LABORATOIRE DE PHYSIQUE NUCLEAIRE

UNITE ASSOCIEE AU CNRS/IN2P3 (UA 57)

2, rue de la Houssinière 44072 NANTES CEDEX 03

UNIVERSITÉ DE NANTES

I N2 P3 CNRS

TIME SCALES FOR SPINODAL DECOMPOSITION IN NUCLEAR MATTER WITH PSEUDO-PARTICLE MODEL

D. Idier, B. Benhassine, M. Farine, B. Remaud, F. Sébille

Rapport Interne LPN - 93-02

UNIVERSITE DE NANTES

Physical Review C

Time scales for spinodal decomposition in nuclear matter with pseudo-particle model

D. Idier, B. Benhassine, M. Farine[1], B. Remaud, F. Sébille

Laboratoire de Physique Nucléaire CNRS/IN2P3, Université de Nantes
2, rue de la Houssinière 44072 Nantes, France

[1] Permanent address: Ecole Navale, Lanvéoc Poulmic, 29240 Brest Marine

ABSTRACT

Dynamical instabilities arising from fluctuations in the spinodal zone for nuclear matter are studied using a large variety of zero range interactions in the frame of a pseudo-particle model. Scale times for spinodal decomposition are extracted and a possible link with decomposition in real heavy-ion collisions is discussed.

The phase space diagram of infinite nuclear matter possesses zones of mechanical instabilities, where an initially homogeneous system is unstable against the growth of density fluctuations and may separate into two phases : liquid drops surrounded by vapor or bubbles inside a liquid phase, depending on the average density of the system. Such a transition could be one of the clusterization processes observed in heavy-ion reactions, specially above 30 MeV/u.

The growth of density fluctuations in infinite Fermi fluids has been analytically treated [1] and applied to the nuclear decomposition [2]; this work is based on a generalization of Landau's kinetic equation and allows the qualitative classification of the behaviors expected in infinite nuclear matter, according to the initial conditions in the density - temperature (n,T) plane. Such an analytical approach however is strictly limited to the linear regime, it provides the domain of critical initial conditions but not the non-linear development of the instabilities. Furthermore, Landau's equation is based on the concept of quasi-particles which is meaningful for small excitation of real particles close to the Fermi level, which is far from being the situation in real heavy-ion collisions.

In another context, using canonical Metropolis simulations, Peilert et al. [3] were able to show that clusters develop at subsaturation energy in nuclear matter. In a dynamical context D. Boal at al. [4] using a quasiparticle model with a simplified interaction have shown, for early times, that the growth of fluctuations is exponential wich a time constant of 25 fm/c.

The background transport theory used in this work is given by the lowest member of BBGKY hierarchy - the 1-body semiclassical 'Vlasov equation'. Then, our model may be first understood as a version of the hydrodynamic model which is added a two-body correction; it is used here to study dynamically the growing of density fluctuations leading to the spinodal decomposition. This paper aims at getting insight in the dynamics of the fluctuation growth: since in actual reactions such a process is in competition with many others (cooling by evaporation, sequential emissions...), time characteristics are then key quantities to determine the conditions under which spinodal decomposition could be observed.

Our numerical treatment is based on the Vlasov phase space transport equation, complemented by a Pauli-blocked Uehling-Uhlenbeck collision term (see [5] for a review). This equation is usually solved using the projection of the phase space density distribution on a set of pseudo-particles, which are gaussians in space and momentum, their widths and numbers being chosen to reproduce the nucleus surface diffuseness and to optimize of the space paving [7]. This pseudo-particle model requires only one run to obtain accurate bulk and surface properties as we have shown [7]; except for the number of gaussians per physical particle and the gaussian widths, no extra parameters are needed.

The pseudo-particles (PP) Hamiltonian in phase space reads :

$$H^{PP} = \frac{\langle p^2 \rangle}{2m} + \langle V_{HF}(\vec{r},\vec{p}) \rangle \qquad (1)$$

where V_{HF} is the Wigner-transformed Hartree-Fock nuclear potential, m the nuclear mass. The brackets indicate that the above quantities are smeared out by the (here gaussian) form factor of the pseudo-particles; the solution of the Vlasov equation gives the time evolution of a swarm of pseudo-particles moving in the field of equation (1) and undergoing binary collisions when allowed by the phase space availability. The cross section of pseudo-particles is scaled on the nucleon-nucleon cross section such that their average mean free path is kept equal to the nucleon one [5]. It is to notice that inside the region where the spinodal decomposition is studied - low temperature and low density - the number of collisions is very low, thus the effect of collisional term is not the most significant.

We first report briefly here on infinite matter calculations, detailed calculations are reported in [7]. Infinite nuclear matter is simulated by a cubic box with periodic boundary conditions; the system is taken homogeneous in r-space with a Fermi-Dirac momentum distribution; its initial phase space distribution then reads :

$$f(\vec{r},\vec{p};t=0) = \frac{1}{n_g}\sum_{i=1}^{N} g_x(\vec{r}-\vec{r}_i)\,g_\phi(\vec{p}-\vec{p}_i) \qquad (2)$$

and the spatial density n is :

$$n(\vec{r};t=0) = \frac{1}{n_g}\sum_{i=1}^{N} g_x(\vec{r}-\vec{r}_i) \qquad (3)$$

Gaussian functions are normalized with a width Δ ; the (r_i,p_i) coordinates of each gaussian are randomly drawn according to the probability density law $d(\varepsilon)$:

$$d(\varepsilon_i) = \theta(\varepsilon_F - \varepsilon_i) \qquad \text{for } T = 0$$
$$d(\varepsilon_i) = \left\{1 + \exp\left[(\varepsilon_F - \varepsilon_i)/T\right]\right\}^{-1} \qquad \text{for } T \neq 0 \qquad (4)$$

The Fermi energy ε_F is constrained on the initial nuclear density n_0; the number N of pseudo-particles then follows as :

$$N = n_0 L^3 n_g \qquad (5)$$

L being the linear dimension of the cube and n_g the number of pseudo-particles associated with each nucleon.

We compare the nuclear Equation Of State (EOS) calculated with the pseudo-particles model against the analytical one in Hartree-Fock approximation; in the case of interaction Skm* [8] the one body potential reads,

$$V_{HF}(\vec{r}) = \frac{3}{4}t_0 n(\vec{r}) + \left[\frac{3t_1 + (5+4x_2)t_2}{16}\right]\int \frac{p^2}{2m} f(\vec{r},\vec{p})\,d\vec{p}$$
$$+ \frac{1}{32}\Delta n(\vec{r})\left[(5+4x_2)t_2 - 9t_1\right] + \frac{3}{8}t_3(\gamma+2)n(\vec{r})^{\gamma+1} \qquad (6)$$

where n is the density, r, the position, p the momentum and t_0, t_1, t_2, t_3, x_2, γ are parameters of the effective interaction written in local density formalism .

Figure 1 shows that one can reproduce with a great precision the exact EOS, as soon as n_g is sufficiently large [7]. For these calculations a value of n_g = 42 has been used. Note that for the whole range of temperatures and densities the gaussian widths of (2) are set constant.

The spinodal zone for the case of Skm* is displayed on figure 2a; it was obtained by solving the implicite equation K(n,T)=0, where K is the incompressibility of infinite nuclear matter at density n and temperature T. We do claim that the spinodal region calculated in that way (Hartree-Fock approximation) is very close from the one of our system because of the quality of our fit of the EOS.

In figure 2b, we show two snapshots of a system initially prepared in the spinodal zone of instability at coordinates (n=0.02 fm^{-3}, T=0 MeV). At initial time, the pseudo-particles (here 852) are randomly scattered. Due to the low number of pseudo-particles as early as 60 fm/c, strong inhomogeneities show up : large clusters of nuclear liquid embedded in a vapor phase. These structures are stable with time; they do not look like nuclei; in particular due to the absence of Coulomb field which would help breaking them into smaller pieces. As expected, for a spinodal decomposition in infinite nuclear matter, the actual number of cluster found is 1 using a 3D generalization of the percolation algorithm of Gawlinski and Stanley [12].

The box size L is 16 fm, sufficiently large (for zero-range interactions) to get independance of the results on the boundary conditions; L is a critical parameter, using a too small box would prevent inhomogeneities to develop.

Our calculations characterize the degree of clusterization by the inhomogeneity factor : $r = \langle n \rangle_t / n_0$ where n_0 is the initial density and,

$$\langle n \rangle_t = \int \frac{n(\vec{r})^2}{A} d^3\vec{r} \qquad (7)$$

Observable <n> has to be understood as a correlation function in configuration space whose time evolution gives pictures of the inhomogeneity of the system. Putting it differently, this quantity is the average density computed *where* the gaussians are. For an homogeneous system the average <n> is equal to A/V where A is the number of nucleons and V the volume of the box, whereas for an inhomogeneous system, <n> is always greater than A/V. Therefore, the factor $r = \langle n \rangle_t / n_0$, n_0 being A/V starts at 1 and grows as soon as inhomogeneities develop.

Time evolutions of this factor are shown in figure 3 for a cold (T=0), dilute (n_0 is less than 1/3 of cold nuclear matter saturation density) initial system, with several samplings. In all our calculations, such curves exhibit a typical S-shape when spinodal decomposition occurs; three regimes are showing up; an initial regime where the r factor rises slowly, it corresponds to the progressive building up of the fluctuations; the decomposition regime where the initial stable state is destroyed by the fluctuations and clusters are formed as shown by the rapid upsurge of the r-factor; finally an asymptotic regime where this factor keeps its limit value which depends on the initial preparation of system.

The decomposition regime corresponds to the rapid amplification of the initial fluctuations present in the system which intervene as 'seeds' of the process. In our simulation, most initial fluctuations are purely numerical : mainly uncomplete sampling of the phase space.

Obviously the behaviour of the system is very phase space sampling dependent. Less pseudo-particles means more initial fluctuations, then the system needs less time to build up the fluctuations which leads to a shorter first regime .

The duration of the first regime of the S-shape curve is then meaningless since 'sampling-dependent' : in particular it depends on the random generator seeds. In the case of a complete paving of the phase space we would get no fluctuations at all (infinite time to build them up !). Our choice was simply to have a good description of the EOS and enough numerical fluctuations to simulate some physical ones. Note that calculations using PP-model with n_g below 20-25 are not physically relevant [7] and calculations with n_g over 50 are not yet performed because of the computational burden.

The second regime is rather similar for a number of gaussians per nucleon greater than 35-40. This means that the system looses memory of its initial preparation as expected in a chaotic transition. It is then possible to define a characteristic time of the decomposition as the non-ambiguous time duration of the second regime, namely the $t_{10\text{-}90}$ time of the density evolution.

$$t_{10\text{-}90} = t(r=0.9r_s) - t(r=0.1r_s) \qquad (8)$$

where r_s is the asymptotic r-factor computed by averaging over the third regime.

Figure 4 shows that the Uehling-Uhlenbeck collision term increases by 15% the asymptotic r-factor. The t_{10-90} does not significally change due to the low density of the system while fluctuations building up and early clusters formation. This allows to neglect collisional term in further calculations in order to save CPU time.

In figures 5a and 5b, we evidence the spinodal zone of Skm* interaction by variation of the initial preparation in the (T,n) plane. Firstly, we notice that when prepared inside the spinodal zone the density inhomogeneities do grow, and when prepared outside ($n=0.11$ fm^{-3}) the system remains homogeneous. This illustrates the ability of the PPM model to accurately simulate the genuine Nuclear Equation Of State. Secondly, the characteristic time for decomposition (i.e. the t_{10-90} parameter) is strongly dependent of $n(t=0)$ (figure 5a) and $T(t=0)$ (figure 5b). Closer to the critical temperatures ($T=12$ MeV) the superficial tension almost vanishes and density homogeneities grow very slowly. The more dilute and the cooler the system the faster the process, since the spinodal decomposition leads to the formation of relatively cold drops inside a dilute gas.

In figure 6, one sees that the decomposition clearly depends on the interaction. The small difference between the asymptotic densities being connected with the differences in the excitation energies of the system. All these interactions give more or less the same saturation properties for nuclear matter. Nevertheless they have important differences for quantities like incompressibility K and effective mass m^*/m. Such parameters are expected to have an important role in the evolution of $\langle n \rangle$ in time; surface parameters like the surface energy coefficient a_S have also to be considered because surface phenomena are important in cluster formation.

In our investigations, typical values for t_{10-90} are in between 60 fm/c and 200 fm/c depending on the initial value (n,T). Typical results are summerzed in Table I. These characteristic times should be compared with time durations of heavy-ion collisions. Since the growth of fluctuations is favoured in cold systems (see Table I), we choose to compare with collisions at relatively low energy. For instance, the passing through time of two medium nuclei at 30 MeV/A beam energies can be roughly estimated to 40 fm/c (10 fm divided by the relative velocity 0.25c of the ions). This corresponds to the

lower limit. Calculations with Boltzmann-like equations including effects of mean-field and two-body collisions yields larger values which do not exceed 80-100 fm/c. Then our calculations show that the characteristic time of the spinodal decomposition lies within the upper bound of the average time duration of heavy-ion reactions.

We have been able to characterize the decomposition time in nuclear matter in a way which is independent of the sampling of the phase space. Moreover our approach was not limited to the linear regime as works based on generalizations of Landau kinetics equation. It was shown that this time is strongly dependent on the coordinates (n,T) of the initial condition in the spinodal zone and on the nuclear interaction itself. Decomposition times are ranging between 60 fm/c to 200 fm/c. A realistic interaction like Skm* gives a time around 100 fm/c in the most favorable case of cold and dilute nuclear matter.

During heavy-ion collisions the compound system could undergo such a decomposition if it spends time enough in the spinodal zone. From previous results such a phenomenon will be difficult to pin out and might be tracked in the core of two very heavy nuclei colliding at low energy around 30 MeV/u.

All those calculations have been performed on a RS/6000 workstation and a complete dynamical computation, up to 270 fm/c (i.e 360 time steps) takes about 10 hours for a system of 8200 gaussians.

The authors are grateful to Pr.D.H. Boal for interesting e-mail exchanges.

Table I : Typical time scales for spinodal decomposition using several interactions. Starting density is $n=0.049\ fm^{-3}$, temperatures T = 0, 6 MeV.

	t_{10-90} (fm/c)	t_{10-90} (fm/c)
$n = 0.049\ fm^{-3}$	T = 0	T = 6 MeV
Skyrme III	61.5	129
Zamick (K=300 MeV)	78	147
Zamick (K=228 MeV)	84	165
Skyrme VI	85	150
*Skm**	112	177
Tondeur To78	165	228
Tondeur T5	175	> 300

References

[1] C.J. Pethick and D.G. Ravenhall, Ann. Phys. (N.Y.) 183,131 (1988).

[2] H. Heiselberg, C.J. Pethick and D.G. Ravenhall, Phys. Rev. Lett. 61, 818 (1988).

[3] G. Peilert, J.Randrup, H.Stöcker and W.Greiner, Phys. Lett. B 260,271 (1991).

[4] D.H. Boal and J.N. Glosli, Phys. ReV. C42, 502 (1990).

[5] S. Das Gupta and G.F. Bertsch, Phys. Rep. 160, 189 (1988).

[6] C. Grégoire, B. Remaud, F.Sebille, L. Vinet and Y.Raffray, Nucl. Phys. A465, 77 (1987).

[7] D.Idier, B.Benhassine, M.Farine, B.Remaud and F.Sebille, to be published.

[8] J.Bartel, P.Quentin, M.Brack, C.Guet and H.B.Hakansson, Nucl. Phys. A386, 79 (1982).

[9] M.Beiner, H.Flocard, N.V.Giai and P.Quentin, Nucl. Phys. A238, 29 (1975).

[10] F.Tondeur, M.Brack, M.Farine and J.M.Pearson, Nucl. Phys. A420, 297 (1984).

[11] F.Tondeur, Nucl. Phys. A315, 353 (1987).

[12] E.T.Gawlinski and H.E.Stanley, J.Phys. A 14 (1981) L291-L299

Figure captions

Figure 1 : Comparison between Hartree-Fock calculations and PP-model : total energy per nucleon (E/A) versus density (n) at T=0,5,10 MeV, for Skyrme Skm* force.

Figure 2 : Snapshots of the (x,y) positions of 852 pseudo-particles at t=0 and t=60 fm/c for Skm* force at T=0 and n(0)=0.02 fm^{-3}.

Figure 3 : Dynamical computation of average density <n(t)> for different samplings (ng=31, 42, 52, 62) at T=0 and n(0)=0.049 fm^{-3}

Figure 4 : Effect of the Uehling-Uhlenbeck collision term (here ng=31).

Figure 5a : Skm* spinodal zone. Time-evolution of the average density at T=3 MeV, for several initial densities : 0.020, 0.049, 0.080 and 0.110 fm^{-3}. The last point (0.110 fm^{-3}) is outside of the Skm* spinodal zone.

Figure 5b : Skm* spinodal zone. Time-evolution of the average density <n> at several initial temperatures : T=0,3,6,9 and 12 MeV. Starting density is 0.049 fm^{-3}

Figure 6 : Dynamical computation of average density <n(t)> for several Skyrme type forces SIII and SVI [9], T1 and T5 [10], To78 [11]. Zam 228 and Zam 300 are simplified (t0,t3) Skyrme interactions with K=228MeV and K=300MeV. The starting density is 0.049 fm^{-3} and initial temperature is T=0.

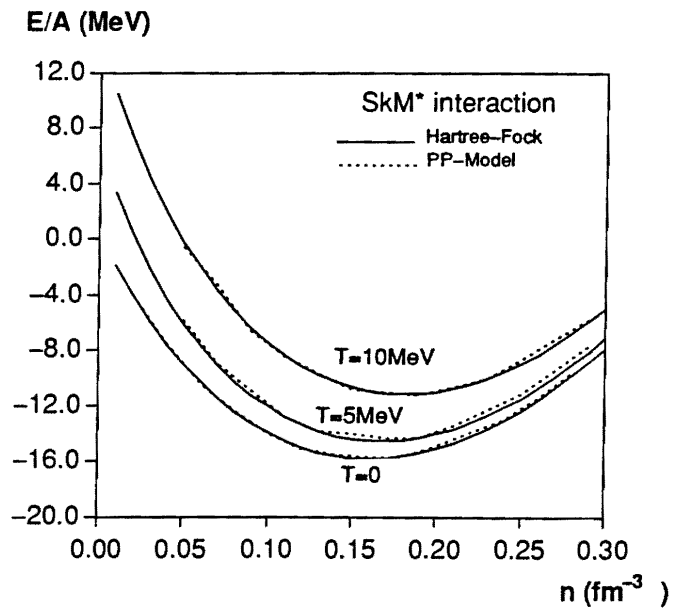
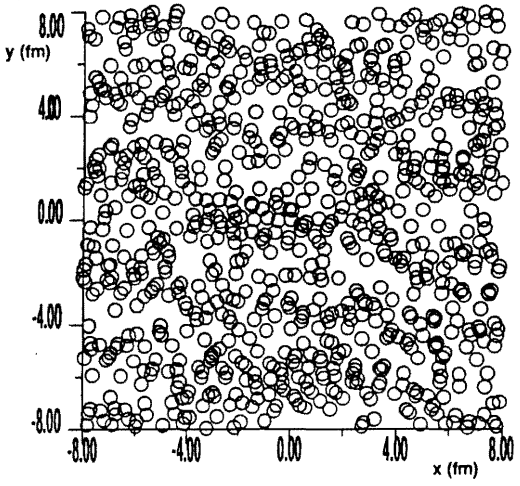
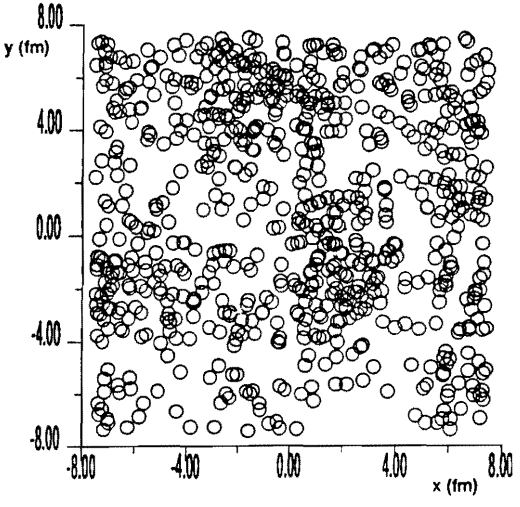


Figure 1



t=0



t = 60 fm/c

Figure 2

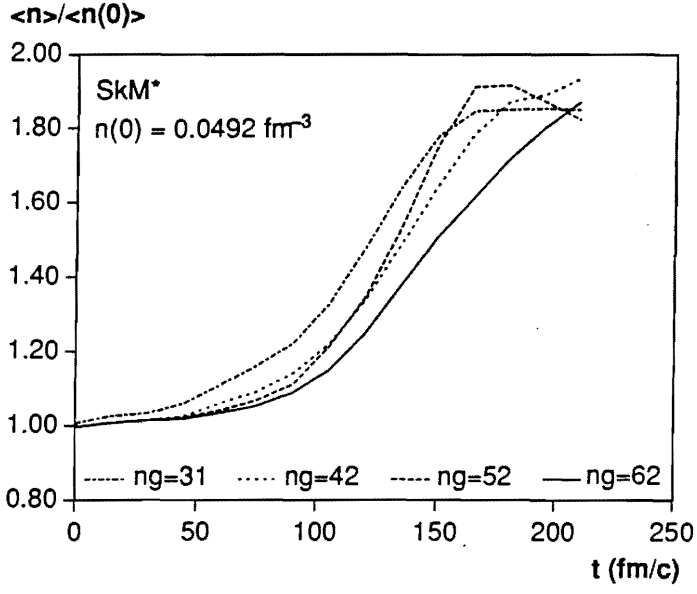


Figure 3

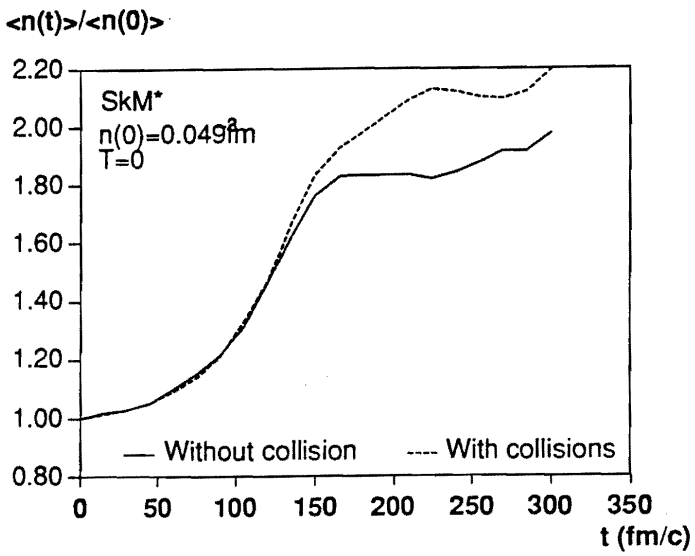


Figure 4

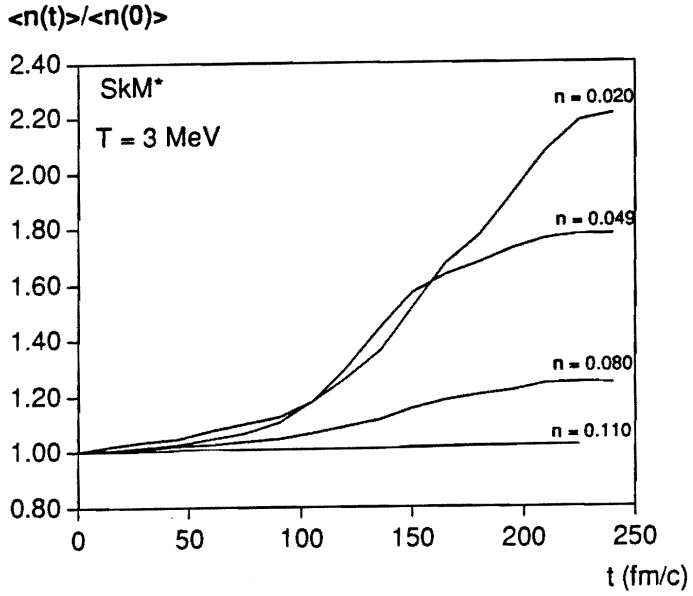


Figure 5a

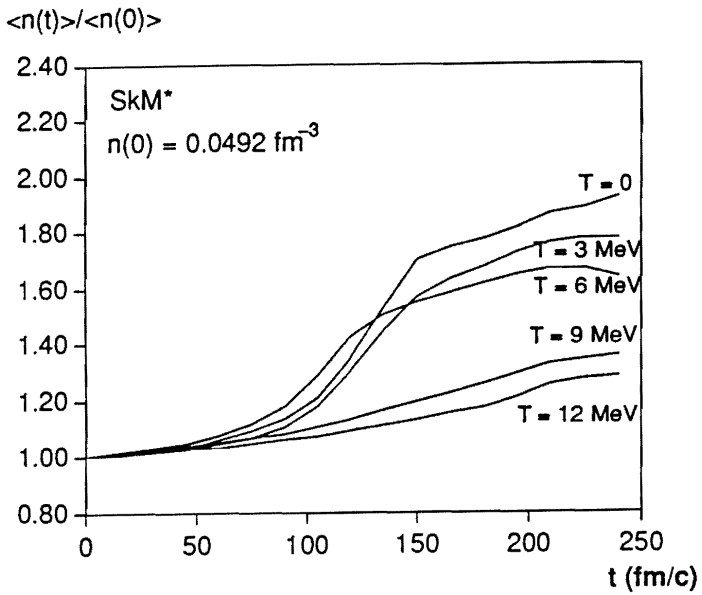


Figure 5b

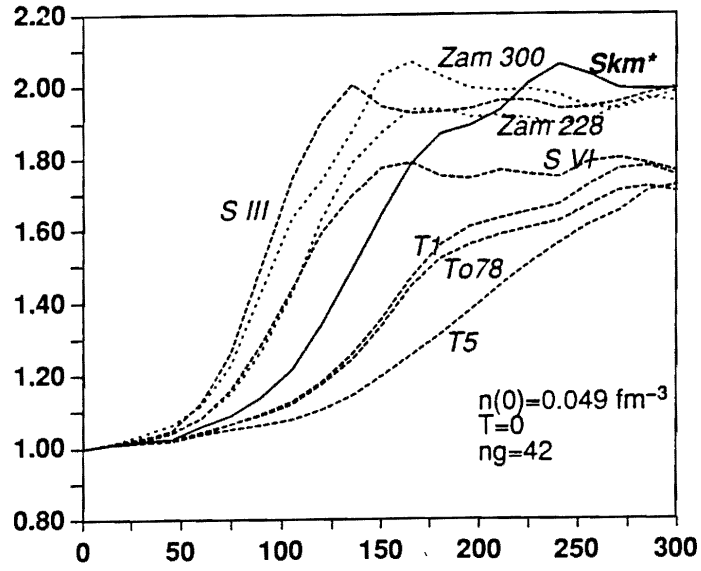


Figure 6