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I. Phase Evolution of Disassembling Nuclei

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Quasi-Classical Simulation of Nuclear Dynamics
I. Phase Evolution of Disassembling Nuclei *

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Abstract:

A recently developed quasi-classical simulation model is employed for studying the dynamics of nuclei that have been compressed to double density and heated to temperatures from 3 to 10 MeV. The evolution of a system is mapped onto the equation of state for the corresponding static system. A systematic change in the disassembly process is observed as the initial temperature is raised: at low temperatures the compressional energy is released by blowing off the outer layer of nucleons leaving a single liquid residue, whereas for high temperatures the system experiences a rapid spinodal composition into an expanding gas of nucleons and small clusters. The filamentary character of this process may lead to experimentally observable multifragment correlations.

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1 Introduction

Heavy-ion induced reactions at intermediate energies produce unique physical scenarios and offer special opportunities for studying non-equilibrium effects in small many-body systems. Conversely, the interpretation of nuclear collision experiments relies heavily on our understanding of nuclear dynamics far from equilibrium. Significant progress has been made in recent years on developing dynamical models for nuclear collisions at intermediate energies. Most notable are those based on the Nordheim approach (VUU, BUU, ...), in which nucleons move in a time-dependent one-body field while experiencing Pauli-blocked two-body collisions with each other, and those based on classical equations of motion, in which the nucleons interact directly via a suitable two-body interaction.

We have recently developed a model of this latter type which seeks to take approximate account of the exclusion principle by means of a repulsive Pauli potential depending on the separation between two nucleons in phase space [1,2], an approach first suggested by Wilets et al.[3]. When the Pauli potential developed in [1] is augmented with a suitable internucleon potential, it is possible to construct a model giving a fairly good reproduction of general thermostatic nuclear properties.[2] In the present paper we report on the first application of that model for dynamical studies, namely the evolution of a compressed and heated system containing 40 protons and 40 neutrons. The dynamical trajectory of the innermost half of the nucleons is projected onto the equation of state associated with ^{40}Ar. The finite system ^{40}Ar provides a more natural reference than infinite nuclear matter, to which dynamical simulations have often been referred.

In the present approach, the nuclear system is modelled as a quasi-classical system of interacting particles (nucleons). The exclusion principle, which acts to prevent identical nucleons with the same spin and isospin components from being close in phase space, is simulated by a momentum-dependent repulsive two-body potential (hence the term "quasi"-classical). Thus the many-body Hamiltonian is given by

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{i<j}[V_P(p_{ij}, r_{ij}) + V_N(r_{ij}) + e^2 \frac{z_i z_j}{r_{ij}}] \ . \tag{1}$$

Here the Pauli potential is $V_P = V_P^0(\hbar/p_0 q_0)^3/\exp(p_{ij}^2/2p_0^2 + r_{ij}^2/2q_0^2)$ with V_P^0=34.32 MeV, p_0=2.067 MeV·10^{-22} s/fm, and q_0=6.00 fm.[1] Furthermore, the nuclear interaction is given by a modified Lennard-Jones potential,

$$V_N(r) = V_N^0 \ [(\frac{r_1}{r})^{p_1} - (\frac{r_2}{r})^{p_2}] \ \frac{1}{1 + e^{\alpha(r-d)}} \ , \tag{2}$$

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where V_N^0=18.263 MeV, p_1=6.2, p_2=3.0, r_1=1.7456 fm, r_2=1.7324 fm, and the parameters for the modulation factor are d=3.350 fm, α=1.2 fm^{-1}.[1] This Hamiltonian gives reasonable results for the specific energy of nuclear matter over a broad range of densities and temperatures as well as for the sizes and bindings of finite nuclei. It therefore presents an interesting tool for gaining insight into the properties of dynamical processes.

2 Thermodynamic Quantities

It is instructive to discuss the dynamical evolution in terms of thermodynamic quantities, such as density, temperature, and pressure. It is therefore necessary to devise methods for extracting such quantities from general (*i.e.* non-equilibrium) states. In the present context, the problem can be stated as follows: Imagine that we are presented with a configuration (or several configurations) sampled from an equilibrium ensemble with definite but unknown values of the characteristic thermodynamic quantities. Our task is then to estimate the values characterizing the ensemble from which the given configuration is picked. More generally, one would like to calculate those values that would characterize the statistical equilibrium of the system, also when the actual system is far from equilibrium. We describe below how we proceed to achieve this.

In principle, the local density of particles, $\rho(\mathbf{r})$, can be obtained by counting the number of nucleons in a suitable neighborhood of the specified point $\mathbf{r}$. In practice, the smallness of the particles number imposes severe limits the degree of detail that can be reliably obtained. We therefore restrict our considerations to the mean density of the innermost portion of the system. Specifically, we calculate the *rms* radius q of the innermost half of the nucleons. For a uniformly filled sphere of radius R we have $q^2 = \frac{3}{5}R^2$. This relation can be used to define the effective volume $V_{\text{eff}} = (4\pi/3)R^3$ occupied by the A nucleons (in the present case A=80/2=40). The mean density then follows as $\rho_{\text{eff}} = A/V_{\text{eff}}$, and the specific volume is $v = V_{\text{eff}}/A = 1/\rho_{\text{eff}}$.

This procedure has the advantage of being well-defined and generally applicable. However, it should be noted that rather large values for ρ_{eff} may result when the density profile is very diffuse, as is the case with the systems considered here. In order to illustrate this feature, let us assume that the total system has a Gaussian density distribution, with a dispersion $\sigma = r_0 A^{1/3}/\sqrt{5}$ that leads to the standard equivalent sharp radius. The mean density of the innermost half of the nucleons then exceeds the saturation value ρ_0 by 52% and, moreover, when the prescription

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[1]These values are those determined in the work reported in [2]. Unfortunately, in that paper a preliminary set of values was inadvertently quoted, though the correct final values (those quoted here) were employed in the calculations. We are thankful to Georg Peilert whose perseverance was instrumental in our unveiling this regrettable oversight. The most important difference between the preliminary value set quoted in [2] and the actual final set listed above is that the strength parameter V_N^0 has dropped from $\approx$26 to $\approx$18 MeV.

described above is employed the extracted mean density is even larger, $\rho_{\mathrm{eff}} \approx 1.94\rho_0$. Fortunately, this feature causes little practical inconvenience, since the same method is used for calculating both the dynamical quantities and the static equation of state onto which they are mapped.

It is often of interest to calculate an effective temperature, even though the system may be far from equilibrium. Since the interaction has a momentum dependence (via the Pauli potential), the momentum of a nucleon is not simply related to its velocity and so the extraction of the effective temperature requires some care. Using the fact that the temperature is a measure of the average kinetic energy, and replacing the time average employed in equilibrium systems by an average over the particles considered, we arrive at the following expression [4],

$$\tau_{\mathrm{eff}} \;=\; \frac{1}{3A}\sum_i \mathbf{p}_i \cdot \dot{\mathbf{r}}_i \;=\; \frac{1}{3A}[\sum_i \frac{p_i^2}{m_i} \;-\; \sum_{i<j} \frac{p_{ij}^2}{p_0^2}\,V_P(p_{ij}, r_{ij})] \;, \tag{3}$$

which provides a general means for extracting a useful effective temperature τ_{eff}.

The stress tensor $\overset{\leftrightarrow}{T}$ is directly related to the momentum transport and is therefore more suitable for systems away from equilibrium. A convenient expression for $\overset{\leftrightarrow}{T}$ can be obtained by replacing the time average in the Virial Theorem by an instantaneous average over the particles in the system [5], leading to

$$3\,\overset{\leftrightarrow}{T}\,V \;=\; \sum_i (\mathbf{p}_i \frac{\partial H}{\partial \mathbf{p}_i} \;-\; \frac{\partial H}{\partial \mathbf{r}_i}\mathbf{r}_i) \tag{4}$$

$$= \; \sum_i \frac{\mathbf{p}_i \mathbf{p}_i}{m_i} \;+\; \sum_{i<j} \mathbf{p}_{ij}\frac{\partial V_P}{\partial \mathbf{p}_{ij}} \;+\; \sum_{i<j} \mathbf{r}_{ij}\frac{\partial(V_P + V_N + V_C)}{\partial \mathbf{r}_{ij}} \;.$$

The sums include the A particles situated closest to the origin. The effective pressure in the system is then given as the trace of the stress tensor, $P = \mathrm{trc}\,\overset{\leftrightarrow}{T}$. Invoking the effective density $\rho_{\mathrm{eff}} = A/V_{\mathrm{eff}}$, we obtain the pressure as

$$P_{\mathrm{eff}} \;=\; \rho_{\mathrm{eff}}[\tau_{\mathrm{eff}} \;+\; \frac{1}{3}\sum_{i<j} r_{ij}F_{ij}] \;, \tag{5}$$

where $F_{ij} = -\partial V/\partial r_{ij}$ is the force between nucleons i and j. The first term is the standard form for an ideal gas, while the second term represents the contribution from the interparticle forces. It should be noted that F_{ij} contains the force arising from the position dependence of the Pauli potential V_P, while the momentum dependence of V_P is incorporated into τ_{eff}.

.3   Calculated Results

In order to have a useful reference for the dynamical results, we first calculate the equation of state for an isosymmetric system with 40 nucleons. In order to ensure that the system be approximately uniform, we require that each nucleon be situated with a designated spatial cell. These cells are constructed by first dividing the

spherical volume into five concentric shells of equal volume and then subdividing each of the shells into octants of equal volume. A Metropolis sampling is then performed with the additional demand that the nucleons remain within their assigned cells. This constraint is particularly important for densities below the saturation value where the the nucleons would otherwise tend to cluster. Because of the cell constraint, the consideration of finite temperatures poses no additional problem. The resulting Pv phase diagram, commonly called the equation of state, is shown in fig. 1. It exhibits a behavior typical of selfcohesive systems and quantitatively similar to what is expected for nuclei.

In the calculation of the equation of state in fig. 1, we have included all the nucleons when extracting the effective density and pressure. Table 1 contains a comparison of these values with corresponding values obtained by considering the innermost 40 nucleons in a system with 80 nucleons. It is seen that the differences are rather immaterial.

We have applied our quasi-classical simulation model to the evolution of nuclei that have been compressed and heated. Specifically, we consider systems having 40 protons and 40 neutrons. Using a ten-layered octopartitioned sphere to constrain the position vectors, these systems are prepared in states corresponding to a compression by a factor of two, and with a range of initial temperatures τ_0.

A visual impression of the character of the dynamical evolution can be obtained by displaying the projected positions of the nucleons as a function of the elapsed time. An instructive example is shown in fig. 2, which displays such snapshots taken at the same time ($=5 \cdot 10^{-22}$s) for four different initial temperatures. These pictures reveal a distinct change in the dynamical process as the initial temperature is raised. At low temperatures the temporal evolution is fairly slow and a considerable fraction of the system remains as a single entity, whereas for high temperatures the system quickly "explodes" into individual nucleons and loosely bound structures that often have a filamentary character.

In order to gain insight into the thermodynamic conditions prevailing in the interior of the system, we have extracted the specific volume v and the effective pressure P_{eff} associated with the innermost half of the nucleons and referred the ensuing phase evolution to the Pv equation of state for a static ^{40}Ar system shown in fig. 1. [It should be noted that the system consisting of the innermost 40 nucleons is only a configuration of ^{40}Ar if half of these happen to be protons, otherwise it is a manifestation of one of its isobars.] Such a dynamical Pv evolution is depicted in fig. 3 for a single system. In order to achieve an impression of the general behavior of the systems, we follow a number of similarly prepared systems, each ensemble containing 15 or 20 systems. In fig. 4 the resulting phase evolution is shown for four initial temperatures.

At the lowest preparation temperature, $\tau_0=3$ MeV, the energy stored in the initial compression is quickly carried off by the outermost nucleons, leaving a single nucleus exhibiting damped monopole oscillations and having a temperature not far from the initial one. This behavior gradually changes as the initial temperature is

raised and the resulting overall outwards motion begins to dominate.

At the highest initial temperature, $\tau_0 = 10$ MeV, the system shows an explosion-like disassembly where all the matter is moving rapidly outwards, in the form of individual nucleons or small clusters. In this scenario, the competition between the radial flow produced by the high pressure and cohesion due to the nuclear interaction leads to a spontaneous breaking of the initial (approximate) spherical symmetry, in each individual event. The resulting filamentary structures formed are akin to what is observed for splashing drops of ordinary fluids. This behavior is characteristic of the spinodal composition occurring when the system moves through the unstable region of the phase diagram.[6] It should also be noted that the persistence of nuclear binding, as evidenced by the emergence of bound clusters, is reflected in the fact that the extracted dynamical pressure falls below the coldest isotherm for the static ^{40}Ar system.

When the thermodynamic properties are sampled at the same points in time for all the different systems in the same ensemble, as in fig. 4, the specific volume will be endowed with fluctuations, since the fluctuations in the initial states give rise to different dynamical histories of each individual event. [These fluctuations are not shown on the figures in order not to clutter the display; typically the dispersion in v is ≈ 0.5 fm^3.] In order to eliminate this effect, one may instead sample each system at those (fluctuating) times when given values of the specific volume have been reached. This procedure then yields the pressure as a function of the volume, rather than the temporal trajectory in the Pv plane. We call the corresponding diagram the *thermodynamic evolution*. Fig. 5 shows this kind of result for the case of $\tau_0 = 10$ MeV. In this case the points follow closely the dynamical trajectory, because the disassembly proceeds so quickly that no backbending of the dynamical Pv trajectory occur. The multi-valued dynamical trajectories characteristic of the lower temperatures are also transformed into single-valued graphs by this construct.

4 Concluding Remarks

Interesting insight into the dynamics of small many-body systems has been obtained previously by Pandharipande *et al.*[7] with classical equations of motion that simulate argon droplets. Since the characteristic parameters for argon differ substantially from those of nuclei, our present model, which approximates nuclear systems much better, should be of more direct utility for the exploration of nuclear dynamics. In the present paper, we report on a first application of our recently developed quasi-classical simulation model to dynamical nuclear processes.

First, we have established general means for extracting thermodynamic quantities (density, temperature, and pressure) from many-body systems that are not in equilibrium. On this basis, we have calculated the equation of state, *i.e.* the relationship between pressure density for fixed temperature, for finite nuclear systems. Subsequently, we have calculated the dynamical evolution of disassembling nuclear systems. Specifically, we have discussed the temporal evolution of compressed and

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hot ^{80}Zr nuclei in terms of the effective density and pressure prevailing in their interior, mapping the trajectories of these thermodynamic variables onto the equation of state for a static ^{40}Ar nucleus, which provides a better reference system than infinite nuclear matter.

The change in the character of the disassembly process as a function of the initial temperature is noteworthy. For low temperatures most of the system remains in the liquid phase, in the form of a hot compound nucleus. As the temperature is raised, the size of the liquid residue shrinks, and at high temperatures, the system quickly turns into an expanding gas of nucleons and small clusters. This explosive disassembly typically proceeds via filamentary structures, as is common in association with spinodal decomposition of ordinary liquids. This feature should manifest itself in observable multifragment correlations, since the final fragments should be clustered with respect to solid angle. Modern (existing and planned) multifragment detector systems might be able to test whether such dynamics actually occurs in nuclear disassembly.

In the present discussion, we have focussed on the thermodynamic quantities, which describe the general physical environment. Because of the microscopic nature of the system, it is also of interest to understand how bound clusters arise and develop. Furthermore, since our model contains the full many-body information about the system, a cluster analysis is feasible, in contrast with one-body approaches. We are currently studying this aspect.

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Table 1: Thermostatic quantities

| τ		40 nucleons	80 nucleons
3	P	2.48 $\pm$ 0.40	2.51 $\pm$ 0.35
	v	2.12 $\pm$ 0.20	2.11 $\pm$ 0.25
5	P	3.20 $\pm$ 0.40	3.42 $\pm$ 0.35
	v	2.15 $\pm$ 0.20	2.11 $\pm$ 0.20
10	P	5.25 $\pm$ 0.80	5.51 $\pm$ 0.40
	v	2.06 $\pm$ 0.20	2.06 $\pm$ 0.20

The pressure P and the specific volume $v = 1/\rho$ calculated for a static isosymmetric nucleus with either 40 or 80 nucleons, for three different temperatures τ. The temperature is in MeV, the pressure is in MeV/fm^3, and the volume is in fm^3.
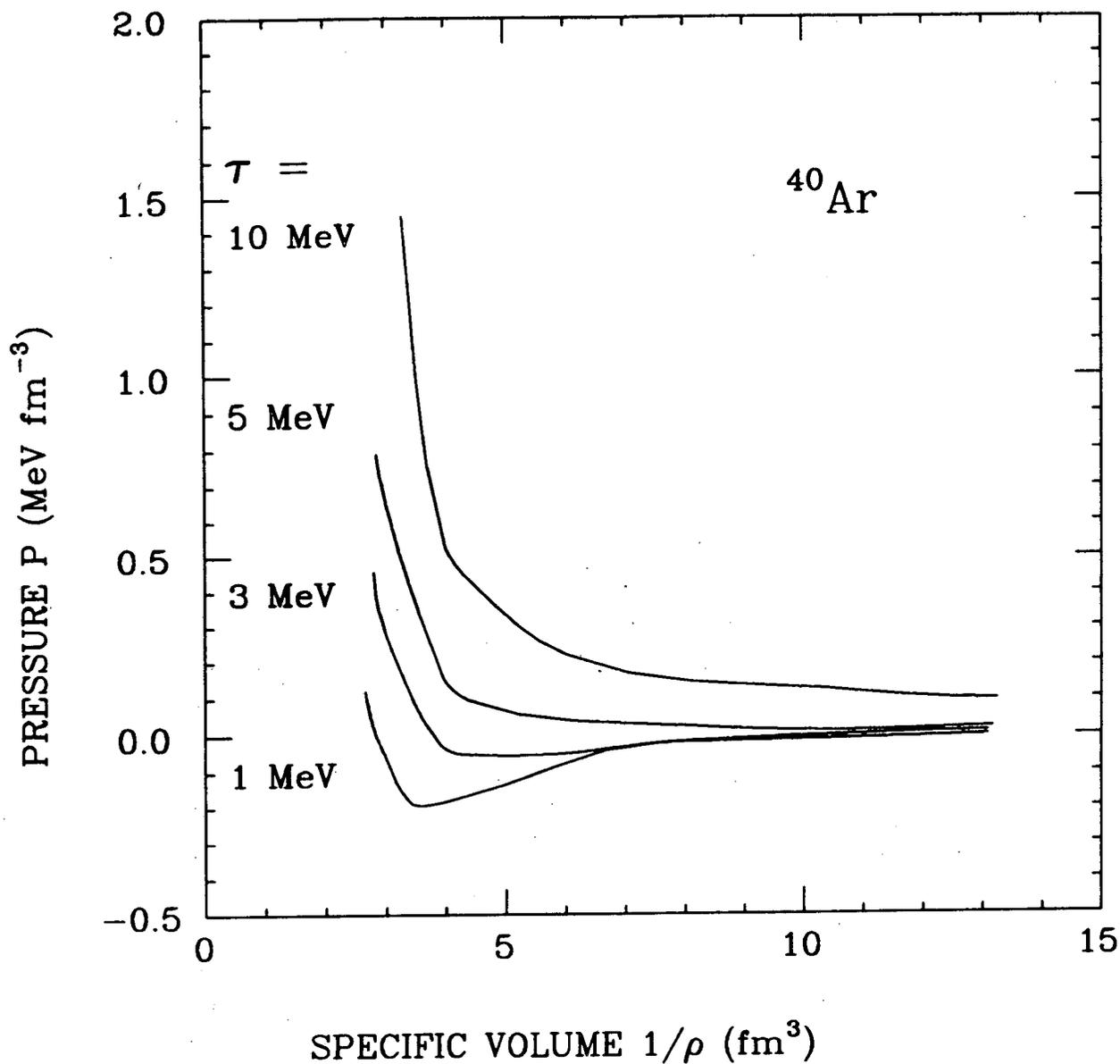
Figure 1: Equation of state for ^{40}Ar

The pressure P in a nuclear system with 20 protons and 20 neutrons constrained to be approximately uniformly distributed within a sphere of specified volume V. The specific volume is given by $v = V/A = 1/\rho$. The curves show the results obtained when the imposed temperature is taken as τ=1, 3, 7, and 10 MeV. The statistical errors associated with the calculated pressure is typically 0.05 MeV/fm^3.
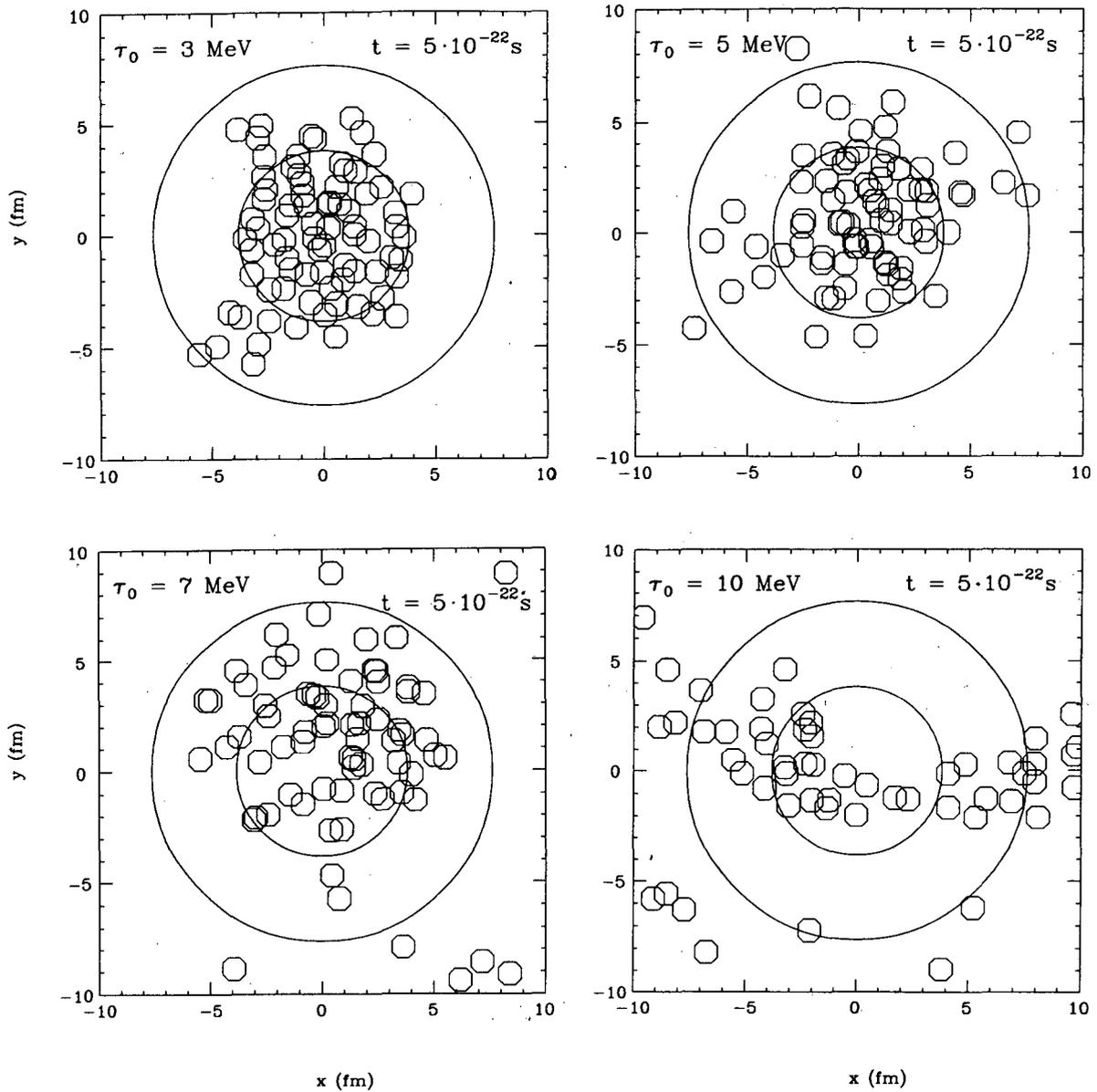
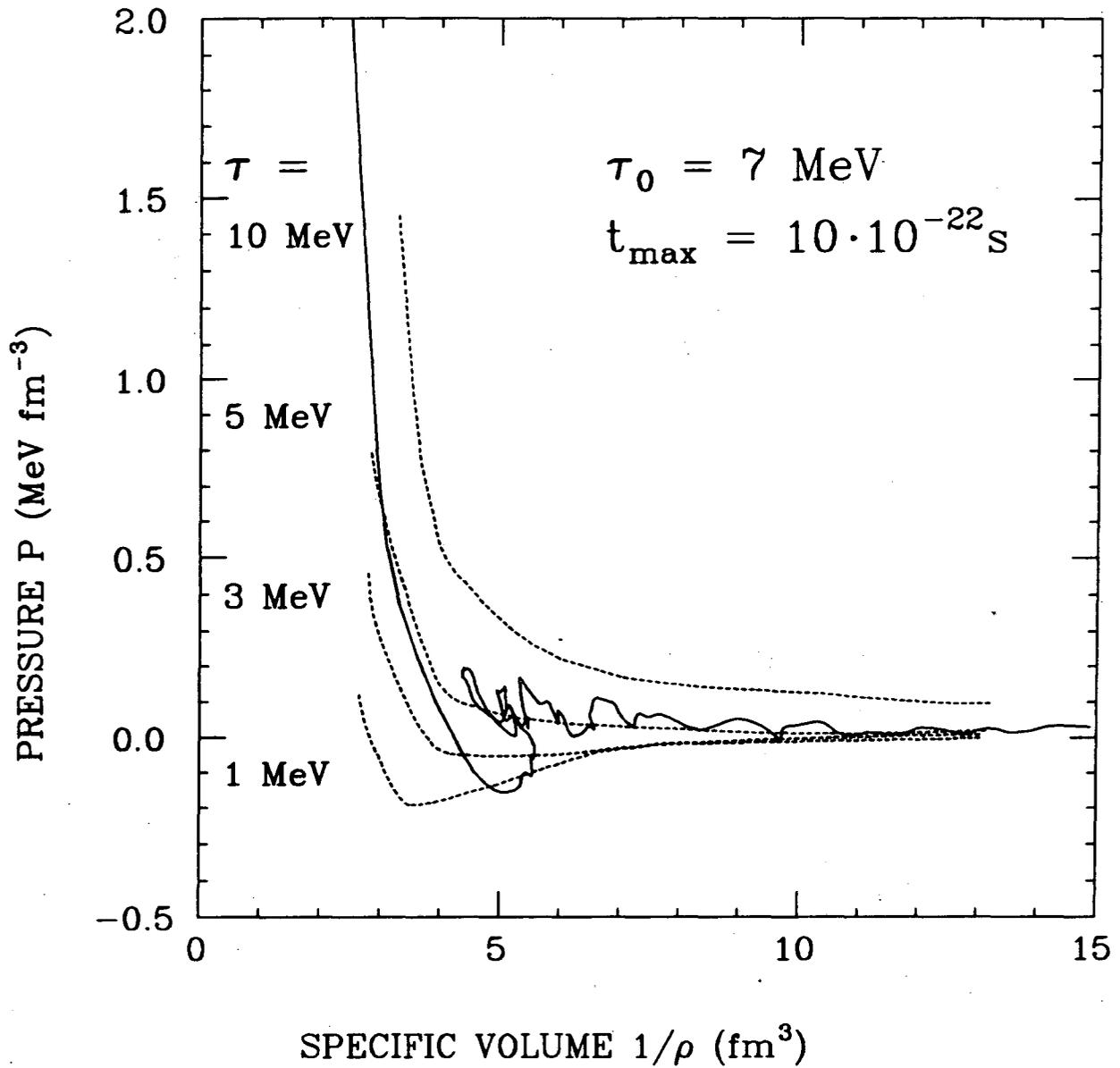Figure 2: Snapshots of the dynamical evolution
The figues show the projected locations of the 80 individual nucleons in the disassembling systems, for the first member of the considered ensembles with initial temperatures of $\tau_0 = 3, 5, 7$, and 10 MeV. These snapshots are taken after a time of $5 \cdot 10^{-22}$s has elapsed after the confining sphere has been removed. The innermost of the two concentric circles has a radius corresponding to the initial volume, while the outermost one has twice that value.

$\tau =$

10 MeV

5 MeV

3 MeV

1 MeV

$\tau_0 = 7$ MeV

$t_{max} = 10 \cdot 10^{-22}$ s

PRESSURE P (MeV fm^{-3})

SPECIFIC VOLUME $1/\rho$ (fm^3)

Figure 3: Phase evolution of a single event

The evolution in the Pv phase plane of the first member of the ensemble with an initial temperature of $\tau_0 = 7$ MeV. The dynamical trajectory joins points corresponding to time intervals of $0.1 \cdot 10^{-22}$ s and the time associated with the last point shown, t_{max}, is indicated.
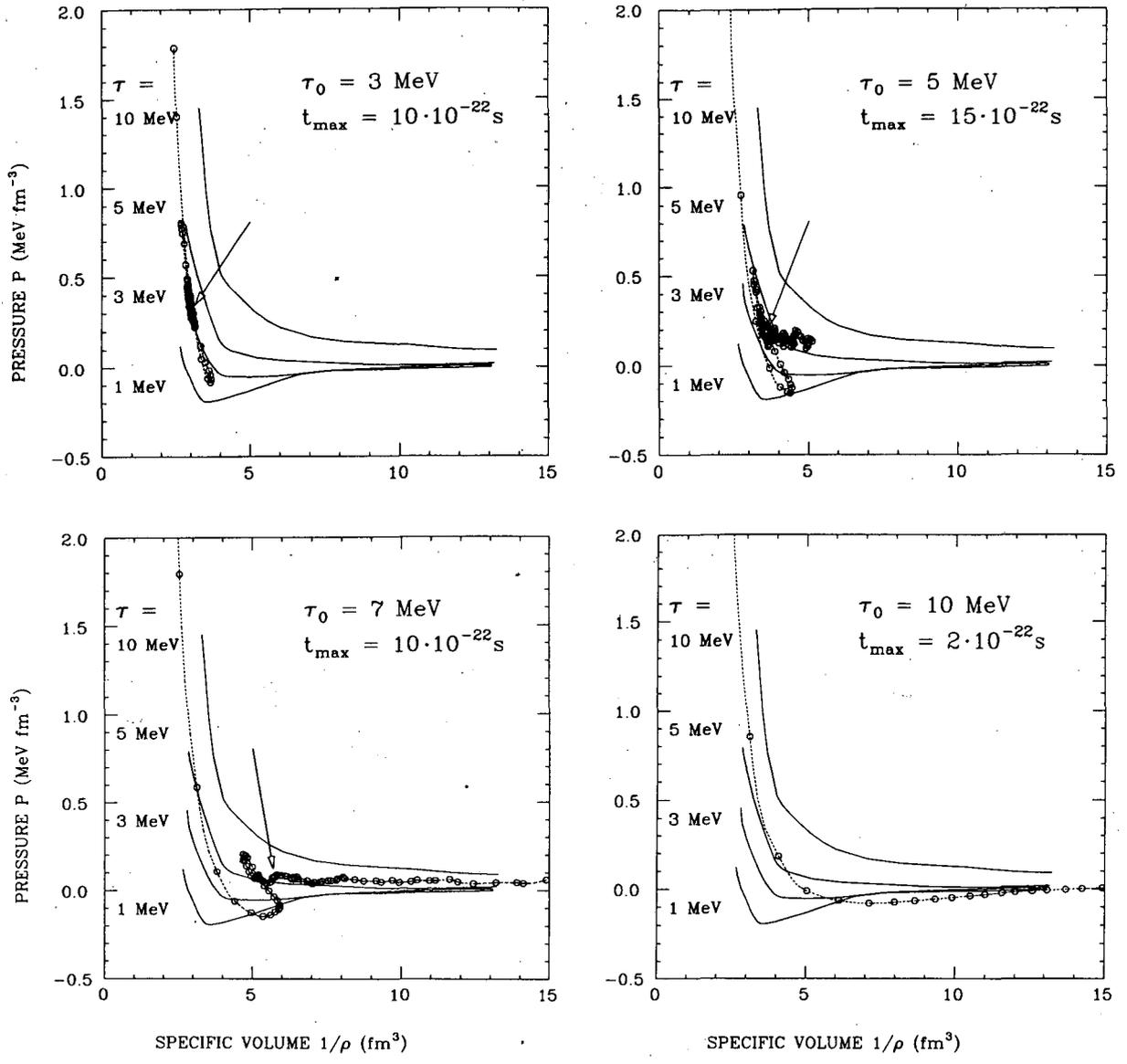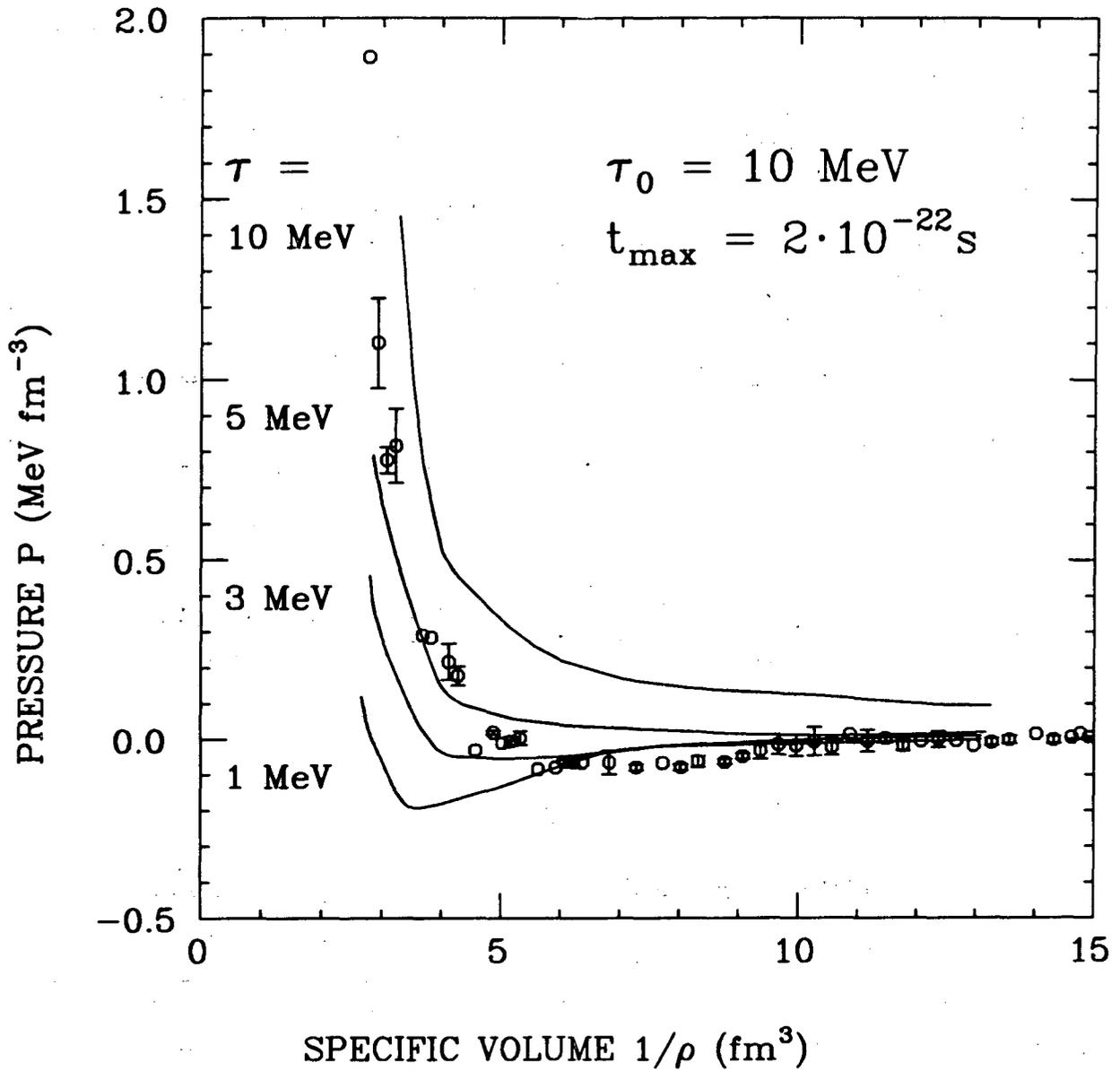
Figure 4: Phase evolution
The evolution in the Pv plane of four ensembles of systems, prepared at double density with the temperatures $\tau = 3$, 5, 7, and 10 MeV. The ensembles contain 15 or 20 individual disassembly events. The arrows point to the location of the systems at the time when the snapshots displayed in fig. 2 are taken.

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Figure 5: Thermodynamic evolution
This figure depicts the last of the processes shown in fig. 4, but sampled according
to specific density rather than time, thus eliminating the fluctuations in v.

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