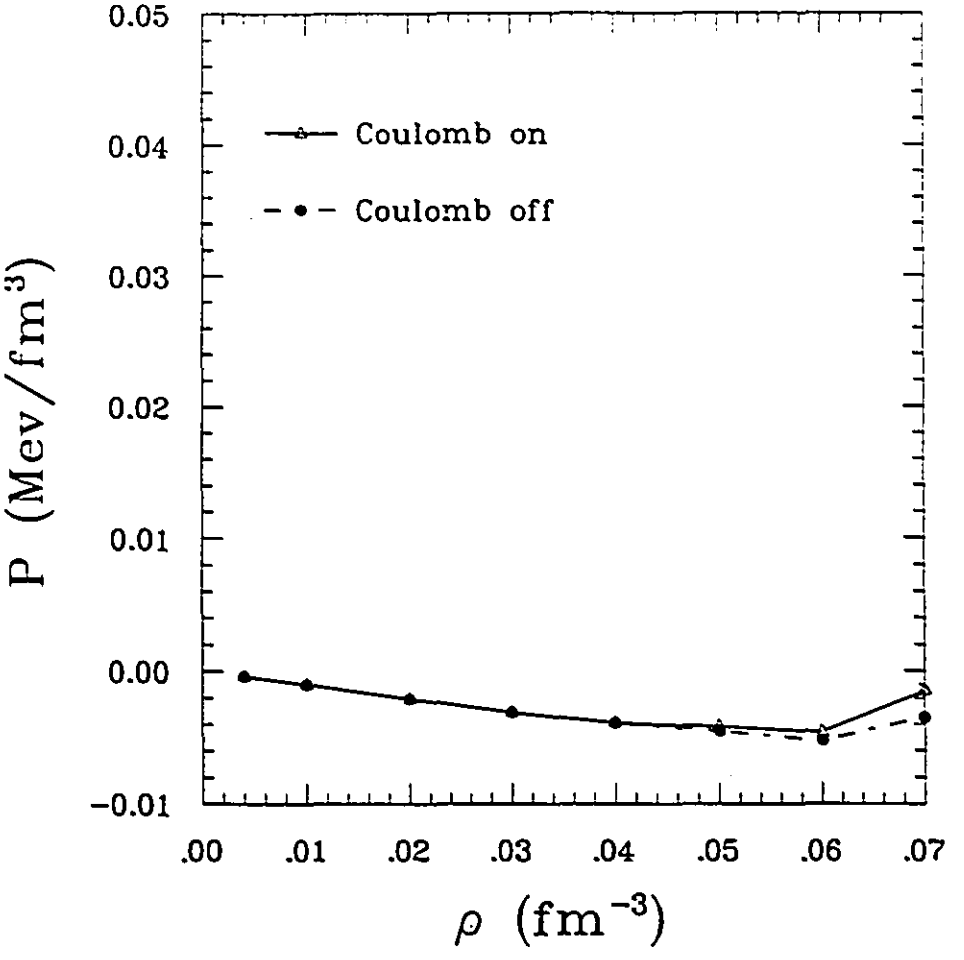

Figure 3.4: Pressure versus density, obtained taking into account the Coulomb repulsion between two protons, at temperature 0.3 MeV. Note, that scales are chosen corresponding to the Figure 3.3.

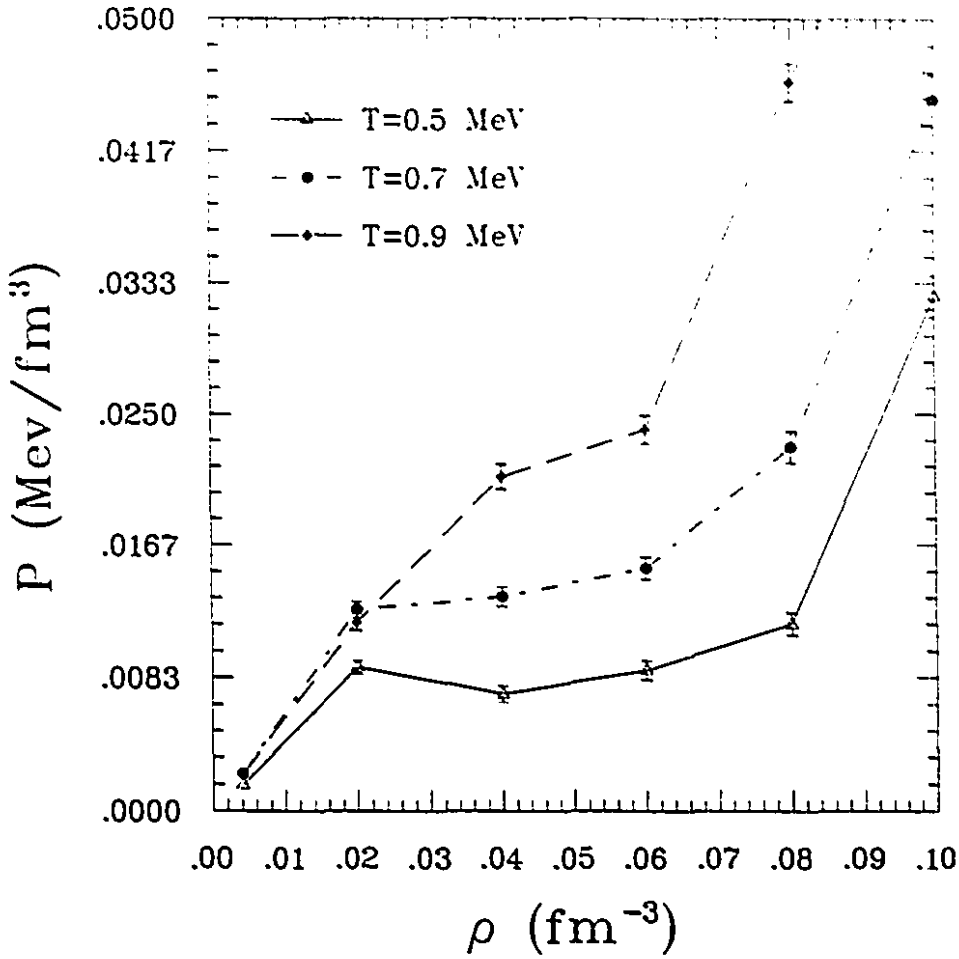

Figure 3.5: Data of the pressure obtained taking into account Coulomb repulsion between two protons.

the critical temperature is around 0.9 MeV and that the critical density is still around 0.04 fm^{-3}. Taking into account Coulomb force has to cause critical parameters to decrease. But in our model the accuracy of the method turns out not to be high enough to detect the difference between critical parameters for phase transition of the system of 85 particles interacting through two-body nuclear and Coulomb potentials and for a system of 85 nucleons interacting just through nuclear potential. However, we believe the accuracy to be adequate to our purposes.

Chapter 4

Finite size effects on the critical phenomena

In the chapter we investigate the influence of finite number of particles N on thermodynamical properties. As in Monte-Carlo calculations the goal is to determine the canonical ensemble averages, it has certain limitations drawn from the fact that on a macroscopic scale the size of a sample is extremely small. Typically, N is order of $0.5 \cdot 10^3$ or less. The time used to evaluate forces and potential energy is proportional to N^2. In order to minimize surface effects and thereby to simulate more closely the behaviour of an infinite system, it is customary to increase the number of particles as much as we can. A common method to do this is to use periodic boundary conditions [14]. However there are certain disadvantages in the utilization of periodic boundaries. Applied to our system it makes very difficult to take into account long-ranged interactions such as the Coulomb interaction [14]. Since in our study we are interested in the determination of the phase transition as well as in the Coulomb influence on it, we use the other way of approaching the thermodynamical limit.

4.1 200 nucleons interacting through the nuclear potential

The problem of finite size effects or, namely, of surface effects can be addressed by increasing the number of participating nucleons as close to the thermodynamical limit as we can. Our ability to consider an infinite system is always limited by the fact that in a Monte-Carlo computer simulation the number of particles is connected directly to the CPU time spent. At the same time, let us remember that the problem

we investigate is a heavy ion collision that forms a finite system of a few hundred nucleons. The number of particles in reality participating in a reaction is far from the thermodynamical limit. We therefore feel that a couple of hundred of nucleons will take us one step towards the thermodynamical limit, while still representing a practical number with some connection with the physical problem at hand.

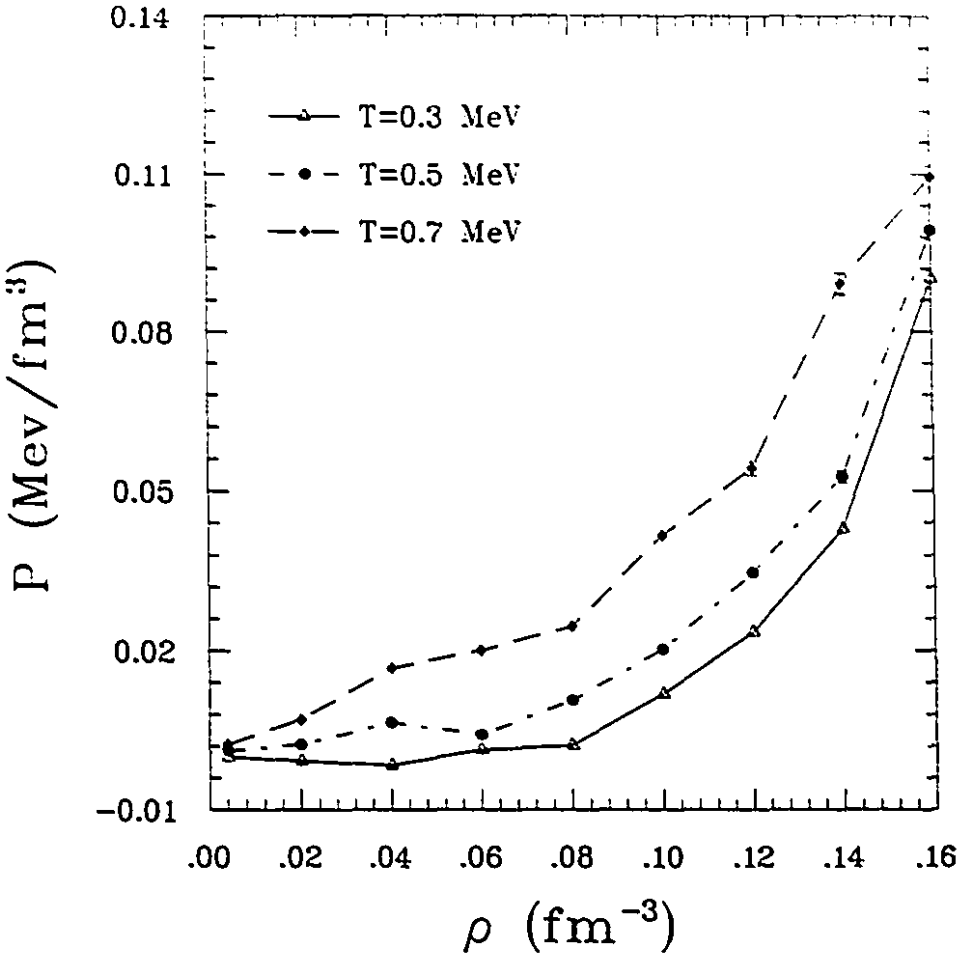

Figure 4.1: Pressure versus density for 200 nucleons system

We consider the system of 200 nucleons with equal numbers of neutrons and protons. Again, the choice of 200 particles represents a reasonable compromise. For an Alpha workstation, the simulation of 8000 events requires approximately one hour of CPU time.

The Coulomb interaction initially is turned off.

The thermodynamic data accumulation was carried out in the same way as in previous chapters. Namely, we used the leapfrog algorithm of particle propagation

from Equations 2.7, 2.8 for a given interparticle potential law from Equations 2.1, 2.2. Cooling time was chosen to be 100 timesteps that corresponds to $0.5 \cdot 10^{-13}$.

Pressure data were obtained making use of the virial theorem (Equation 2.17) for a two-body nucleon-nucleon interaction ignoring the Coulomb repulsion between protons. In Figure 4.1 one can see the results obtained.

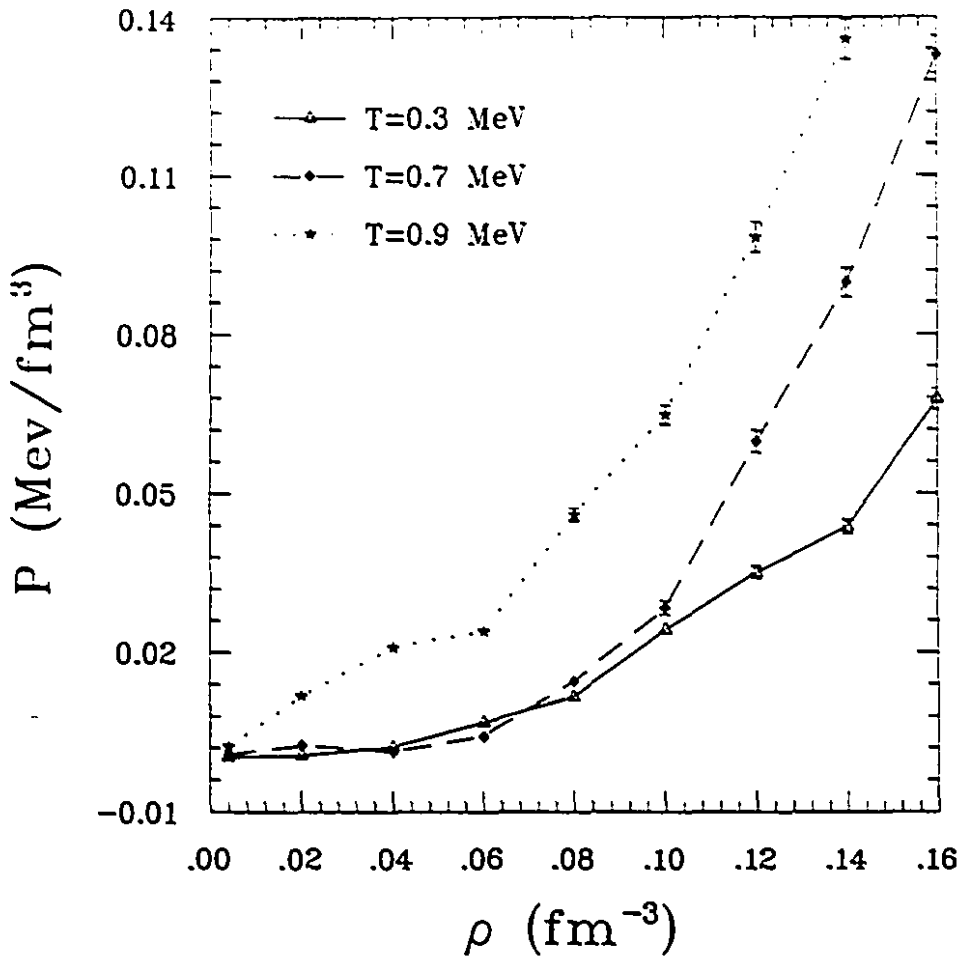

Figure 4.2: Pressure versus density for 85 nucleons system. Scales are chosen to fit Figure 4.1.

As one compares Figure 4.1 and Figure 4.2, representing the data on pressure for 85 nucleons system (obtained earlier and shown in Figure 2.8 in different scale), one will see that the pressure behaviour does not differ significantly for systems of 85 and 200 nucleons. Qualitatively it remains the same: we still can see the same plateau in the pressure graph for the same temperatures in about the same range of densities.

Let us note though that the critical temperature for 200 nucleons system will be

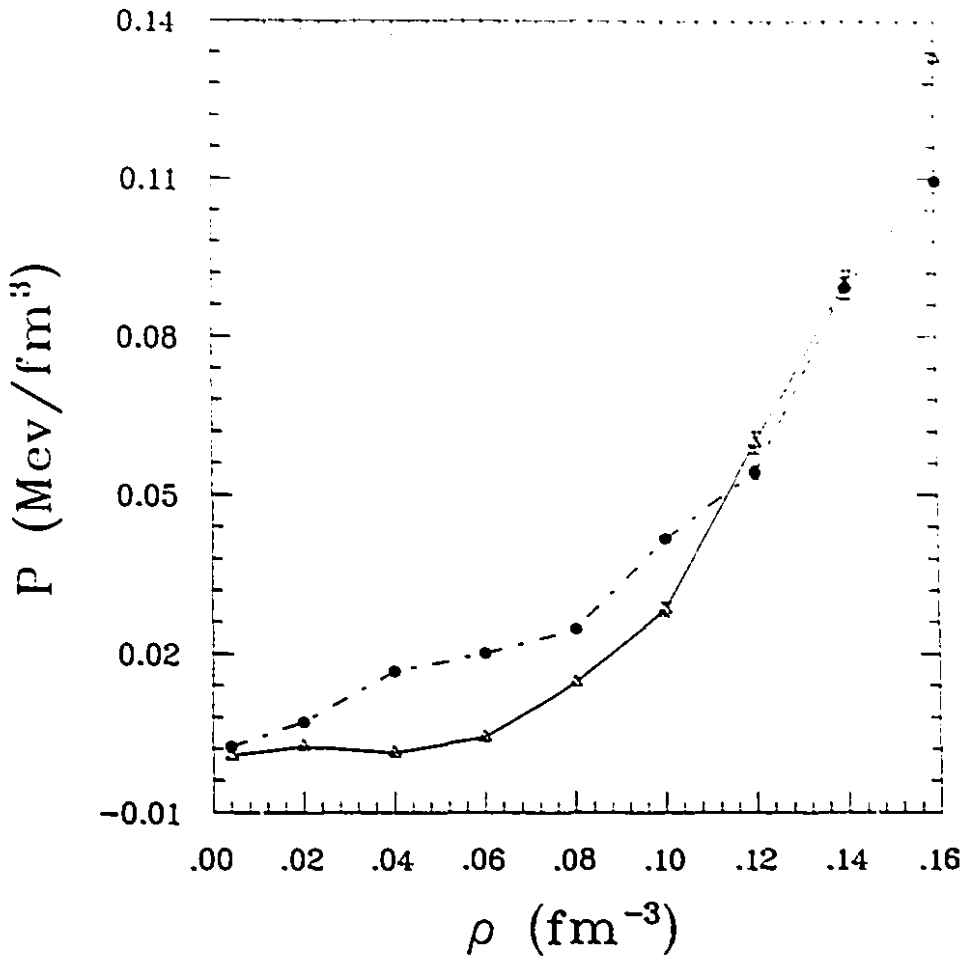

Figure 4.3: Pressure versus density for different number of nucleons at temperature $T = 0.7\,MeV$. Circles correspond to the 200 nucleon system and triangles - to 85 nucleons.

slightly lower than for the 85 nucleons system. Figure 4.3 represents the pressure against density at temperature $T = 0.7\,MeV$ for those systems. One can see that for the 85 nucleons system the temperature $T = 0.7\,MeV$ is still in phase coexistence region while for the system of 200 nucleons the temperature $T = 0.7\,MeV$ is much nearer to the critical temperature.

The heat capacity graph for the 200 nucleons system does not exhibit any significant peak within the investigated regions of temperatures and densities.

4.2 Coulomb effects on the 200 nucleon system

Let us include into consideration now the Coulomb interaction between charged protons. In such a way we get the most realistic picture of the heavy ion collisions process that is possible to get in the classical molecular dynamics model.

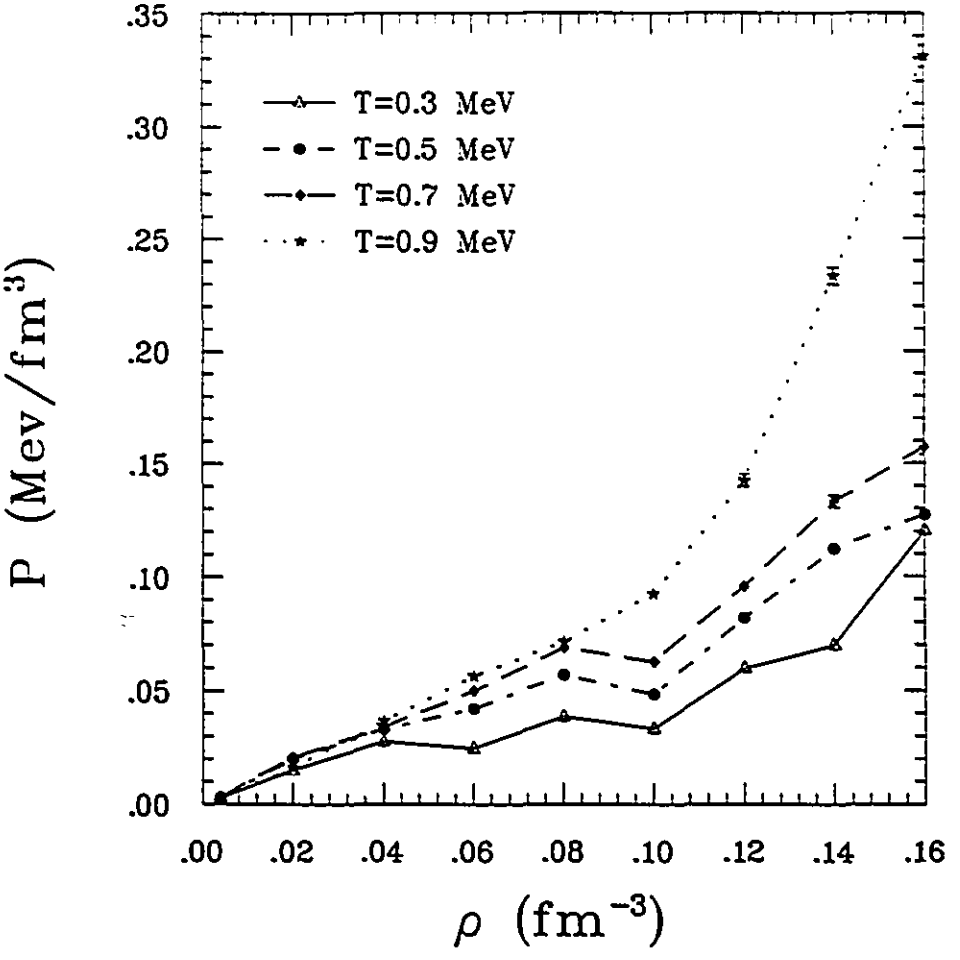

Figure 4.4: Pressure versus density, obtained taking into account the Coulomb repulsion between two protons for the system of 200 nucleons.

As can be seen from the Figure 4.4 the results for the pressure as a function of density for the system of 200 nucleons with Coulomb interaction turned on are roughly the same as those obtained for the 85 nucleons system and represented in Figure 4.5, except perhaps at higher densities. We note although that the value of critical density grows slightly. As one could expect taking into account the similarities obtained in previous section, the number of participating nucleons, interacting through nuclear

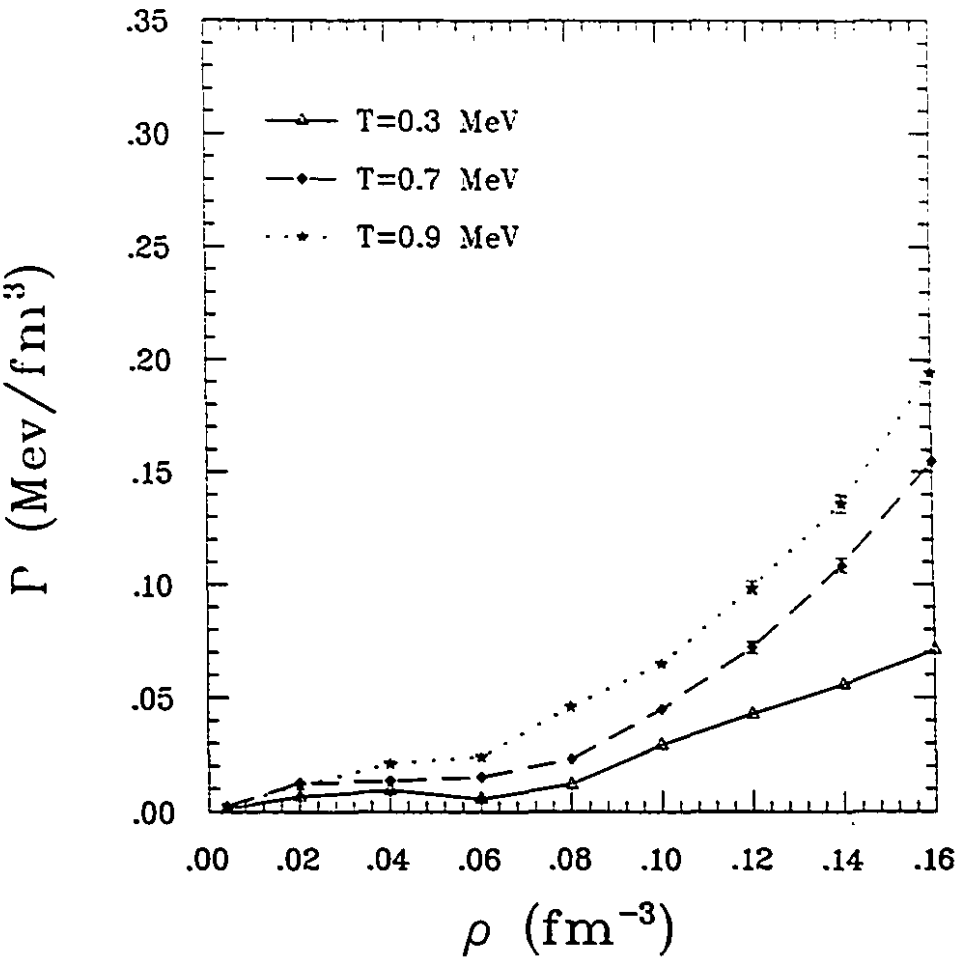

Figure 4.5: Pressure versus density for 85 nucleons system with turned on Coulomb interaction. Scales are chosen to fit Figure 4.4.

and Coulomb potential, does not affect the critical parameters of the nuclear phase transition significantly.

Conclusion

In conclusion it makes sense to summarize the results obtained.

We have shown that the classical molecular dynamics model, applied to the description of nuclear multifragmentation, gives us opportunity to study nuclear matter fragmentation as a nuclear liquid-gas phase transition.

We used the Monte Carlo technique for a computer simulation of the transition stage in heavy ion collisions. Since the molecular dynamics computer simulation allows us to study the properties of the system starting far away from equilibrium, it is important to define the initial configuration properly. Different kinds of starting configuration have been considered. In order to satisfy the energy conservation law, different methods of particles propagation have been studied. Finally the "leap-frog" finite difference method was found to be the best. To simulate the dynamics of canonical ensemble evolution we have investigated two ways of keeping the kinetic temperature constant. One of them, based on the velocities rescaling, turns out to be a crude method of solving the equations of motion. Another one, constraint method, has been proven to give results of high precision.

We studied the system of 85 identical nucleons interacting through two-body nucleon-nucleon potential. The calculations of thermodynamic quantities show the presence of nuclear liquid-gas phase transition. Data of thermodynamic quantities gives the values of critical parameters: the critical density about $\rho_c = 0.04\, fm^{-3}$ and the critical temperature near $T_c = 0.9\, MeV$.

The computer simulation was carried out for the case of distinguishable protons and neutrons. The Coulomb interaction between charged protons was included. The data on various thermodynamic quantities also have been obtained. The phase transition in the presence of Coulomb field has been detected. The specific heat data shows that the critical temperature is about $0.9\, MeV$ and the critical density is about $0.04\, fm^{-3}$.

To estimate the influence of the finite number of particles, or surface effects, on the critical behaviour of the system, we considered a system of 200 nucleons and compared the thermodynamical quantities obtained with those for the a 85 nucleons system. Calculations have been carried out initially ignoring the Coulomb interaction and then taking it into account, in complete accordance with our previous scenario for the 85 nucleons. Remarkable similarities have been observed leading us to conclude that number of particles taken in consideration, as well as the Coulomb interaction, in

our model does not affect significantly the accumulating thermodynamical quantities, only slightly pull them down, at least for the case of the transition from 85 to 200 nucleons. In Figure 4.6 the results for differently sized system are represented with and without the Coulomb interaction.

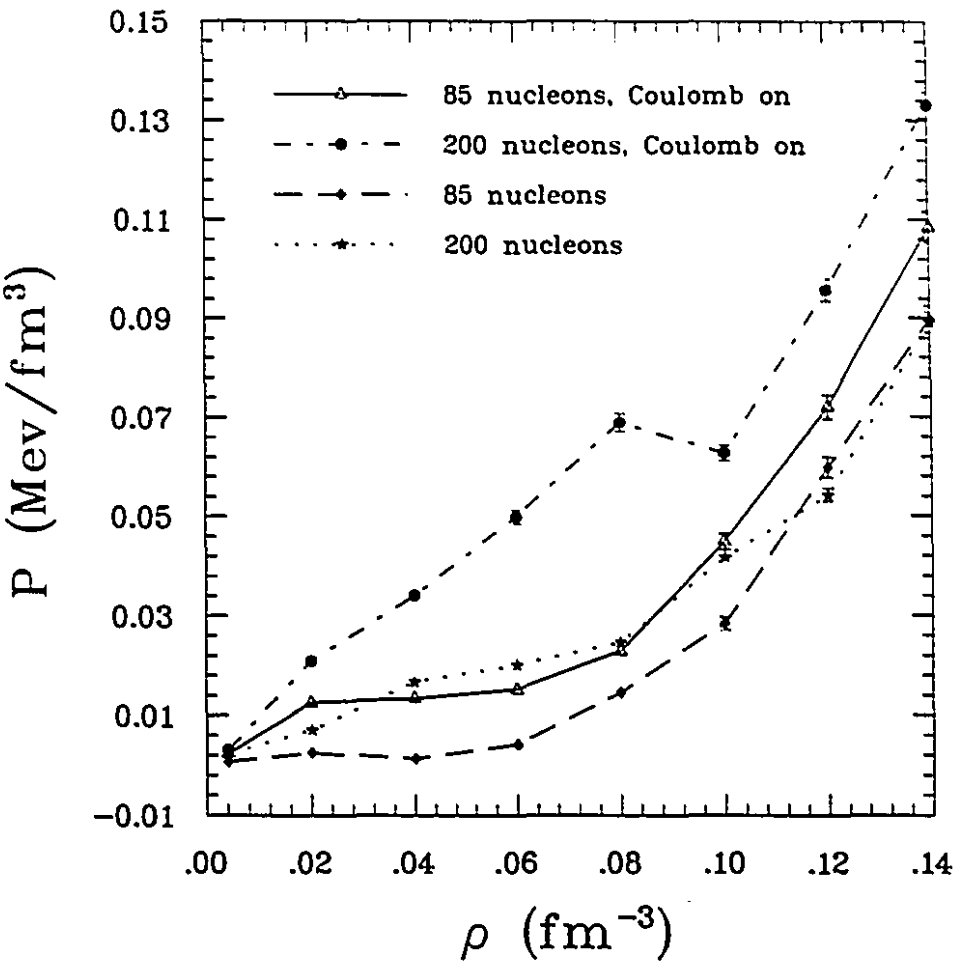

Figure 4.6: Pressure against density isotherms $T = 0.7\,MeV$ for systems of 85 and 200 nucleons with and without Coulomb contribution.

As one can see the molecular dynamics model works well in sense of detecting the phase transition existence, but the critical parameters are quite hard to determine accurately. If we could have unlimited computer time and a number of particles close to the thermodynamical limit, the problem of statistical errors would be solved. Let us not forget also that we described a quantum system by means of a classical model, partially neglecting quantum effects such as Pauli repulsion principle and so on. It would be interesting to perform a similar work taking care of quantum effects in the

heavy ion system as it was done in fermionic molecular dynamics [25, 26, 27]. Only then can statements with potential impact on experimental measurements be made. Work along those lines is in progress.

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