FR 9003504

CEA-CONF - -10111

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THERMODYNAMICAL DESCRIPTION OF EXCITED NUCLEI

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November 13, 1989

Abstract

In heavy ion collisions it has been possible to obtain composite systems at rather high excitation energies corresponding to temperatures of several MeV. The theoretical studies of these systems are based on concepts borrowed from thermodynamics or statistical physics, such as the temperature.

In these lectures, we present the concepts of statistical physics which are involved in the physics of heavy ion as they are produced nowadays in the laboratory and also during the final stage of a supernova collapse. We do not attempt to describe the reaction mechanisms which yield such nuclear systems nor their decay by evaporation or fragmentation. We shall only study their static properties.

The content of these lectures is organized in four main sections. The first one gives the basic features of statistical physics and thermodynamics necessary to understand quantum mechanics at finite temperature. In the second one, we present a study of the liquid-gas phase transition in nuclear physics. A phenomenological approach of the stability of hot nuclei follows. The microscopic point of view is proposed in the third part. Starting from the basic concepts derived in the first part, it provides a description of excited or hot nuclei which confirms the qualitative results of the second part. Furthermore it gives a full description of most properties of these nuclei as a function of temperature. Finally in the last part, a microscopic derivation of the equation of state of nuclear matter is proposed to study the collapse of a supernova core.

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*lectures given at the second Sorak school, June 26-30, Korea

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1. INTRODUCTION TO STATISTICAL PHYSICS

In this first part, we give an overlook of the concepts we will need subsequently. First we recall the definition and properties of density operators. Then we introduce the statistical entropy as a measure of the missing information. Taking into account the knowledge of the system one has, the appropriate choice of the density operator is done by mean of a variational method with suitable Lagrange multipliers. This procedure yields the equilibrium density of a system together with its partition function. According to the choice of the physical variables, we define the canonical and grand canonical ensemble. The connection with thermodynamics is briefly given without detailed justifications, only the relation between the Lagrange multiplier associated with the energy and the temperature is discussed. Finally, several thermodynamical potentials are defined together with the Legendre transforms which allow to express each of them in term of another one.

For further discussion, it will be fruitful to refer to the chapter 2 to 5 of the book by R. Balian: "Du microscopique au macroscopique" [1]).

1.1. STATISTICAL MIXTURE – DENSITY OPERATORS

A physical state of a system is usually represented by a ket $|\Psi\rangle$ of a Hilbert space $\mathcal{H}$ associated to the quantum system. We shall assume below that the dimension of this Hilbert space is finite to avoid mathematical complications. The experimental measure of a physical quantity A described by an operator $\hat{A}$ is the average of $\hat{A}$ taken over the state $|\Psi\rangle$: $\langle A\rangle = \langle\Psi|\hat{A}|\Psi\rangle$. The state of the system is then known exactly, this is a pure state.

We want to describe more complex, and richer, cases where the actual state of the system is not well known. In such case, the only thing we may obtain is the probability q_λ that the state is described by a ket $|\Psi_\lambda\rangle$. As for any probability law, the q_λ must be non negative real numbers and their sum must be 1. The system is represented by the statistical mixture of states: $\{q_\lambda ; |\Psi_\lambda\rangle\}$. When the system is in a pure state $|\Psi_\lambda\rangle$ the measure of the observable A is given by $\langle\Psi_\lambda|\hat{A}|\Psi_\lambda\rangle$, as the probability of this ket is q_λ, one can see that the mean value of A will be:

$$\langle A\rangle = \sum_\lambda q_\lambda \langle\Psi_\lambda|\hat{A}|\Psi_\lambda\rangle \quad . \tag{1.1}$$

We have assumed the kets $|\Psi_\lambda\rangle$ normalized to unity, the above result still holds when they are not orthogonal. The density operator $\hat{D}$ associated to the statistical mixture $\{q_\lambda ; |\Psi_\lambda\rangle\}$ is defined as:

$$\hat{D} = \sum_\lambda |\Psi_\lambda\rangle q_\lambda \langle\Psi_\lambda|. \tag{1.2}$$

Thus equation (1.1) takes the from:

$$\langle A\rangle = \mathrm{tr}(\hat{D}\hat{A}) \quad . \tag{1.3}$$

This result shows that only $\hat{D}$ is needed to calculate $\langle A\rangle$. All the relevant information concerning the quantum system is contained in the density operator.

These operators satisfy the following properties:

$$
\begin{array}{llll}
i) & \hat{D} = \hat{D}^\dagger & \text{hermiticity} & (q_\lambda \text{real}) \\
ii) & \text{tr}(\hat{D}) = 1 & & (\sum_\lambda q_\lambda = 1) \\
iii) & \langle \Phi | \hat{D} | \Phi \rangle \geq 0 & \text{non negative} & (q_\lambda \geq 0, \forall \lambda)
\end{array}
\tag{1.4}
$$

We have listed in parenthesis the properties of q_λ which imply those of $\hat{D}$. Conversely, one can show that any operator satisfying these properties can be viewed as a density operator represented by a statistical mixture which can be constructed in principle.

Up to now we have assumed that the number of particles is given. If one only knows its mean value, it is still possible to generalize the above results by considering the Fock space which is the direct sum of all the Hilbert spaces having a given number of particles. For any observable A which conserves the particle number, $[\hat{A}, \hat{N}] = 0$ (where $\hat{N}$ is the particle number operator), the measure of A is still given by (1.3).

1.2. STATISTICAL ENTROPY

We want now to determine for a given quantum system its density operator as its knowledge allows to calculate all mean values of observable. For a system which is not exactly known one has to define a quantitative measure of the missing information, or equivalently an estimation of the amount of disorder. This amount of missing information is measured from the density operator $\hat{D}$ by the statistical entropy S:

$$
S(\hat{D}) = -k \, \text{tr}(\hat{D} \lg \hat{D}) \quad , \tag{1.5}
$$

where k is the Boltzmann constant.

When $\hat{D}$ is given by its spectral representation (see eq. 1.2), the entropy becomes:

$$
S(\hat{D}) = -k \sum_i (p_i \lg p_i) \quad .
$$

The statistical entropy defined according to (1.5) satisfies some elementary properties which justifies it as a measure of the dis·.·der:

1. It remains invariant under a unitary transform which does not modify the system: the disorder does not increase nor decrease.

2. The statistical entropy reaches a minimum of value zero for a pure state, and conversely. No disorder and zero statistical entropy are equivalent statements.

3. The statistical entropy is maximum when all events p_i are equiprobable. For N such equiprobable events, $p_i = 1/N$ and $S = k \lg N$. This result shows that the entropy is a valid measure of the disorder. Equiprobable events correspond to a state for which the disorder reaches a maximum: there is no good physical reason to choose any state instead of the other.

For a system built from two sub-systems a et b, the Hilbert space of the total system is the tensorial product of the Hilbert spaces $\mathcal{H}^a$ and $\mathcal{H}^b$ of the sub-systems. Let $\hat{D}$ be the density operator of the total system and A an observable defined by an operator $\hat{A}_a$ acting only in $\mathcal{H}^a$. To calculate its mean value, $Tr(\hat{D}\hat{A}_a)$, one can take its trace in the space $\mathcal{H}^b$

where $\hat{A}_a$ does not act and define: $\hat{D}_a = \mathrm{tr}_b(\hat{D})$. As $\hat{D}_a$ satisfies the properties (1.4), it can be viewed as the density operator of the sub-system a attached to $\mathcal{H}^a$. Similarly, one can define the density operator $\hat{D}_b$ by taking the trace of $\hat{D}$ in $\mathcal{H}^a$.

When both sub-systems are statistically independent, $\hat{D}$ is equal to the tensorial product $\hat{D}_a \otimes \hat{D}_b$ of the density operators of the sub-systems. The total statistical entropy is then exactly the sum of the entropies calculated in each sub-space: $S(\hat{D}) = S(\hat{D}_a) + S(\hat{D}_b)$. When this is the case, there is no correlations and no information from one of the sub-systems can teach us something about the other.

On the other hand, when the sub-systems a and b are correlated, $\hat{D}$ contains more informations than $\hat{D}_a$ et $\hat{D}_b$ altogether. The knowledge of the total system, with its correlations, is more accurate than the sole knowledge of its two parts: $S(\hat{D}) \leq S(\hat{D}_a) + S(\hat{D}_b)$. The density operator $\hat{D}$ is no longer equal to the tensorial product $\hat{D}_a \otimes \hat{D}_b$.

The last property is a "concavity" property which means that mixing two states of a given system in a unique one increases the disorder. Let us define two states by their density operators $\hat{D}_1$ and $\hat{D}_2$. Let μ_1 and μ_2 be the weighting factors of the mixing ($0 \leq \mu_1, \mu_2 \leq 1$ et $\mu_1 + \mu_2 = 1$) then,

$$S(\mu_1 \hat{D}_1 + \mu_2 \hat{D}_2) \geq S(\mu_1 \hat{D}_1) + S(\mu_2 \hat{D}_2) \qquad .$$

Finally the variation of S with respect to $\hat{D}$ is:

$$\delta S(\hat{D}) = -k \, \mathrm{tr}(\delta \hat{D}(\lg \hat{D} + 1)) \qquad . \tag{1.6}$$

1.3. CHOICE OF THE DENSITY OPERATOR

Up to now we have formally defined a density operator and given an estimation of the disorder through the entropy. The next step is to calculate $\hat{D}$, taking into account our knowledge of the system.

When nothing is known, one has to count the number of pure states as they are equiprobable. For N such available states, the entropy is maximum and equal to $k \lg N$. For states at least partly known, one must take explicitly into account all the available information. An "exact" one will be included in the construction of the Hilbert space. For instance, if the particle number N is exactly known, it is natural to choose the Hilbert space $\mathcal{H}^N$ built on the eigenstates of the particle number operator with the eigenvalue N. In other cases the information is only known by mean values, e.g. the energy $U = \mathrm{tr}(\hat{D}\hat{H})$. The most usual cases are:

1. N et U are exactly known, the statistical ensemble of these states is the micro-canonical ensemble.

2. N is known exactly, U by its mean value. This is the canonical ensemble.

3. Finally when both N and U are known in average, one defines the grand canonical ensemble.

In what follows, we assume that exactly known quantities are taken care of by an appropriate definition of the Hilbert space. Let us assume more generally that we know the mean values of an arbitrary number of observables $\hat{A}_i$:

$$\mathrm{tr}(\hat{D}\hat{A}_i) = \langle \hat{A}_i \rangle \qquad . \tag{1.7}$$

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We want to find the statistical equilibrium distribution realized by the density operator $\hat{D}$, taking into account the constraints (1.7). For that purpose, we shall use the fact that the entropy is maximum when the disorder is maximum. To generalize this concept while taking the constraints into account, one postulates that the equilibrium distribution is such that the entropy is maximal and the constraints are fulfilled. The explicit construction of $\hat{D}$ is achieved with an additional constraint which imposes that the trace of $\hat{D}$ is unity (see (1.4)). The variational method of the Lagrange multipliers results in the search of the stationary values of:

$$-\operatorname{tr}(\hat{D}\lg\hat{D}) - \sum_i \lambda_i \operatorname{tr}(\hat{D}\hat{A}_i) - \lambda_0 Tr(\hat{D}) \qquad .$$

Given the constraints on the mean values, the resolution of this problem yields the density operator at equilibrium:

$$\hat{D} = \frac{1}{Z}\exp\left(-\sum_i \lambda_i \hat{A}_i\right) \qquad . \tag{1.8}$$

This expression is called *Boltzmann-Gibbs distribution*. The corresponding entropy is strictly larger than that obtained for any other density operator fulfilling the constraints (1.7): this extremum of S is indeed a maximum. The normalization condition of $\hat{D}$ determines the partition function Z of the system as a function of the Lagrange multipliers λ_i:

$$Z = \operatorname{tr}\left(\exp\left(-\sum_i \lambda_i \hat{A}_i\right)\right) \qquad . \tag{1.9}$$

Finally, the conditions (1.7) give the λ_i as solutions of the equations:

$$\frac{\partial}{\partial\lambda_i}\lg Z(\lambda_j) = -\langle\hat{A}_i\rangle \qquad . \tag{1.10}$$

By a simple calculation, the equilibrium entropy can be related to the Boltzmann-Gibbs distribution:

$$S(\hat{D}) = k\lg Z + k\sum_i \lambda_i\langle\hat{A}_i\rangle \qquad , \tag{1.11}$$

or equivalently, because of (1.10):

$$S = k\lg Z - \sum_i \lambda_i\frac{\partial}{\partial\lambda_i}(k\lg Z) \qquad . \tag{1.12}$$

For a small displacement of the equilibrium associated to an infinitesimal variation of the $\langle\hat{A}_i\rangle$, and thus of the λ_i which are related, one has:

$$d(\lg Z) = \sum_i \frac{\partial}{\partial\lambda_i}(\lg Z)d\lambda_i = -\sum_i\langle\hat{A}_i\rangle\,d\lambda_i \qquad ,$$

and, due to (1.12)

$$dS = k\sum_i \lambda_i\,d\langle\hat{A}_i\rangle \qquad . \tag{1.13}$$

These last two relations illustrate that the natural variables of the partition function are the Lagrange parameters, whereas for the entropy they are the mean values $\langle \hat{A}_i \rangle$. Taking these mean values as variables, one gets from (1.13):

$$\frac{\partial S}{\partial \langle \hat{A}_i \rangle} = k\,\lambda_i \qquad . \tag{1.14}$$

The transformation (1.12) is a Legendre transformation which connects $k\lg Z$, function of the λ_i, to the entropy S, function of the $\langle \hat{A}_i \rangle$ conjugate variables of the λ_i. The inverse transformation, which is also a Legendre transformation, reads as:

$$k\lg Z = S - \sum_i \langle \hat{A}_i \rangle \frac{\partial S}{\partial \langle \hat{A}_i \rangle} \qquad . \tag{1.15}$$

In the canonical ensemble, the particle number N and the volume Ω are given exactly. The energy is given in average, $U = \mathrm{tr}(\hat{D}\hat{H}_N)$, where $\hat{H}_N$ is the hamiltonian in the Hilbert space of N particles. The Lagrange parameter associated is traditionally called β.

In the grand canonical ensemble, both the energy U and the particle number N are given in average. The Lagrange parameters associated to U and N are β and $-\alpha$. The underneath table summarizes the expressions of $\hat{D}$, Z and S.

$\hat{D}=\frac{1}{Z_c}\exp\left(-\beta\hat{H}_N\right)$	$\hat{D}=\frac{1}{Z_G}\exp\left(-\beta\hat{H}+\alpha\hat{N}\right)$
$Z_C(\beta,N)=\mathrm{tr}\exp\left(-\beta\hat{H}_N\right)$	$Z_G(\alpha,\beta)=\mathrm{tr}\left(\exp\left(-\alpha\hat{H}+\beta\hat{N}\right)\right)$
$S(U)=k\lg Z_C + k\beta U$	$S(U,N)=k\lg Z_G + k\beta U - k\alpha N$

Finally let us give the relations between U and N, mean values of observables, and β and α, relations derived from (1.10) and (1.14)

$$\frac{\partial}{\partial\beta}\lg Z_G = -U \qquad , \qquad \frac{\partial}{\partial\alpha}\lg Z_G = N \qquad , \tag{1.16}$$

and the inverse relations:

$$\frac{1}{k}\frac{\partial S}{\partial U} = \beta \qquad , \qquad \frac{1}{k}\frac{\partial S}{\partial N} = -\alpha \qquad . \tag{1.17}$$

In the grand canonical ensemble, the generalization to the case of several species of particles can be done without particular difficulties. Starting from the general expressions (1.8) to (1.15), one introduces as many particle number operators $\hat{N}_i$ as needed with corresponding Lagrange multipliers α_i.

1.4. RELATION WITH THERMODYNAMICS – TEMPERATURE

In the preceding section we have constructed the Boltzmann-Gibbs equilibrium distribution. Our aim is now to make the connection with thermodynamical concepts. In what follows, we shall only introduce the temperature and the different thermodynamical potentials.

Let us work in the canonical ensemble. Let a and b be two independent systems at thermal equilibrium. They are characterized by Lagrange parameters β_a et β_b. As they are thermally isolated, there are no correlations between themselves. We bring them into contact by means of a perturbation small enough to be neglected in front of the hamiltonians. Its role is to allow energy transfer between a and b without perturbing the total system so that the total energy remains constant. As a result, the new density operator depends upon a single Lagrange parameter β, as there is a unique constraint on the total energy. This thermal contact yields thus the equality of β_a and β_b. The Lagrange parameter β *plays the role* of a temperature. The new energy partition between a and b is obtained by calculating the mean values of the hamiltonians of the sub-systems with the new equilibrium distribution.

To achieve the relationship between β and the temperature, we make use of the fact that the energy U is a decreasing function of β, a result we have not proven but which comes from the entropy concavity (see section 1.2). As the total energy is conserved, the equilibrium is realized for a value of β lying between β_a and β_b. The energy of the *colder* system increases at the expenses of the other, simultaneously, its parameter β decreases: β varies as the inverse of a temperature.

Under an infinitesimal transformation of an isolated system, we can associate the part dQ of the variation dU of U coming from the variation of $\hat{D}$ to heat (no variation of $\hat{H}$). Similarly an infinitesimal variation of work dW can be related to the variation of $\hat{H}$ itself. Thus we have $dU = dQ + dW$ with:

$$dQ = \mathrm{tr}(\hat{H}d\hat{D}) \qquad , \tag{1.18}$$

$$dW = \mathrm{tr}(\hat{D}d\hat{H}) \qquad . \tag{1.19}$$

For a system which remains at thermal equilibrium during a transformation, the heat variation can be related to the entropy by:

$$dS = k\beta \, \mathrm{tr}(\hat{H}d\hat{D}) = k\beta \, dQ. \tag{1.20}$$

The comparison of this result with the relation $dS = dQ/T$ between the entropy and heat variations during a quasi-static transformation of a system at thermal equilibrium shows that one can identify β with the inverse of the temperature: $\beta = 1/kT$. We shall not elaborate further in these lectures on the correspondence between the microscopical scale we used to introduce the Boltzmann-Gibbs distribution and the macroscopical scale of thermodynamics.

1.5. THERMODYNAMICAL POTENTIALS

A thermodynamical potential is a function of some variables which characterizes a system, this function presents an extremum at equilibrium and its partial derivatives have simple physical interpretations. The entropy is an example of such thermodynamical potential, it depends upon the internal energy U, the particle number N, and other possible variables x_α, such as the volume V or an external field. The total differential of S is (see equations (1.13), (1.16) et (1.17)):

$$dS = k\beta \, dU - k\alpha \, dN - k\beta \sum_\alpha X_\alpha \, dx_\alpha \qquad .$$

It is written in terms of pairs of conjugate variables: U and $k\beta$, N and $-k\alpha$,...

In thermodynamics, one distinguishes extensive variables which are proportional to the volume at the macroscopic limit, from intensive variables which do not depend upon it. The variables U and N are extensive, the conjugate variables $k\beta = 1/T$ and $-k\alpha$ are intensive.

Most of the time the internal energy $U(S, N, x_\alpha)$ is used instead of the entropy $S(U, N, x_\alpha)$. Its total differential is $dU = T\,dS + \mu\,dN + \sum_\alpha x_\alpha\,dx_\alpha$. The internal energy is useful for adiabatic transformations. The conjugate variable of N, $\mu = \alpha/\beta$, is the chemical potential. One can also use the temperature T rather than the entropy as variable. Then an appropriate Legendre transformation gives the free energy:

$$F(T, N, x_\alpha) = U(S, N, x_\alpha) - S\frac{\partial U}{\partial S} = U - TS \qquad , \qquad (1.21)$$

The natural variables of F are $T = 1/k\beta$, N and the volume. They are these of the canonical ensemble. The free energy is relevant for the study of quasi-static isothermal transformations. If one of the x_α is the volume, the work received by the system for a variation dV of the volume is, according (1.19):

$$dW = \operatorname{tr} \hat{D}\frac{\partial \hat{H}}{\partial V}\,dV = -P\,dV \qquad .$$

where the pressure P is the conjugate variable to the volume:

$$P = -\frac{\partial F}{\partial V} \qquad . \qquad (1.22)$$

The pressure, as a function of the temperature, of the particle number and of the volume is called the equation of state of the system. The quantity $-P\,dV$ represents the amount of work due to the pressure forces for a variation of the volume, similarly $\mu\,dN$ plays the role of a work associated to a variation of the particle number. It can be viewed as the quantity of energy received by a system when one adds or removes one particle. In nuclear physics, it is the opposite of the separation energy in the limit of low temperature. For exchange of particles at constant temperature, it is easier to use the chemical potential $\mu = \alpha/\beta$ rather than the Lagrange parameter α.

When T and μ are chosen as variables, one introduces the grand potential A by means of a double Legendre transformation on the internal energy:

$$A(T, \mu, x_\alpha) = U(S, N, x_\alpha) - S\frac{\partial U}{\partial S} - N\frac{\partial U}{\partial N} = U - TS - \mu N = F - \mu N \qquad .$$

The natural variables, $T = 1/k\beta, \mu, V, \cdots$ are those of the grand canonical ensemble. The equation of state (1.22) is given by the parametric representation:

$$\begin{aligned}
P &= -\partial A(T, \mu, V)/\partial V \qquad , \\
N &= -\partial A(T, \mu, V)/\partial \mu \qquad .
\end{aligned}$$

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The grand potential depends upon only one extensive variable, namely the volume, therefore

$$\frac{A(T,\mu,V)}{V} = \frac{\partial A}{\partial V} \tag{1.23}$$

For a homogeneous medium, the pressure is equal to minus the grand potential per unit volume:

$$P = -A/V \quad . \tag{1.24}$$

The entropy maximization, which is our starting point, amounts to the minimization either of F or A. The underneath table summarizes the definitions and properties of the free energy and the grand potential, as well as the variables upon which these quantities depend:

$F(T,N,V)$	$= U - TS$	$A(T,\mu,V)$	$= F - \mu N$
	$= -kT \lg Z_c(\beta,N,V)$		$= -kT \lg Z_G(\beta,\alpha,V)$
dF	$= -S\,dT + \mu\,dN - P\,dV$	dA	$= -S\,dT - N\,d\mu - P\,dV$
P	$= -\partial F/\partial V$	P	$= -\partial A/\partial V = -A/V$

To use only the intensive variables T, μ and P to define a thermodynamical potential, one has to perform the Legendre transformation: $A - V\,\partial A/\partial V$. However one gets an identically zero potential according to (1.23). The differential form of this "result" reads:

$$S\,dT - V\,dP + N\,d\mu = 0 \quad . \tag{1.25}$$

This relation is the *Gibbs-Duhem relation*, It tells us that to characterize a fluid with three variables, at least one of them must be extensive. We shall encounter a simplified form of this relation in the following section for a homogeneous infinite system.

As an exercise, it is suggested to calculate the partition function, the internal energy and the entropy of a system composed of N bosons occupying either one of two levels separated by an energy ϵ. Show that: for $\beta \to \infty$, one obtain the ground state of the system ($U = 0$, $S = 0$); for $\beta \to 0$, the internal energy is: $U = -N\epsilon/2$ and the disorder reaches a maximum: $S = \lg(N+1)$; finally if β decreases and goes to $-\infty$, then: $U \to N\epsilon$ and $S \to 0$: one gets again a pure state where all bosons have been excited. In such a case – only two degrees of freedom – it is difficult to speak of temperature, (which becomes "negative"!). We are far away from the macroscopic limit necessary to use thermodynamical concepts.

It is also instructive to study the system made of a single particle in an oscillator well (one particle, but an infinite number of degrees of freedom).

2. PHASE TRANSITION – STABILITY OF HOT NUCLEI

In this second part, we study the stability of hot nuclei which we describe as the coexistence limit of two phases, a gas and a liquid one. After a short introduction recalling the physical context we derive the liquid-gas coexistence equations from an equation of state for infinite nuclear matter. Finally we show the specificity of the nuclear problem characterized by a small number of particles and a strong coulomb field.

2.1. THE SITUATION IN HEAVY ION PHYSICS

During a collision between heavy ions, a large part of the reaction cross section is due to the formation of a composite system. The experimental determination of this fraction requires an accurate selection of the different events [2-7]), and has given evidences for the compound nucleus formation up to rather high excitation energies corresponding to temperatures of the order of 5 MeV. The study of the stability limit of these hot nuclei will gives new insight on the properties of hot nuclear matter.

The possible coexistence of two distinct phases in nuclear matter has been pointed out in numerous theoretical works [8-13]). These studies are based on the phase diagram of nuclear matter isotherms which have a typical van der Waals shape with two stable regions corresponding to a dense phase (liquid) and a more dilute one (gas). As temperature increases, these isotherms are deformed, and the distinction between the two phases disappears at a critical temperature T_C which has been interpreted as the temperature limit for the stability of the nucleus [14-19]).

Microscopic calculations [20,21]) which will be presented in the next part have shown that a correct description of a compound nucleus within statistical physics implies the consideration of a nucleus in equilibrium with a surrounding gas built from the evaporated particles. This vapor comes from unbound components of the nuclear wave function due to open decay channels. The equilibrium between the nucleus and the gas is interpreted as the coexistence of two distinct phases of nuclear matter. Matter within the nucleus is in a liquid dense phase whereas the external vapor is in a gaseous phase.

We introduce below a phenomenological model [22,23]) to describe the equilibrium of a nucleus immersed in its own saturating vapor. This model reproduces qualitatively the microscopical results [20,21]). Furthermore it gives an adequate ground to discuss the importance of the nuclear surface and the charge. It is a liquid drop model at finite temperature similar to that used in astrophysics[24-26]). One replaces the nucleus by a drop of nuclear matter with an abrupt surface with a constant density and a uniform temperature. The pressure inside is given by the equation of state of the infinite nuclear matter of the liquid phase. Outside, the vapor is described by the equation of state of the infinite nuclear matter of the gaseous phase.

2.2. LIQUID-GAS COEXISTENCE EQUATIONS

Before introducing the nuclear equation of state, let us recall how to describe a liquid-gas equilibrium from the concepts developed in the first part of these lectures.

Let us consider a container of volume V with N particles at a thermal equilibrium defined by the temperature T. We suppose that N_n of them are condense in a liquid drop within a volume V_n, the remaining $N_v = N - N_n$ being the surrounding gaseous phase in the volume $V_v = V - V_n$. The variables of this problem are the volume, the temperature and the particle number, they are these of the canonical ensemble. It is thus natural to write the free energy of the system as the sum of two terms,

$$F(T,V,N;V_n,N_n) = F_n(T,V_n,N_n) + F_v(T,V-V_n,N-N_n) \quad , \quad (2.1)$$

where F_n and F_v are respectively the free energy of the liquid drop (or the nucleus) and of the vapor. The two additional variables N_n and V_n determine the partition of the particles between the two phases in the container, their values result from the minimization of the free energy, which yields the standard coexistence equations:

$$\partial F/\partial V_n = 0 \quad \Rightarrow \quad P_n = -\partial F_n/\partial V_n = -\partial F_v/\partial V_v = P_v \quad , \quad$$
$$\partial F/\partial N_n = 0 \quad \Rightarrow \quad \mu_n = -\partial F_n/\partial N_n = -\partial F_v/\partial N_v = \mu_v \quad . \quad (2.2)$$

The first one expresses the equality of the pressures across the liquid-gas interface. The second gives a similar condition for the chemical potentials: the same amount of energy is required to transfer a particle from one phase to the other. These two reasonable conditions are thus based on the principle of maximal entropy.

For the time being, we include no surface tension and no coulomb effect. The two phases are homogeneous so that their free energies are proportional to their volume. For the nucleus phase one has: $F_{on}(T,V_n,N_n) = V_n f_{on}(T,\rho_n)$, where f_{on} is the liquid free energy per unit volume at the density $\rho_n = N_n/V_n$. The subscript "o" means the absence of surface tension and charge. The chemical potential and the pressure are:

$$\mu_{on} = \frac{\partial F_{on}}{\partial V_n} = V_n \frac{\partial f_{on}}{\partial \rho_n}\frac{\partial \rho_n}{\partial N_n} = \frac{\partial f_{on}}{\partial \rho_n} \quad , \quad (2.3)$$

$$P_{on} = -\frac{\partial F_{on}}{\partial V_n} = -f_{on} - V_n\frac{\partial f_{on}}{\partial \rho_n}\frac{\partial \rho_n}{\partial V_n} = \rho_n\,\mu_{on} - f_{on} \quad , \quad (2.4)$$

They depend only upon temperature and density. The derivation of the pressure with respect to the density yields:

$$\frac{\partial P_{on}}{\partial \rho_n} = \mu_{on} + \rho_n\frac{\partial \mu_{on}}{\partial \rho_n} - \frac{\partial f_{on}}{\partial \rho_n} = \rho_n\frac{\partial \mu_{on}}{\partial \rho_n} \quad , \quad (2.5)$$

which is a simplified version of the Gibbs-Duhem relation (1.25) for an homogeneous medium. For the gaseous phase one has similarly: $F_{ov} = V_v f_{ov}$. The relations (2.3) and (2.4) are still correct for the chemical potential μ_{ov} and for the pressure P_{ov}. The coexistence equations read as:

$$P_{on} = -(f_{on} - \rho_n\,\mu_{on}) = -(f_{ov} - \rho_v\,\mu_{ov}) = P_{ov} \quad , \quad$$
$$\mu_{on} = \partial f_{on}/\partial \rho_n = \partial f_{ov}/\partial \rho_v = \mu_{ov} \quad . \quad (2.6)$$
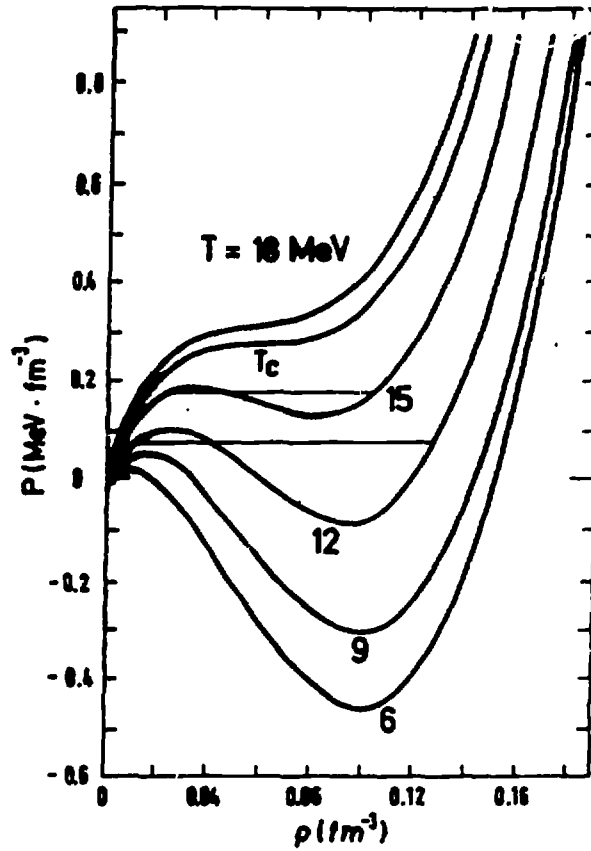
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Figure 1: Isotherms of the pressure calculated with the equation of state (2.7). Horizontal lines at $T = 12$ and 15 MeV indicate the coexistence pl~ eau between the liquid and the gaseous phases in the absence of surface tension and coulomb effect.

2.3. EQUATION OF STATE – PHASE DIAGRAM

In order to solve the coexistence equations, one needs an equation of state. Instead of using a van der Waals equation to study the liquid-gas transition, we shall work in the context of nuclear physics. It is possible to derive a nuclear equation of state from an effective force of the Skyrme type. This has been done and yields rather complicated expressions. We use below a simplified version [11] which gives qualitatively correct results and at the same time allows a better understanding of the underlying physics:

$$P_o(T,\rho) = T\rho - a'_o(T)\rho^2 + a_3(1+\sigma)\rho^{2+\sigma} \qquad , \qquad (2.7)$$

$$a'_o(T) = a_o - \frac{1}{2^{5/2}g}\left(\frac{2\pi\hbar^2}{m}\right)^{3/2} T^{-1/2} \qquad .$$

The chemical potentials μ_{on} and μ_{ov} are calculated up to an additive constant $\mu_o(T)$ from the Gibbs-Duhem relation:

$$\tilde{\mu}(T,\rho) = \mu(T,\rho) - \mu_o(T) = T\lg(\rho) - 2a'_o(T)\rho + a_3(2+\sigma)\rho^{1+\sigma} \qquad (2.8)$$
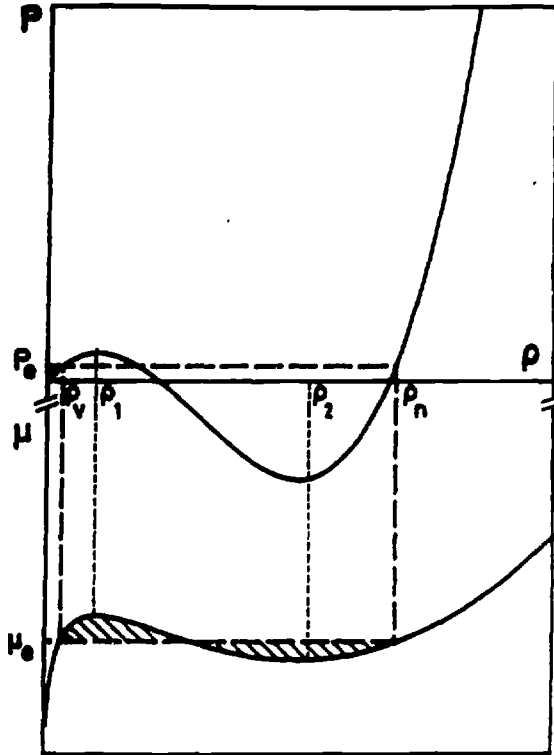
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Figure 2: Pressure and chemical potential for a temperature $T < T_C$ as a function of the density ρ. The solution of the coexistence equations is indicated by the dashed line.

In the definition of the pressure, m is the nucleon mass and $g = 4$ the spin-isospin degeneracy. The parameter σ determines the stiffness of the equation of state; together with a_o and a_3, it is related to infinite nuclear matter properties [11]. This equation of state results from an approximation of low density and high temperature.

The isotherms calculated with this equation of state are shown on figure 1. They have a typical van der Waals shape with a critical point at $T_C = 17.22$ MeV for $\rho_c = 0.057$ fm^{-3} and $P_c = 0.27$ MeV fm^{-3}. Below the critical temperature, there are two stable regions where the derivative of the pressure with respect to ρ is positive; the vapor corresponds to the low density region, the liquid to the high density one. These two phases are separated by an unphysical region where the derivative $\partial P / \partial \rho$ is negative.

As equation (2.6) tells us that the chemical potentials of the two phases are equal, the exact determination of $\mu_o(T)$ is useless. Figure 2 shows an example of chemical potential at a temperature below the critical one ($T < T_C$). Because of the Gibbs-Duhem relation, the minima and maxima of $\mu(\rho)$ and $P(\rho)$ correspond to each other. The liquid phase, $P_{on}(\rho_n)$ and $\mu_{on}(\rho_n)$, corresponds to densities $\rho_n > \rho_2$ (minimum of P and μ), whereas the gaseous phase, $P_{ov}(\rho_v)$ and $\mu_{0v}(\rho_v)$, corresponds to densities $\rho_v < \rho_1$ (maximum of P and μ).

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The coexistence equations can be solved by iteration, they give the two densities ρ_v and ρ_n, the pressure P_e and the equilibrium chemical potential μ_e. When drawn in the (P, μ) plane (see fig. 3), the isotherm has a typical shape with two cusps corresponding to the extrema of $P(\rho)$ and $\mu(\rho)$. The gaseous phase corresponds to the almost vertical branch, the unphysical region lies in between the two cusps and the liquid phase is represented by the last branch. This representation provides a nice way of solving graphically the coexistence equations.

The Maxwell construction determines the vaporization plateau by the law which says that the algebraic sum of the areas comprised between the plateau and the pressure isotherm, as a function of the volume, is zero. One can verify this law from the Gibbs-Duhem relation written under the form (2.5) of the relation. One can also show that when the isotherm is drawn as a function of the density, it is the algebraic sum of the areas comprised between the plateau and the chemical potential isotherm which is zero! (the hatched areas on figure 2).

2.4. SURFACE TENSION – COULOMB INTERACTION

We consider now the nucleus as a liquid drop having a uniform charge and to the free energy, we add a surface term and the coulomb energy of the drop. The contribution of the nucleus to the total free energy (2.1) becomes:

$$F_n(T, V_n, N_n) = F_{on}(T, V_n, N_n) + F_{surf}(T, S_n) + F_{coul}(V_n) \qquad .$$

For a sphere of radius R_n with a uniform charge Z and a surface tension $\alpha(T)$ which depends upon temperature, these terms are:

$$F_{surf}(T, S_n) \quad = \alpha(T) \, 4\pi \, R_n^2 \qquad , \tag{2.9}$$

$$F_{coul}(V_n) \quad = (3/4) \, Z^2 e^2 / R_n \qquad . \tag{2.10}$$

A detailed study of the surface tension $\alpha(T)$ has been done in ref. [25]. In the results we present below, the simpler form has been used [27]:

$$\alpha(T) = \alpha_o \left(1 + \frac{3}{2} \frac{T}{T_C} \right) \left(1 - \frac{T}{T_C} \right)^{3/2} \qquad ,$$

where T_C is the critical temperature. At zero temperature, $\alpha_o = 18/4\pi \, r_o^2 = 1.14$ MeV fm^{-2}, this is the usual value found in semi-empirical mass formulae with $r_o = 1.12$ fm. As we are mainly interested in the qualitative origin of the nucleus instability, we shall not introduce separately protons and neutrons. The charge Z of the nucleus is defined by $Z = xA$ where x is a fixed parameter to be determined for each nucleus.

With these additional terms, the coexistence equations becomes:

$$\begin{aligned} P_{on}(T, \rho_n) + \delta P_n(T, \rho_n, A) \quad &= P_{ov}(T, \rho_v) \qquad , \\ \mu_{on}(T, \rho_n) + \delta \mu_n(T, \rho_n, A) \quad &= \mu_{ov}(T, \rho_v) \qquad , \end{aligned} \tag{2.11}$$

with,

$$\begin{aligned} \delta P_n = \quad P_{coul} + P_{surf} \quad &= (4\pi \rho_n / 3A)^{1/3} \left[Z^2 e^2 \rho_n / 5A - 2\alpha(T) \right] \qquad , \\ \delta \mu_n \quad = \mu_{coul} \quad &= (4\pi \rho_n / 3A)^{1/3} \, 6xZe^2 / 5 \qquad . \end{aligned} \tag{2.12}$$
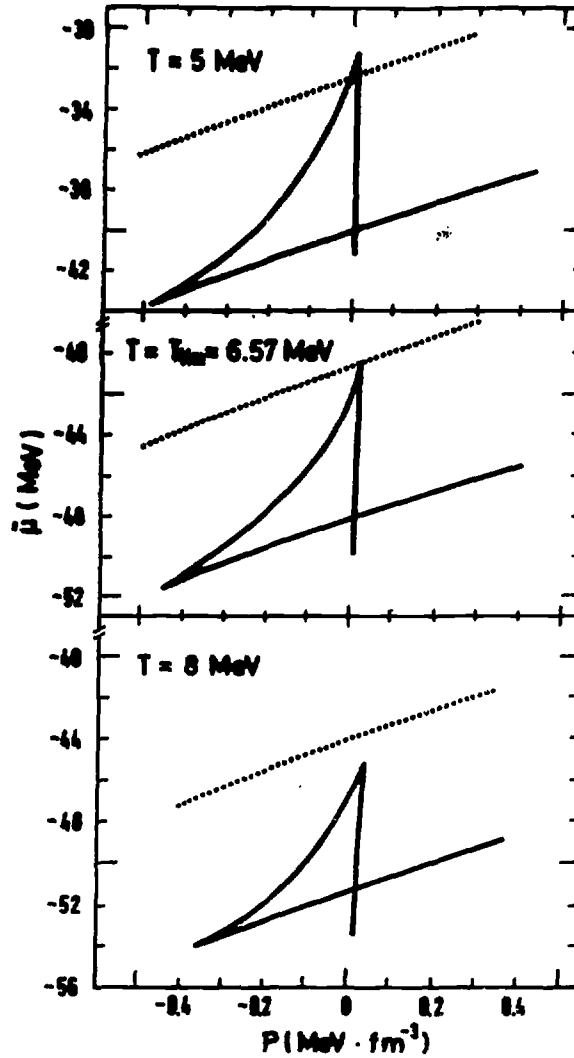
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Figure 3: Isotherms $T = 5$ MeV, $T = 6.57$ MeV and $T = 8$ MeV. The isotherms in solid line include infinite nuclear matter contribution only, these in dashed line take surface and coulomb effects into account.

There is no surface tension contribution to the chemical potential. The coulomb repulsion induces a positive term to the pressure, contrary to the surface tension which reduces the internal pressure. The pressure necessary to hold the nucleus stable is the result of a balance between the surface tension which tends to bind the nucleus and the coulomb repulsion. The coulomb term gives a modification of the chemical potential proportional to the fraction x of protons inside the nucleus.

Figure 3 shows the isotherms $T = 5$ MeV, $T = 6.57$ MeV and $T = 8$ MeV in the plane (P, μ) for the nucleus ^{109}Ag. The solid lines represent the isotherms with the three branches: vapor, unphysical and liquid. The coexistence point for infinite nuclear matter is at the crossing of the liquid and the gas branches. The dashed lines give the total pressure $(P_{on} + \delta P_n)$ as a function of the total chemical potential
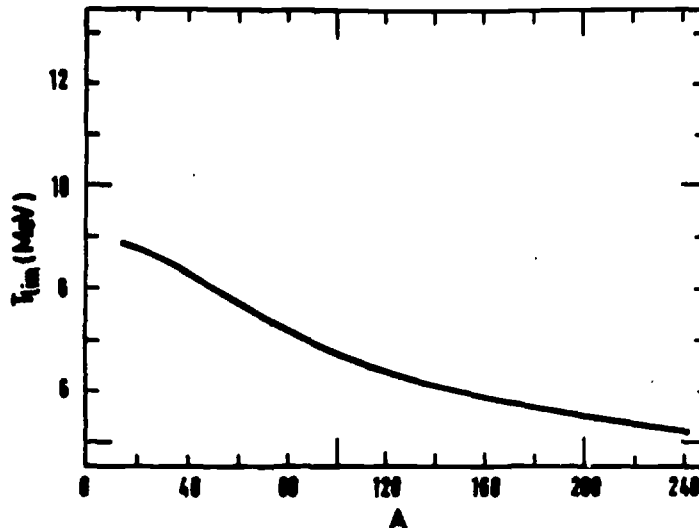
Figure 4: Variation of T_{lim} along the valley of stability.

$(\mu_{on} + \delta\mu_n)$. The intersection of these curves with the vapor vertical branches defines the new solution of the coexistence equations (2.11). One observes that at a limiting temperature $T_{lim}(= 6.57\text{Mev})$, this intersection reaches the border of the gas phase and that there is no solution beyond this temperature.

The disappearance of the solution for $T > T_{lim}$ implies that there is no equilibrium where the liquid and gaseous phases may coexist. At temperatures larger than T_{lim} it is no longer possible to equilibrate the internal pressure of a nucleus: an expansion out of equilibrium will occur with charged particle emission or fragmentation of the nucleus [28,29]). This expansion will stop only when new equilibrium conditions will be matched at lower temperatures for the fragments or the residual nucleus.

This model shows that there exists a limiting temperature which depends upon the nucleus. This temperature is always lower than the critical temperature T_C. Figure 4 shows this dependence along the nuclear stability line approximated by the relation $Z = A/2 - 0.3.10^{-2} A^{5/3}$. The value of T_{lim} decreases with A, the decreasing rate being smaller for larger A. This can be interpreted from the expressions (2.12) of the pressure and the chemical potentials. The coulomb part P_{coul} of δP_n and $\delta\mu_n$ increase with A, which implies a lowering of the temperature at which nuclei become unstable.

2.5. SUMMARY

We have proposed a simple model to study the possible occurrence of a liquid-gas phase transition for nuclei at high temperature. As a matter of fact we have observed the existence of a limiting temperature at which the nucleus becomes unstable mainly because of the coulomb repulsion. This limiting temperature T_{lim} depends upon the nuclear matter properties: equation of state and surface tension. In principle it is possible to study this dependence by the measure of T_{lim} for different nuclei. The

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isospin has been taken care of in an approximate way, one should introduce explicitly the neutron and proton contributions in the free energy. Such an improvement has been done recently [30]. In any case, this attempt remains qualitative as the matter density of a nucleus is still approximated by a sharp distribution with an abrupt edge.

To conclude the second part of these lectures, let us make three comments.

1) The experimental signature of the coulomb instability is a sudden reduction of the compound nucleus formation rate together with an increase of the emission of unequilibrated particles. Fragmentation [29,31] is expected at temperatures higher than T_{lim}.

2) The question remains whether this coulomb instability can be associated to a phase transition. For a nucleus enclosed in a finite box, the coulomb instability does correspond to a first order phase transition toward a state where all the matter is ejected and sticks to the surface of the box [21]. Such a transition resembles the bubble-nucleus transition found in the core of a supernova [26,32] where the nuclear medium is electrically neutral (see the last part of the lectures). However, it is irrelevant for the physics of nuclear reactions.

3) Finally few words concerning other approaches. In ref. [11], finite size effects and the coulomb field are included directly in the equation of state for infinite nuclear matter. This produces a lowering of the critical temperature T_c itself. However, the coulomb interaction is a long range force, its range is actually larger than the size of the nucleus. It seems therefore not appropriate to include such a force in an equation of state for an infinite medium. The separate treatment of the coulomb force that we have proposed shows that there is indeed a instability which cannot be related to a thermodynamical effect. It is more likely to be of a dynamical nature, rather than coming from a modification of the critical temperature.

In another work [33] the coulomb force has been included separately, however the nucleus is enclosed in a box without including open channels for particle emission. In our approach, unbound single particle levels by which this emission occurs are included through the external saturating vapor which matches adequately the nucleus. The coulomb instability triggers when this matching is no longer possible. Finally, in references [18] and [19], the coulomb force is apparently not included.

3. MICROSCOPIC DESCRIPTION OF HOT NUCLEI

In this third part, our aim is to propose a completely microscopic version of the description of hot nuclei. For that purpose we shall use the formalism developed in the first part of these lectures for a system made of independent particles. The hamiltonian contains only a one-body potential associated to a set of single particle states. This first step toward a microscopic calculation allows the derivation of the occupation numbers without having to deal with the full complexity of the two-body forces. However, the difficulty coming from the presence of states in the continuum is present and it will be possible to infer a method to take them into account properly.

To include a two-body force in the hamiltonian, we shall introduce the mean field approximation before using the variational method described in the first part of the lectures, this will lead to the Hartree-Fock equations at finite temperature. Properties of nuclei as a function of temperature are calculated with a Skyrme effective two-body interaction: root mean square radii, chemical potentials, entropy, charge and matter density profile, life time and stability limit.

3.1. INDEPENDENT PARTICLE SYSTEM

Let us work in the grand canonical ensemble where both the energy and the particle number are known by their mean values. The density operator reads as:

$$\hat{D} = \frac{1}{Z_G} \exp\{-\beta(\hat{H} - \mu \hat{N})\} \qquad . \qquad (3.1)$$

The system consists of independent particles, its hamiltonian is a one-body operator $\hat{H} = \sum_i \epsilon_i \hat{n}_i$, with $\hat{n}_i = a_i^+ a_i$. The particle number operator is $\hat{N} = \sum_i \hat{n}_i$. The a_i and a_i^+ obey the fermion anticommutation relations. The operator $\hat{D}$ becomes:

$$\hat{D} = \frac{1}{Z_G} \exp\left(-\sum_i \alpha_i a_i^+ a_i\right) \qquad ,$$

with $\alpha_i = \beta(\epsilon_i - \mu)$. One calculates the partition function in the Fock basis associated to the hamiltonian $\hat{H}$: $Z_G = \prod_i (1 + e^{-\alpha_i})$. The mean value f_i of the occupation number operator $\hat{n}_i$ for a given state i is given by:

$$f_i = \langle \hat{n}_i \rangle = -\frac{\partial}{\partial \alpha_i} \lg Z_G = \frac{1}{1 + e^{\alpha_i}} = \frac{1}{1 + e^{\beta(\epsilon_i - \mu)}} \qquad . \qquad (3.2)$$

These occupation numbers are also called Fermi factors. As a function of the f_i, the grand potential is:

$$A = -kT \lg Z_G = -kT \sum_i \lg(1 + e^{-\alpha_i}) = kT \sum_i \lg(1 - f_i) \qquad . \qquad (3.3)$$

Similarly, the particle number, the internal energy and the entropy are:

$$
\begin{aligned}
N &= & \langle \hat{N} \rangle & = \sum_i f_i & , \\
E &= & \langle \hat{H} \rangle & = \sum_i \epsilon_i f_i & , \\
S &= & (E - \mu N - A)/T & = k \sum_i (f_i \alpha_i + \lg(1 - f_i)) & .
\end{aligned}
$$

In the above expression of S, one can eliminate α_i and the entropy takes its usual form in terms of the Fermi factors:

$$S = -k \sum_i \left(f_i \lg f_i + (1 - f_i) \lg (1 - f_i) \right) \qquad . \qquad (3.4)$$

The Fermi factors f_i (3.2) lie between 0 and 1, they decrease with ϵ_i: higher energy states are less occupied than low energy ones. In the limit of low temperature, α_i goes to infinity with the sign of $\epsilon_i - \mu$. Hence, for states below μ, f goes to 1, whereas for those above, f goes to 0. In this limit, one recovers a pure state corresponding to the Slater determinant built from the single particle states lying below the Fermi level, those above remaining empty. One is also welcome to verify on the expression (3.4) that the entropy is indeed 0 in the limit of zero temperature.

3.2. SYSTEM OF INTERACTING PARTICLES

Let us return now to the general case where the hamiltonian of the system contains a two-body potential. In the grand canonical ensemble, the expression of the density operator is still given by (3.1); however the hamiltonian reads as:

$$\hat{H} = \sum_{i,j} \langle i|t|j \rangle \, a_i^+ a_j + \frac{1}{2} \sum \langle ij|V|kl \rangle \, a_i^+ a_j^+ a_l a_k \qquad .$$

This expression of $\hat{D}$ is far too complicated as it involves the exponential of a two-body operator. We want to find an approximate expression for $\hat{D}$, for that purpose, let us return to the variational principle which has allowed us to derive the expression of $\hat{D}$ by maximization of the entropy, or equivalently by minimization of the grand potential A. The mean field approximation amounts to minimize A amongst a restricted class of density operators defined as the exponential of one-body operators:

$$\hat{D}_o = \frac{1}{Z_o} \exp\left(-\sum_i \alpha_i a_i^+ a_i \right) \quad , \qquad (3.5)$$

The form postulated for $\hat{D}_o$ is identical to that obtained for one-body hamiltonian in section 3.1. The results of this section are still valid insofar as they do not imply the relation between α_i and ϵ_i:

$$
\begin{aligned}
Z_o &= & \prod_i \left(1 + e^{-\alpha_i} \right) & , \\
f_i &= \langle \hat{n}_i \rangle & = -\partial(\lg Z_o)/\partial \alpha_i = 1/\left(1 + e^{\alpha_i} \right) & , \\
N &= \langle \hat{N} \hat{D} \rangle & = \sum_i f_i & , \\
S &= -kTr(\hat{D} \lg \hat{D}) & = -k \sum_i \left\{ f_i \lg f_i + (1 - f_i) \lg(1 - f_i) \right\} & .
\end{aligned}
\qquad (3.6)
$$

The internal energy $E = Tr(\hat{H}\hat{D})$ and the grand potential however are given by:

$$E = \sum_i f_i \langle i|t|i \rangle + \frac{1}{2} \sum_{ij} f_i f_j \left\{ \langle ij|V|ij \rangle - \langle ij|V|ji \rangle \right\} \qquad , \qquad (3.7)$$

$$A = E - \mu \sum_i f_i + kT \sum_i \left\{ f_i \lg f_i + (1 - f_i) \lg(1 - f_i) \right\} \quad . \qquad (3.8)$$

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The minimization of A with respect to the parameters which generate the class of trial density operators $\hat{D}_o$ is described in the references [32] et [34]). The variation with respect to the single particle states $|i\rangle$ yields to the Schrödinger equation:

$$h|i\rangle = e_i|i\rangle \quad , \qquad (3.9)$$

where the one-body hamiltonian h is given by:

$$h_{ij} = \langle i|h|i\rangle = \langle i|t|i\rangle + \sum_k f_k \{\langle ik|V|ik\rangle - \langle ik|V|ki\rangle\} \quad . \qquad (3.10)$$

We now minimize with respect to the α_i. As the expression (3.6) defines f_i as a monotonic function of α_i and as the grand potential depends only upon f_i, it is simpler to minimize A with respect to f_i, which yields: $f_i = 1/(1 + e^{\beta(e_i - \mu)})$ with $\alpha_i = \beta(e_i - \mu)$. We find thus a result quite similar to that of a one-body potential (see section 3.1) for the potential $\hat{h} = \sum_i e_i a_i^+ a_i$.

There is however an essential difference as the one-body hamiltonian $\hat{h}$ is the solution of the non-linear equations (3.9): the Hartree-Fock equations. This hamiltonian $\hat{h}$ is also called the Hartree-Fock mean field. In the limit of zero temperature, one recovers the usual Hartree-Fock equations.

Another difference lies in the calculation of the internal energy and of the grand potential or of the partition function. Let $\hat{D}_o$ be the density operator of the independent particle system corresponding to $\hat{h}$. The internal energy E_o calculated from $\hat{D}_o$ is: $E_o = \sum_i f_i \epsilon_i$, whereas the Hartree-Fock internal energy of the system is according to (3.7):

$$E_{HF} = \sum_i f_i \epsilon_i - \frac{1}{2} \sum_{ij} f_i f_j V_{ij} = E_o - \langle V \rangle \quad .$$

The additional term, equal to the mean value of the potential, is the generalization of the term already present in the Hartree-Fock energy at zero temperature. In the mean field approximation, the Hartree-Fock grand potential is written as: $A = A_o - \langle V \rangle$, where A_o is the grand potential associated to $\hat{h}$. Let Z_o be the partition function associated to $\hat{D}_o$, the Hartree-Fock approximation Z_{HF} to the exact partition function of the interacting system is: $Z_{HF} = Z_o \exp(\beta \langle V \rangle)$. These modifications to E_o and Z_o are the direct consequence of the non linearity of the Hartree-Fock equations as derived within the mean field approximation [35,36]).

These equations are solved by iteration, as done in the usual case of zero temperature. Given a trial mean field, one solves equation (3.9), this gives the single particle spectrum and wave functions. The chemical potentials are obtained from the e_i by demanding that the sums of the proton and neutron occupation numbers are equal to the corresponding nucleon numbers. Finally, the Hartree-Fock field is recalculated from (3.10). One has then to iterate the process until convergence.

3.3. CONTINUUM STATES – ONE-DIMENSIONAL MODEL

In an independent particle model, the energy E and the particle number N of a system are given by:

$$N = \sum_i g_i f_i \quad .$$
$$E = \sum_i g_i f_i \epsilon_i \quad , \qquad (3.11)$$

where the coefficients g_i are the degeneracy factors of the orbits.

The difficulty comes from positive energy states which introduces a continuum of states whose exact treatment is out of reach numerically. As soon as the temperature rises, the number of particles in the continuum, proportional to $\int_0^\infty f(\epsilon)d\epsilon$, can become important. When a continuum state is occupied with a non negligible probability, the nucleus is no longer stable but is in a diffusion state.

In a first approximation, one can eliminate the contribution of the continuum by taking into account only the bound single particle states [37,38] and truncating the sums in the expressions (3.11). However, the contribution coming from the resonances is also eliminated at the same time. At low temperature, this rather drastic method can be justified, arguing of the negligible occupation of the continuum. At higher temperature however, it is necessary to include their contribution in an appropriate manner.

We propose below a simple one-dimensional model to show how to include this contribution by means of a subtraction procedure based on a phase shift analysis [39,40] for a calculation of the partition function [41-43]. Let $V(x)$ be a short range potential defined on a segment of length $2R$. The wave functions which vanish at $x = -R$ behave as $\sin(kx + kR + \delta)$ in the vicinity of $x = R$, where k is the wave number $(2mE/\hbar^2)^{1/2}$ and $\delta(E)$ the phase shift. The positive energy states are given by the quantization condition $2kR + \delta(E) = n\pi$. And their density is thus $f(E) = dn/dE$. Upon replacing $f(E)$ in the grand potential and writing explicitly the bound state contribution, one has:

$$A = kT \sum_{i:\epsilon_i<0} \lg(1 - f_i) + \frac{kT}{\pi} \int_0^\infty \lg(1 - f) \frac{d\delta}{dE} dE + 2R\frac{kT}{\pi} \int_0^\infty \lg(1 - f) \frac{dk}{dE} dE \quad .$$

$$(3.12)$$

In the above equation, the first term comes from the bound states, the second represents the finite contribution to the grand potential arising from the continuum. The last one diverges with the length of the segment, it is equal to the grand potential obtained in the absence of the interaction $V(x)$. The finite part $\tilde{A}$ of the grand potential is thus obtained by the subtraction: $\tilde{A} = A(V) - A(V = 0)$.

This model suggests to define the grand potential describing a nucleus in equilibrium with its vapor as the difference between the grand potential of the total system, nucleus plus vapor, and that of the vapor alone (where the nuclear interaction is set to zero). A more detailed justification of this subtraction method is given in ref. [20], with a similar model design to include a Coulomb field in a three-dimensional space.

3.4. APPLICATION TO NUCLEI

Hartree-Fock calculations in a cell of radius R for a given temperature and chemical potential give in general two distinct solutions. One of them is obtained by starting the iterative method proposed in section 3.2 from a Saxon-Woods potential; it describes a nucleus located at the cell center and surrounded by an external gas. The other one, which resembles a vapor-like dilute nuclear matter, is obtained while starting the iterations from a zero potential. In the absence of Coulomb force, the matter density of this solution is nearly uniform; at large distances, it is equal to the

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density of the other solution. Subsequently, we denote ρ and $\tilde{\rho}$ the matter densities corresponding respectively to the nucleus and vapor-like solutions, in addition, we distinguish explicitly neutrons and protons, introducing two distinct chemical potentials μ_n and μ_p.

According to the discussion of section 3.3, it is natural to define the grand potential of a hot nucleus as the difference between the grand potentials A and $\tilde{A}$ calculated with the one-body density matrices ρ and $\tilde{\rho}$ respectively. In the absence of Coulomb field, this definition is satisfactory as the difference $\bar{A} = A - \tilde{A}$ defining the nucleus converges toward a value which turns out to be independent of the cell as its radius R is increased.

The Coulomb field introduces an additional difficulty: when the cell size increases, the Coulomb repulsion becomes so large that protons are driven out to the cell surface. The presence of a gas outside the nucleus is the signature of an evaporation: we are somehow simulating a dynamical mode of evaporation by a permanent regime calculation where the gas represents the evaporated particles. As it is reasonable to neglect the Coulomb interaction between two evaporated protons, we shall neglect the Coulomb interaction in the gaseous phase: evaporated protons only feel the charge of the nucleus. This method has the advantage of eliminating spurious divergences.

The Coulomb energy is calculated accordingly from the subtracted proton density: $\rho_p - \tilde{\rho}_p$, and the corresponding subtracted grand potential is:

$$\bar{A} = A_N(\rho) - A_N(\tilde{\rho}) + \frac{1}{2} \int [\rho_p(r) - \tilde{\rho}_p(r)] \frac{e^2}{|r - r'|} [\rho_p(r') - \tilde{\rho}_p(r')] \, dr \, dr' + E_{cx} \qquad . \tag{3.13}$$

The term E_{cx} comes from the Coulomb exchange potential calculated in the Slater approximation. The index N added to the grand potentials $A(\rho)$ and $A(\tilde{\rho})$ means that they only contain the nucleon-nucleon interaction.

The minimization of $\bar{A}$, with respect to both ρ and $\tilde{\rho}$, yields two set of coupled Hartree-Fock equations quite similar to equation (3.9). The nucleus solution contains a Coulomb potential obtained by variation of the Coulomb energy included in (3.13), The same occurs for the vapor solution.

The calculations presented in the next section have been done with two nucleon-nucleon effective forces of the Skyrme type [44,45]. These interactions consist of the sum of a two-body force and of a density dependent term, both of range zero. The corresponding Hartree-Fock equations are local in coordinate space. Their explicit derivation is given in reference [32] together with the parameters of the forces SIII [45] and Skm [46] which are presently used. The detailed expression of the Coulomb field for the nucleus and vapor solutions can be found in reference [20].

3.5. RESULTS

3.5.1. Condition of validity. First of all we have to check that our subtraction method describes the physics of a hot nucleus and not that of the container or the cell in which we have put the nucleus to perform the calculation!

Table 1 gives results obtained for ^{208}Pb at 4 MeV temperature with Skm, the cell radius ranges from 12 to 18 fm. The convergence is quite good for the subtracted entropy, energy and mean square radii. At the edge of the cell, the densities of the nucleus and the vapor are already very close to each other for a cell of radius 14 Fermi ($\rho_n \sim \tilde{\rho}_n$ and $\rho_p \sim \tilde{\rho}_p$) and the difference decreases rapidly when the radius increases. On the other hand, the $R = 12$ fm cell is slightly to small. Practical calculations have been performed with $R = 16$ fm.

R	S	E^*	r_n	r_p	ρ_n	ρ_p	$\tilde{\rho}_n$	$\tilde{\rho}_p$
12	130.75	280.14	5.785	5.607	8.8000	0.9200	8.2600	0.7800
14	130.71	280.06	5.784	5.606	8.1600	1.1500	8.1300	1.1400
16	130.65	279.86	5.784	5.606	8.0814	1.5139	8.0811	1.5136
18	130.70	280.02	5.784	5.606	8.0745	1.8821	8.0741	1.8820

Table 1: Subtracted values of the entropy S, the binding energy E^* (MeV), and the neutron and proton radii r_n and r_p (fm) as a function of the cell radius R for ^{208}Pb at $T = 4$ MeV with Skm. The densities at the edge of the cell are given for the nucleus and vapor solutions in unit 10^{-4} fm^{-3}.

3.5.2. Lifetime. One can get an estimation of the nucleus lifetime by evaporation in the following way. The external gas produces exactly the amount of pressure necessary to hold the nucleus at equilibrium. The grand potential $\tilde{A}$ of this uncharged gas is equal to the opposite of the pressure multiplied by the volume: $\tilde{A} = A(\rho) + PV$. The minimization of $\tilde{A}$ is identical to that of $A(\rho)$ with the constraint that the system occupies the volume V, the corresponding Lagrange parameter is then $-P$. Hence, the gas directly characterizes the stability of the nucleus. For example, the lifetime of a hot nucleus can be estimated from the standard formula used in nucleosynthesis to calculate reaction rates [47]: $1/\tau = n\langle \sigma v \rangle = \langle \sigma j \rangle$, where n is the density of the external gas, σ the neutron capture cross section, v the speed of the external nucleons and j their current. The notation $\langle \sigma v \rangle$ represents the statistical average over the gas states. If one replaces σ by the geometrical cross section, $\sigma = \pi R^2$, where R is the radius of the nucleus, one finds for ^{208}Pb ($R = 7$ fm, $\mu_n = -8$ MeV) a lifetime of 10^{-18} sec at 1 MeV temperature. This lifetime decreases when the temperature increases: $0.9\ 10^{-20}$ at 2 MeV and $1.3\ 10^{-22}$ at 5 MeV.

To be meaningful, these lifetimes must be larger than the time the system need to thermalize or simply to form. This hierarchy of time seems to be experimentally observed, at least up to temperatures of the order of 5 to 6 MeV: 5 MeV for the heavier nuclei, (see for instance ref [2])) and 6 MeV for the lighter ones [3]).

3.5.3. Other properties. The results we present below have been with the Skm and SIII interaction for the lead nucleus. For temperatures higher than 2 MeV the subtraction procedure is used. AT $T = 1$ MeV the density of the external gas is nearly zero
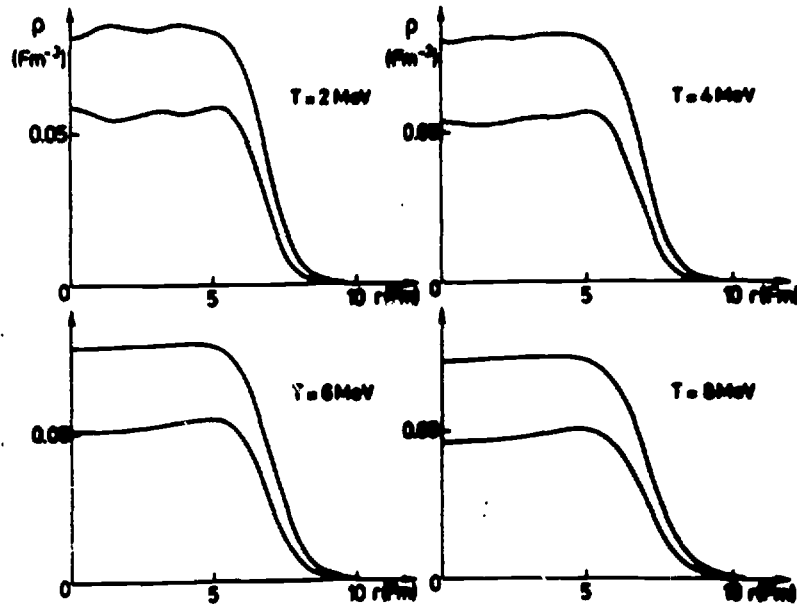
Figure 5: Density profiles for ^{208}Pb calculated with SIII at four different values of the temperature.

and no state in the continuum is significantly occupied. No center of mass correction is done, nuclei are spherical: no deformation effect is taken into account.

Neutron and proton subtracted densities are drawn on figure 5 at four different temperatures for ^{208}Pb with SIII. The surface thickness increases with temperature faster for protons than for neutrons. This difference reflects the importance of the Coulomb field. Density oscillations due to shell effects are washed out as soon as the temperature becomes larger than the shell spacing [38]).

Table 2 summarizes the main results obtained with SIII for ^{208}Pb. Up to 8 MeV temperature, the Skm interaction gives qualitatively similar results, the differences can be attributed to the value of the incompressibility modulus which is smaller for Skm ($K \sim 220$ MeV) than for SIII ($K \sim 380$ MeV). The most spectacular difference between these two interactions is the temperature at which the nucleus becomes unstable. There is no solution with Skm beyond $T=8$ MeV which appears as a limiting temperature for Skm.

3.5.4. Limit of stability. These calculations were possible only over a limited range of temperature. Beyond the limiting temperature observed above, the results depend upon the of the cell in which the Hartree-Fock equations are solved.

Figure 6 shows the density profiles of ^{208}Pb with SIII at 11 MeV. In a 14 Fermi radius cell, one may think that the nucleus is well described by the subtracted densities as they do vanish at the cell edge. However, the same calculation repeated in a 16 Fermi radius cell produces a very different density: the nucleus is no longer stable and nucleons are escaping toward to edge of the cell.

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T(MeV)	E^*(MeV)	S	μ_p(MeV)	μ_n(MeV)	r_p(fm)	r_n(fm)
0	0	0	-5.75	-4.95	5.53	5.65
1	14.65	20.40	-6.30	-5.80	5.53	5.66
2	74.18	60.41	-6.58	-6.24	5.56	5.68
3	154.83	92.86	-7.07	-6.57	5.59	5.71
4	255.96	121.79	-7.81	-6.90	5.63	5.75
5	379.14	149.19	-8.79	-7.28	5.69	5.80
6	523.30	175.42	-9.98	-7.73	5.76	5.87
7	688.00	200.78	-11.36	-8.25	5.85	5.95
8	870.36	225.11	-12.91	-8.87	5.97	6.06
9	1068.05	248.36	-14.61	-9.56	6.12	6.19
10	1291.50	271.93	-16.51	-10.34	6.33	6.39

Table 2: Excitation energy, E^*, entropy, S, proton and neutron chemical potential, μ_p and μ_n, proton and neutron root mean square radii, r_p and r_n for ^{208}Pb with SIII.

In an even larger cell, the calculations give a solution looking like a bubble where matter is glued to the surface of the cell. This transition is irrelevant for an isolated nucleus: there is no physical mechanism which can produce such a cell holding a "bubble nucleus".

It is nevertheless possible to go beyond the limiting temperature by setting artificially the Coulomb field to zero. The corresponding uncharged and fictitious nucleus still exists at temperatures higher than T_{lim}, however it becomes less dense, its surface is more and more diffuse and its radius increases. At even higher temperature, one does not observe a sudden instability, but rather a smooth transition toward a uniform nuclear matter at a temperature slightly lower than the critical temperature for an infinite medium.
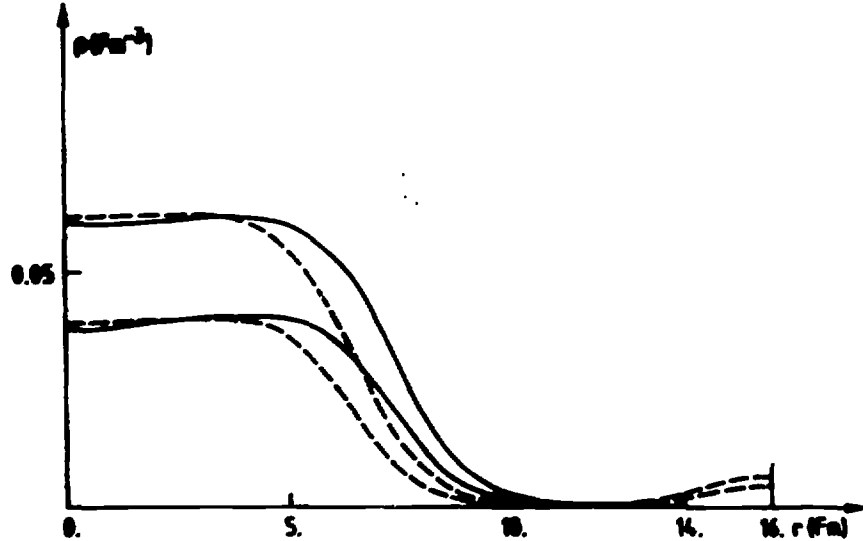

Figure 6: Profiles of neutron and proton subtracted densities for ^{208}Pb at $T = 11$ MeV with SIII in cell of 14 fm (solid lines) and of 16 fm (dashed lines).

3.6. CONCLUSIONS

We have confirmed in a microscopical approach the results obtained in the phenomenological model of the second part of the lectures. The dependence of the limiting temperature with the nucleus mass seems however less pronounced. Microscopical calculations with Skm show that ^{56}Fe and ^{208}Pb are both stable at $T = 8$ MeV and unstable at $T = 9$ MeV. A more detailed study has been done from the root mean square radii[21]: the limiting temperature for ^{208}Pb merely exceeds 8 MeV whereas for ^{56}Fe, it is close to 9 MeV. This difference remains smaller than the prediction of the phenomenological model and a systematic study of the mass dependence of the limiting temperature remains to be done.

Finally, let us stress some theoretical limitations of the above calculations.

1) All the calculations have been performed for spherical nuclei. Deformation may play an important role, especially at lower temperature. It must certainly be included if one is interested in the influence of temperature on fission barriers [48].

2) Angular momentum has not been included either, and one knows that nuclei produced in heavy ion reactions do carry a large angular momentum.

3) The available effective interactions are usually determined so as to reproduce nuclear properties at zero temperature. For the time being, there are no indications that they usage is valid at non zero temperature. The dependence of the mean field upon the temperature due to its non linearity may not be sufficient. However there is also no strong evidence that it is not legitimate to use these forces [49].

4. HOT NUCLEI IN SUPERNOVA

Amongst the different stages of a supernova evolution [50-53] we shall focus only in the collapse of the core. During this final stage, the density reaches values close to the infinite nuclear matter density with a temperature of the order of several MeV. The nuclei which build the core can be described following the method used precedently. However the nuclear medium within a supernova core is electrically neutral and the description of the nuclei will be simpler as the difficulties arising from the long range Coulomb field are no longer present. The physics is also different: beyond the description of a single nucleus, it is the equation of state of the matter inside the core of the star which is important as well as the chemical composition of the core [52,54]. The total pressure inside the core increases as the density to a power γ called the adiabatic index. When the nucleons are bound in nuclei, they do not contribute to the total pressure, it is then solely due to the electrons which form an ultra-relativistic gas and γ is equal to 4/3. On the contrary, when nucleons are free particles, they contribute to the pressure as a non relativistic gas and γ is equal to 5/3. The value 4/3 is of special importance as it determines whether it is possible for the star to resist to gravitation and to stop the collapse: for an adiabatic index larger than 4/3, the star is stable [55]. Furthermore, if the nuclei are still present during the collapse, the neutrinos diffuse coherently. Their mean free path decreases [56,57], and it is no longer possible for them to escape the star before the end of the collapse. Otherwise they might remove too much energy from the core so that the rebounce at the end of the collapse could be not powerful enough to eject the outer layer of the infalling star producing in this way what is observed as a supernova explosion.

The simplest approximation which can be made to estimate the equation of state is to use uniform gases of neutrons, protons and electrons. Such calculations [54] may be considered as useful guides. However, they cannot give any information about the presence of nuclei. An improved version of this simple model is to include nuclei by means of semi-empirical mass formulae [50,56,58]. In these approaches, nuclei are treated as point-like particles in a Boltzmann gas. The first attempt to include the finite size of nuclei, as well as nuclear forces, has been through the compressible liquid-drop model [59,13]. However, since these calculations include only an incomplete description of the nuclear surface, they still need to be improved. This can be achieved by means of Thomas-Fermi [60,61]. An alternate but more microscopic way is to perform Hartree-Fock calculations at non zero temperature [32,62] following the scheme we have given in these lectures. These calculation have been reproduced later within the Thomas-Fermi approximation [63,64], which has open a new way to study the detailed structure of the supernova core [65].

In what follows, we describe more precisely the physical context of the problem. We show how the variational principle introduced in section 1.3 gives the equation of state. We proceed by describing the method of resolution and the main results in a model with a spherical geometry [32,62]. Finally, we present some calculations done in a three-dimensional model [65] but at the cost of a further approximation.

4.1. PHYSICAL CONTEXT

The stellar medium during the collapse [52,66]) has some special features which modify the previous picture we have developed for an isolated nucleus.

The core of the star is made not only of barions but also of electrons and neutrinos whose contributions must be included. As the core is electrically neutral, there are as many protons as electrons. The hydrodynamical description of the collapse assumes an adiabatic evolution: the entropy per barion remains constant. This is actually true only when neutrinos are "trapped" inside the core, which happens at a density of the order of one percent of infinite nuclear matter [50]). Above this density, there is β equilibrium: $p+e^- \rightleftharpoons n+\nu_e$. This condition implies the equality between chemical potentials: $\mu_p+\mu_e = \mu_n + \mu_\nu$. The total lepton number is conserved. The electron and neutrino concentrations, Y_e and Y_ν are the ratio of the particle number of each kind of leptons to the total number of barions. As the barion number is conserved, the lepton concentration remains also constant: $Y_l = Y_e + Y_\nu$.

It is not our purpose to discuss the evolution of the star from the origin till the beginning of the collapse. However, this description is necessary as it defines the conditions of the collapse: an entropy per barion S/A roughly equal to unity [52]) and a lepton concentration Y_l of the order of 0.35 [52,67]). Our goal is to find which phase minimizes the energy. Is this a uniform matter phase or a phase made of nuclei? For the optimal solution, we want the equation of state which tells how the pressure varies with the barion density. In what follows, we are only interested in the final stage of the collapse when the mean density $\bar{\rho}$ of the core is of the order of $\rho_o/10$ to ρ_o, where ρ_o is the infinite nuclear matter density.

For normal nuclear matter, ρ_o is about 0.17 fm^{-3} (3. 10^{14} g/cm^3). A lepton fraction Y_l of 0.35 corresponds to $Y_e \simeq 0.30$. Due to electrical neutrality Z/A is equal to 0.30 instead of the symmetric nuclear matter value of 0.50. The resulting saturation density ρ_o is no longer 0.17 but closer to 0.14 fm^{-3}. Similarly, the incompressibility modulus is roughly 140 MeV instead of 220 MeV.

4.2. MODEL DESCRIPTION OF THE CORE

In the density domain we are considering, the core is expected to be a solid. It can thus be described as a crystal with a nucleus at each site, the interstitial space being filled by a diffuse nucleon gas.

4.2.1. Wigner-Seitz approximation. To derive an equation of state, we use of the Wigner-Seitz approximation [68]). The calculation of the whole core is replaced by the calculation of the properties of a single elementary cell surrounding a given site. This problem is still very difficult because of the rather complicated polyhedral shape of the unit cell. If the gas filling the interstitial space is uniformly distributed, the Wigner-Seitz cell can be replaced by a sphere. Curvature corrections are small when the size of the nucleus is small compared with the size of the cell – i.e. when the distance

between adjacent nuclei is small compared with the mesh size – and when the density of the external gas remains low. This reduces the initial three-dimensional problem to a one-dimensional one. The minimum of a given thermodynamical potential Ω characterizing the core is obtained by calculating its value Ω_c in an elementary cell containing A_c nucleons and by minimizing Ω_c/A_c with respect to A_c.

Two additional conditions have to be fulfilled. The first one is related to the spherical geometry hypothesis: a reasonable matching between two neighboring cell is possible only if the density remains constant in the vicinity of the surface. For a cubic face centered crystal for instance, the density must remain constant over a distance from the surface equal to $2R(1 - (\sqrt{6}\pi/6)^{1/3}) = 0.19 R$ where R is the cell radius. This distance represents the overlap between two adjacent cells obtained by imposing the condition that the volume of the core is equal to that of all cells.

For the Wigner-Seitz approximation to be valid the crystal must be solid: it should not melt. As a first approximation, matter can be considered as a one-component plasma, i.e. a system of point-like nuclei surrounded by a uniform background of negative charges. For such system, matter will be a solid when the plasma parameter, $\Gamma = Z^2 e^2/RkT$, is greater than 155 [69,70]). For lower values of Γ, Coulomb liquid corrections can be included [69,70]). Even in the less favorable cases we shall encountered, these corrections remain negligible.

Finally, the Wigner-Seitz approximation replaces an infinite but periodic system by a unique cell with appropriate boundary conditions. This amounts to replacing each band by a single isolated level: band width corrections are to be expected. It is possible to justify this approximation in the limit of a large number of particles at each crystal site [32]).

4.2.2. Definition of the thermodynamical potential. We choose to work in the grand canonical ensemble and we minimize the grand potential in a single cell:

$$\Omega = \Omega_{n,p} + \Omega_e + \Omega_\nu + V_{p,e} \quad ,$$

where $\Omega_{n,p}$ is the barion grand potential without Coulomb terms, Ω_e is electron one and Ω_ν the neutrino one. The last term is the Coulomb interaction energy between the protons and the electrons: $V_{p,e} = V_{coul}(\rho_p - \bar{\rho}_e)$, where ρ_p is the proton density and $\bar{\rho}_e = Y_e \bar{\rho}$ the electron one which is chosen uniform.

The microscopic calculation of $\Omega_{n,p}$ is performed at the Hartree-Fock approximation with a suitable two-body effective force (see section 3.2). The boundary conditions at the surface of the cell are chosen so that there is a correct matching between adjacent cells. To do so, a given parity is imposed to the single particle wave functions across the surface. The freedom in the choice of this parity can be used as a test of the Wigner-Seitz approximation which must be independent of any reasonable choice.

4.2.3. Electron contribution. The next step is the calculation of the electron contribution Ω_e for a given Y_e. Several simplifications can be made.

First of all electrons are ultra-relativistic. For barion densities larger than 0.02 fm^{-3}, the electron density $\bar{\rho}_e$ is at least of the order of 0.01 and their Fermi momentum

is $k_F^{(e)} = (3\pi^2/\bar{\rho}_e)^{1/3} \gtrsim 0.6$ fm^{-1}. The electron mass is then negligible to better than 10^{-4} and the Fermi energy becomes: $\varepsilon_F^{(e)} = \sqrt{\hbar^2 c^2 k_F^2 + m_e^2 c^4} \simeq \hbar c k_F^{(e)}$.

Electrons can be treated as free particles, for $\bar{\rho}_e \sim 0.01$ fm^{-3} the average distance between two electrons is $a \sim (1/\bar{\rho}_e)^{1/3} \gtrsim 5$ fm. Their Coulomb interaction energy, $e^2/a \lesssim 0.3$, MeV is much smaller than the Fermi energy, $\varepsilon_F^{(e)} \gtrsim 120$ MeV.

Finally as temperatures are always one order of magnitude lower than $\varepsilon_F^{(e)}$ during the collapse, low temperature expansions can be used:

$$\frac{\Omega_e}{N_e} = -\theta_F \left\{ \frac{1}{4} + \frac{\pi^2}{6}\left(\frac{T}{\theta_F}\right)^2 + \cdots \right\} \quad , \tag{4.1}$$

$$\mu_e - E_o = \theta_F \left\{ 1 - \frac{\pi^2}{3}\left(\frac{T}{\theta_F}\right)^2 + \cdots \right\} \quad , \tag{4.2}$$

where the electron number in the cell N_e is equal to the proton number and θ_F is the Fermi temperature: $\theta_F = \hbar c k_F^{(e)}$. The chemical potential μ_e is shifted by the lattice Coulomb energy E_o which comes from the proton electron interaction $V_{p,e}$. For T, $\bar{\rho}_e$ and ρ_p given in the cell, the calculation of Ω_e and μ_e follows [1].

4.2.4. Method of resolution. From the previous history of the star, the entropy per barion and the lepton concentration are known at the beginning of the collapse: $S/A = 1$ and $Y_l = 0.35$. Three successive choices have to be made:

1. Y_e – which we arbitrarily fixed to some value lower than Y_l, e.g. 0.30. The electron density is then given by: $\bar{\rho}_e = Y_e\, \bar{\rho}$.

2. T – of the order of 1 MeV for the lowest density we shall consider.

3. A_c – The number of nucleons in the cell.

These three quantities are not known a priori, they can be guessed from a previously converged calculation for a neighboring density. The numerical resolution is performed in three steps:

- Given A_c, Y_e and $\bar{\rho}$, one deduces N, Z and the cell radius. The mean field equations (3.9) are solved for the chosen temperature. The grand potential $\Omega_{n,p}$, the chemical potentials μ_n and μ_p, and the barion entropy $S_{n,p}$ are calculated from their solution.

- Ω_e, μ_e and the electron entropy S_e are derived from the proton density $\rho_p(r)$ and from $\bar{\rho}_e$.

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[1]As an exercise, one can show that if one neglects the lattice energy E_o in (4.2), the electron pressure is proportional to the electron density to the power 4/3.

- The neutrino chemical potential μ_ν is obtained from β equilibrium. Equations (4.1) and (4.2) are valid for the neutrinos, however their degeneracy is 1 – one state of helicity –, and there is no lattice energy ($E_o = 0$ in (4.2)). They give $\bar{\rho}_\nu$, the neutrino concentration Y_ν, the grand potential Ω_ν and the entropy S_ν.

The next step is to obtain the minimum de Ω_c/A_c in the cell as a function of A_c. The temperature is varied until the entropy per barion $S/A = (S_{n,p} + S_e + S_\nu)/A_c$ is equal to 1. For each trial value of the temperature, A_c has to be varied again. Finally the electron concentration Y_e is adjusted so that the sum $Y_e + Y_\nu$ is equal to $Y_l = 0.35$. Again, for each trial Y_e, the two previous variations have to be repeated.

The result of these three variations is the equation of state $P = -\Omega_c/V_u$ as a function of the mean density $\bar{\rho}$. For each value of $\bar{\rho}$, the number of nucleons in the cell is also obtained, as well as the temperature T and the electron concentration Y_e which characterize the collapse.

4.3. RESULTS FOR A SPHERICAL WIGNER-SEITZ CELL

The calculations presented below have been done with the Skyrme interaction Skm [46]). For a given lepton concentration Y_l, the variation of Y_e remains small during the collapse. This can be checked by keeping Y_e constant and calculating the resulting Y_l. In a first calculation the value of Y_e was arbitrarily kept fixed to 0.25. The size of the cell and the temperature are varied to minimize the grand potential $\Omega_{p,n} + \Omega_e$ for an entropy per barion: $(S_{p,n} + S_e)/A_c = 1$. The neutrinos are not included.

T	P	$\bar{\rho}$	A_c	Γ	S/A	Y_l	μ_p	μ_n	μ_e	γ
3.80	0.1357	0.02	300	139.3	0.9992	0.296	-29.38	-1.02	102.23	1.316
4.35	0.2309	0.03	400	225.0	1.0012	0.298	-31.61	-0.78	117.01	1.306
4.75	0.3356	0.04	500	329.0	1.0011	0.299	-33.62	-0.55	128.77	1.299
5.06	0.4482	0.05	600	450.8	1.0009	0.300	-35.46	-0.35	138.80	1.286
5.34	0.5655	0.06	900	892.2	1.0007	0.301	-37.02	-0.20	147.32	1.260
5.53	0.6851	0.07	1000	1081.0	1.0002	0.301	-38.81	-0.12	154.48	1.230

Table 3: Temperature T (MeV), pressure P (MeV/fm^3), density ρ (fm^{-3}), chemical potentials μ_p, μ_n and μ_e (MeV), and nucleon number A_c in the cell along the adiabat $S/A = 1$. The interaction is Skm, Γ is plasma parameter, Y_l the lepton concentration (Y_e is fixed to 0.25), and γ is the adiabatic index.

Table 3 summarizes the main results along the adiabat $S/A = 1$. The concentration Y_l remains remarkably constant, which justifies the approximation of constant Y_e. The plasma parameter Γ is always small enough to ensure that the core of the star is a solid at all considered densities. The calculated entropy per barion is equal to 1 to better than 10^{-3}. The approximation of ultra-relativistic electron gas is very good as μ_e is always larger than
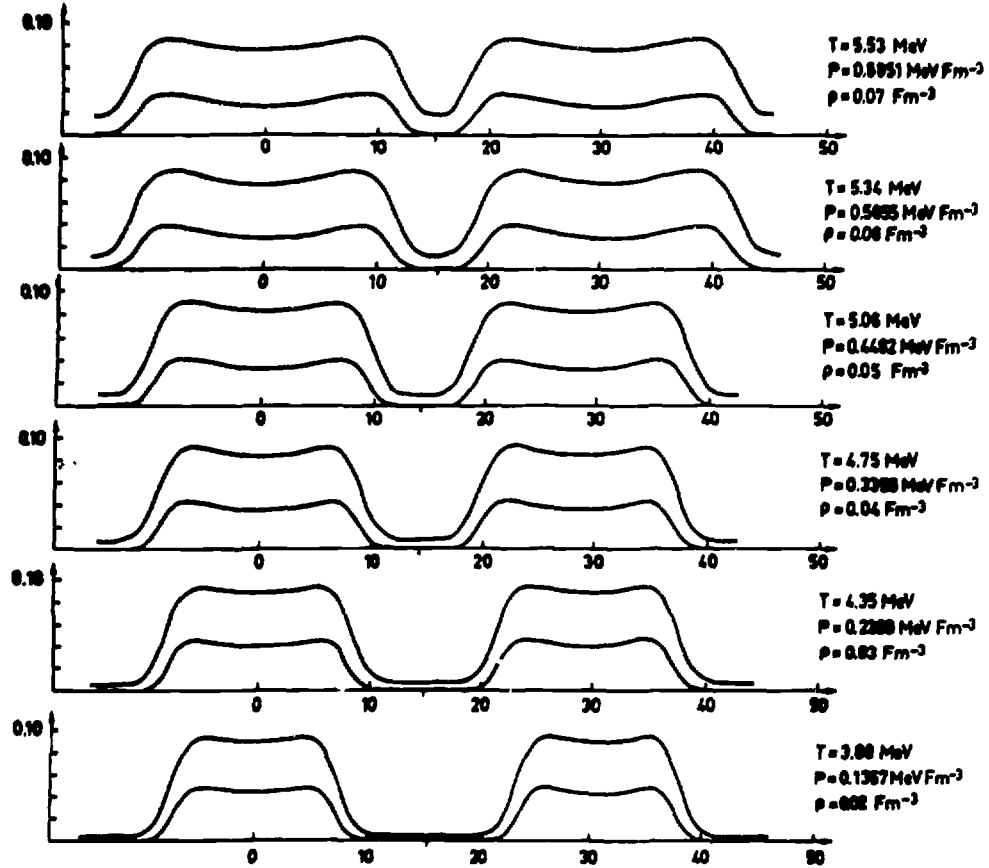
Figure 7: Density profiles (fm^{-3}) of neutrons (upper curves) and protons (lower curves) along a line joining the centers of two cells. Distances along this line are in Fermi. The electron concentration is 0.25.

100 MeV. The adiabatic index, $\gamma = \partial \log P / \partial \log \bar{\rho}$ is given in the last column of Table 3. Its average is 1.29, slightly less than 4/3, which guarantees that the collapse will not stop for densities up to the largest one for which this calculation is done: $\bar{\rho} = 0.07$ fm^{-3}.

These results are illustrated on. For the values of $\bar{\rho}$ listed in table 3, figure 7 shows the neutron and proton densities along a line joining the centers of two adjacent nuclei in the crystal. Up to the largest density, most nucleons are bound in nuclei. Hence, the pressure is expected to come mainly from the electrons and to vary as $\bar{\rho}^{4/3}$.

Between the maximum density of 0.07 and the infinite nuclear matter density, the solution crystal of nuclei is no longer stable and a transition is observed toward a solution where protons have been driven out into the interstitial space by the Coulomb repulsion. Because of the nucleon-nucleon force, the neutrons follow and the final solution corresponds to a crystal of bubbles with a low barion density at the sites previously occupied by nuclei and a connected bath of uniform matter filling the interstitial space. At high density, matter distributions are no longer constant in the vicinity of the surface of the cell: the approximation of spherical cell becomes very questionable.

For the above calculation ($Y_e = 0.25$), the lepton concentration is about 0.30. The study of this equation of state has been repeated with the neutrino contribution

included, varying Y_e until $Y_l = 0.35$ [62]). The contribution of the bubble and uniform matter phases have also been analyzed. For the bubble phase, the approximation of spherical Wigner-Seitz cell is not quite justify: the matter distribution resembles a thin layer glued onto the surface of the cell. Nevertheless, one can compare these different solutions and find out which of them is the most stable one. For that purpose, the appropriate variables are the entropy S, the pressure P and the particle number N. According to the discussion of section 1.5, the relevant thermodynamical potential is the enthalpy. It is obtained from the internal energy which depends upon S, V and N, by the Legendre transformation: $H(S, P, N) = U + PV$ [1,39]). Figure 8 shows the enthalpy per barion as a function of the pressure. The uniform phase has a larger enthalpy for all densities, it is therefore always less bound. At a density of the order of 0.05 nucleons/fm^3, the nucleus phase becomes less bound than the bubble phase. This this is only an indication of a possible phase transition: the approximation of spherical cell being less and less justified as the density is increased.
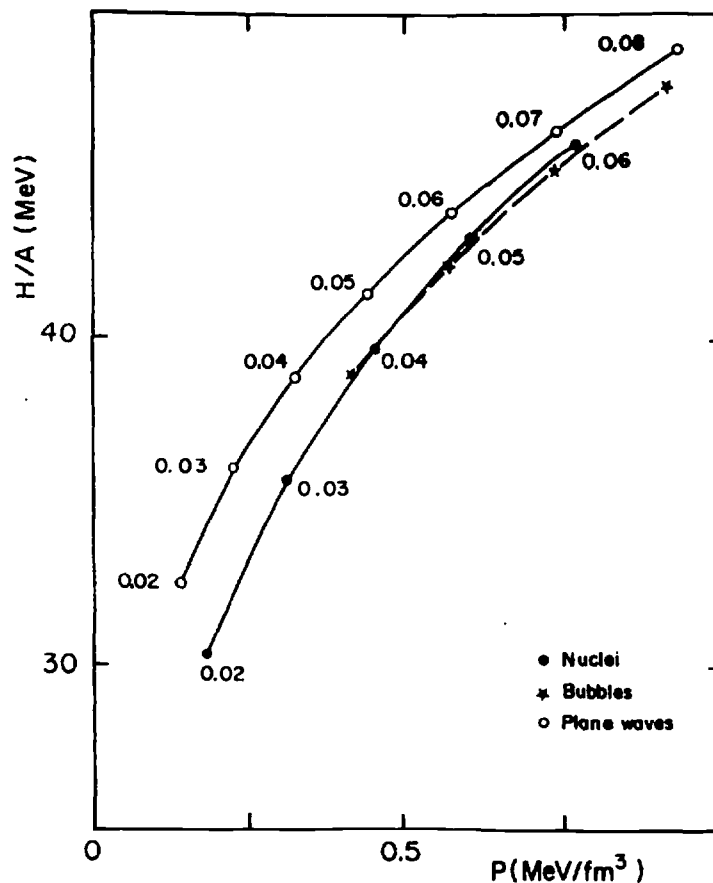

Figure 8: Variation of the enthalpy per barion as a function of the pressure for the nucleus phase (•), the bubble phase (*) and the uniform matter phase (o). The entropy per barion is unity and $Y_l = 0.35$. The values of the density $\bar{\rho}$ at which the calculation has been done are also quoted.

4.4. THOMAS-FERMI APPROXIMATION IN THREE DIMENSIONS

To further confirm this nucleus-bubble phase transition, the calculation must be repeated in a more realistic model with three spatial dimensions.

Unfortunately, the exact resolution of the Hartree-Fock equations in a polyhedral cell is at present out of reach of the most powerful computer. To avoid this numerical difficulty, it has been suggested to solve these equations in an approximate way by utilizing the Thomas-Fermi approximation [63]. It is known that this approximation is too crude to account correctly for the main properties of stable nuclei. It can be improved to take into account shell effects by including higher order terms in the expansion in $\hbar$ from which the Thomas-Fermi approximation is derived [71]. However, at the temperatures encountered inside a supernova, these shell effects are no longer present and the normal Thomas-Fermi approximation is quite sufficient. The calculations presented below are done with this lowest order approximation [63]. The agreement with Hartree-Fock calculations is excellent, which assesses the validity of Thomas-Fermi in this context. This result is very fruitful: whereas the Hartree-Fock functional depends upon a large number of single particle wave functions, hand the Thomas-Fermi approximation involves only the neutron and proton densities and their gradients for the calculation of the energy and the entropy.

It becomes possible to study not only cells with more complex geometries but also different kind of crystal structure. Besides the three-dimensional periodic structures we have considered, namely nucleus or bubble crystals, we can investigate the possibility of two-dimensional structures [72]. In these more exotic phases, nucleons arrange themselves in crystals of rods or tubes, or also in slabs of matter. Thomas-Fermi calculations for symmetric nuclear matter $(N = Z)$ at zero temperature have shown that a microscopic study of these configurations is possible [73].

Different geometries have been studied: [65]

- nuclei or bubble crystal, either cubic centered, or cubic face centered. The elementary cell is then a cube.

- two-dimensional configuration: cylindrical rods of high nuclear density, or a nearly uniform medium with tubular low density regions. In both cases, the cell has a prismatic shape corresponding to a two-dimensional close packed hexagonal crystal. This is realized by imposing a $\sqrt{3}$ ratio between the two dimensions of the cell in the plane of the crystal. The third dimension is irrelevant.

- one-dimensional configuration: nucleons are distributed in slabs of matter arranged in parallel planes, the cell is defined by the only inter-slab distance.

For a given mean density $\bar{\rho}$, several phases may coexist. They appear as local or absolute minima of the variational problem. There is no systematic method to get all these possible minima and also to be sure that one of them is the absolute one. The resolution of the non-linear equations with an iterative algorism gives a minimum close to the trial configuration. Several initial configurations have to be tried to explore as many solutions as possible. On the other hand, each solution can be studied as a function of the mean density $\bar{\rho}$, even when it becomes metastable. In this way for the same cubic cell and the same given density $\bar{\rho}$, it is possible to construct either a cubic centered or a cubic face centered crystal by choosing
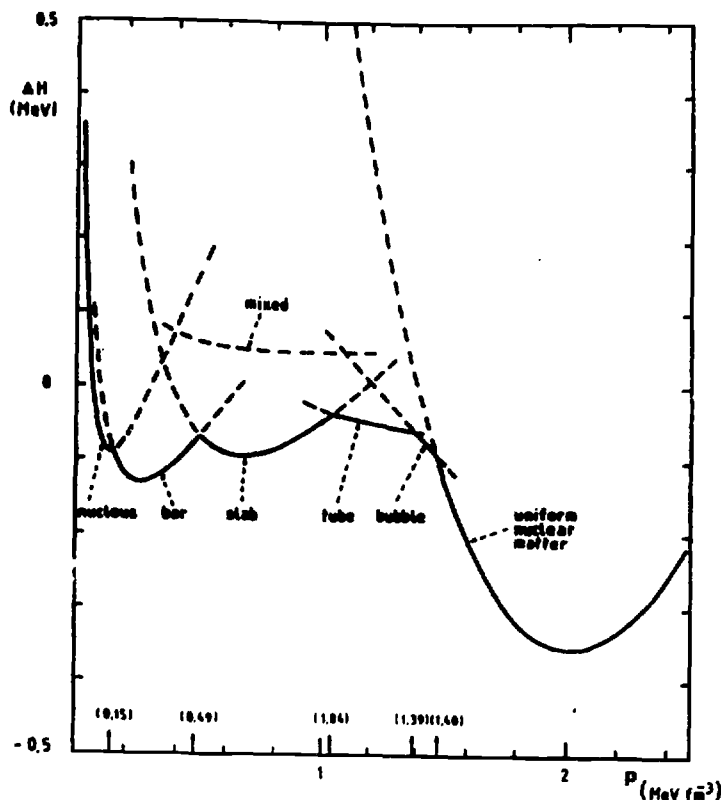
Figure 9: Variation of the enthalpy as a function of the pressure. The quantity ΔH is the difference between the calculated enthalpy H and its average trend $\bar{H}$ (see text).

an appropriate geometry at the starting point of the iterative calculation for the regions of low and high density in space.

Amongst the possible solutions, thermodynamic considerations will decide of the optimal solution. The most stable one has the lowest enthalpy (see section 4.3). Figure 9 shows the enthalpy for different phases as a function of the pressure along the adiabat $S/A = 1$. At a fixed Y_e of 0.285, the lepton concentration is remarkably constant, with a value of 0.35. In the range of studied pressure, the enthalpy varies by more than 50 MeV while the differences between phases rarely exceed 0.2 MeV. To render more evident possible phase transitions, figure 9 gives the enthalpy difference $\Delta H(P)$ with the mean enthalpy $\bar{H}(P)$:

$$\bar{H} = 49.7 + 13.68 \log P + (log P)^2 + 0.09 (\log P)^3 \quad .$$

For the lowest pressure, the most stable configuration is a crystal of nuclei immersed in a neutron gas. The curve drawn on figure 9 corresponds to the cubic centered solution, the cubic face centered crystal has almost the same enthalpy and is not distinguishable from the other on the figure. With increasing pressure, one finds the sequence of phases predicted by Ravenhall [72]: nuclear matter rods, slabs, hollow tubes, the bubble phase we found in the previous section and finally infinite nuclear matter.
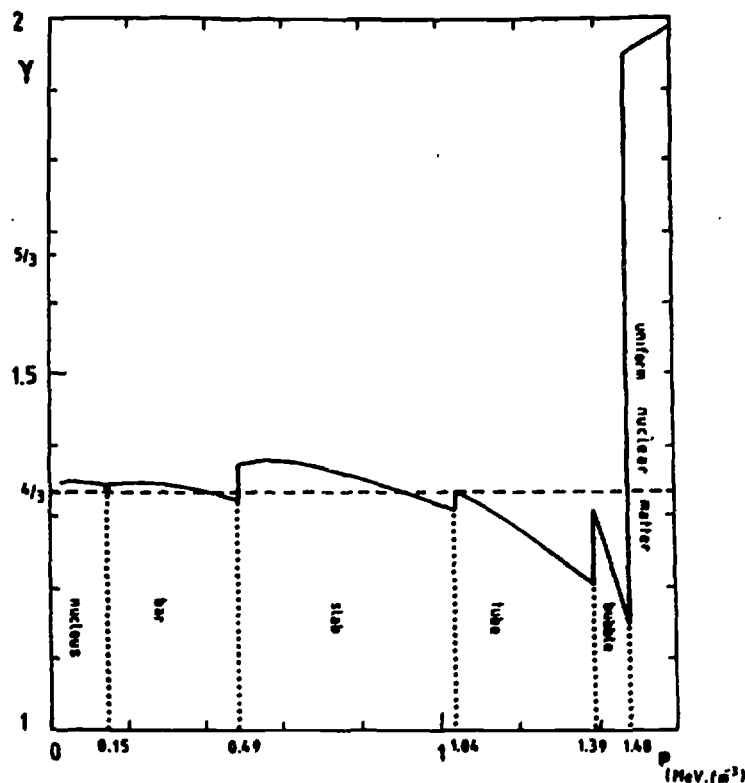
35

Figure 10: Variation of the adiabatic index γ as a function of pressure.

In addition to these solutions, there exists another phase called mixed phase which remains metastable at all pressure. It is made of a crystal of nuclei connected by bridges of matter between nearest neighbors so that both the low and the high density regions are connected. At low pressure, the transition toward a crystal of nuclei is achieved by the breaking of the matter bridges, whereas at high pressure it becomes a bubble crystal by filling the tunnels of low density until the bubbles are isolated from each other.

At low pressure, the rod phase becomes metastable, eventually each rod breaks in an alignment of nuclei, arranged from one rod to the other so as to form a nucleus crystal. At high pressure it is the opposite: the tube phase transforms itself in a bubble crystal.

In the region where the infinite nuclear matter phase is not the most stable, the adiabatic index remains always close to the critical value 4/3. Above the transition to nuclear matter, it reaches 1.9 which is larger than the value corresponding to a free nucleon gas (5/3), because of the nuclear interactions. Figure 10 shows the evolution of γ with the pressure. The discontinuities observed at each intermediate transition, together with the fact that γ is sometimes slightly larger than 4/3, might slow down the collapse of the core, at least in the initial stage. The dynamical consequences of such an equation of state are still to be studied.

It should also be remembered that these results are obtained within the mean field approximation which neglects the effects of thermal fluctuations. In view of the small differences of energy between the phases, these fluctuations may well smooth out the discontinuities and destroy long range correlations [39]). In such a case, only the mean behavior of γ which can be extracted from figure 10 will be relevant for the evolution of the collapse.

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