

2- Nuclear structure in the continuum

1. High excitation energy nuclear reactions

In lecture 1 we have addressed the problem of nuclear reactions when the beam energy is high enough to excite the reaction partners in their continuum states, above the S_n (S_p) threshold of neutron (proton) emission. We have seen that a treatment in terms of quantum statistical mechanics is adequate. In particular, the Hauser-Feshbach theory of compound nucleus decay constitutes, together with the shell model, one of strongest theoretical basis of nuclear physics. Within this theory, the particles emission process is governed by two typical statistical mechanics concepts, namely temperature and chemical potential, defined as:

$$T^{-1} = \frac{\partial \ln \rho}{\partial E} \quad ; \quad \frac{\mu_q}{T} = \frac{\partial \ln \rho}{\partial N_q} \quad (1.1)$$

where $q=n,p$ and

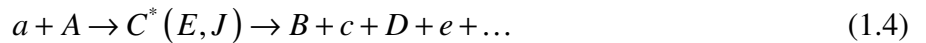
$$\rho(N_n, N_p, E) = \sum_K \delta(E - E_K(N_n = N, N_p = Z)) \quad (1.2)$$

is the level density, summed over angular momentum and parity, of a nucleus with N neutrons and Z protons. It is interesting to remark that, if the definition of a temperature is perfectly legitimate for a finite and isolated object as an excited nucleus, the same is not entirely true for the chemical potential which, for an isolated system, can only be rigorously defined at the thermodynamic limit because the number of particle is an integer variable and not a real variable. Indeed the use of a chemical potential to replace its conjugate variable given by the number of particles (that is: the definition of the *grand-canonical potential*) is justified only if the thermodynamic potential can be differentiated with respect to that variable, that is at the thermodynamic limit. However a grand-canonical modelization for a finite nucleus is still interesting because of great simplifications in the calculations it allows, even if the most advanced realistic nuclear models are rather formulated in the canonical or microcanonical ensemble.

The possibility of exploring nuclei at finite temperature with nuclear reactions comes from the Bohr independence hypothesis which, as we saw in chapter 1, states that the time scales are sufficiently decoupled, or the process sufficiently chaotic, for the compound nucleus decay to be independent of its formation process:



This hypothesis is very well verified, as we have discussed, in the fusion-evaporation reactions. Experimental data show that, if fusion reactions are properly selected, the same hypothesis can be very well verified also at higher excitation energy where many body are present in the exit channel :



An example is given in the following figure. The production cross sections of the different elements obtained with different entrance channels are approximately superposed if in each case a nucleus of comparable size, charge, excitation energy and angular momentum is formed. Such an experimental selection is not easy and subject to considerable systematic errors, which can explain the observed residual deviations. IN particular no angular momentum measurement was available for the systematics of that figure. The approximate scaling thus demonstrates that angular momentum does not play a crucial role in the production probability of the different channels:

$$\frac{\sigma_{\alpha\beta}}{\sigma_{\delta\beta}} = \frac{\sigma_{\alpha}^c}{\sigma_{\delta}^c}(E^*, J) \cong f(E^*). \quad (1.5)$$

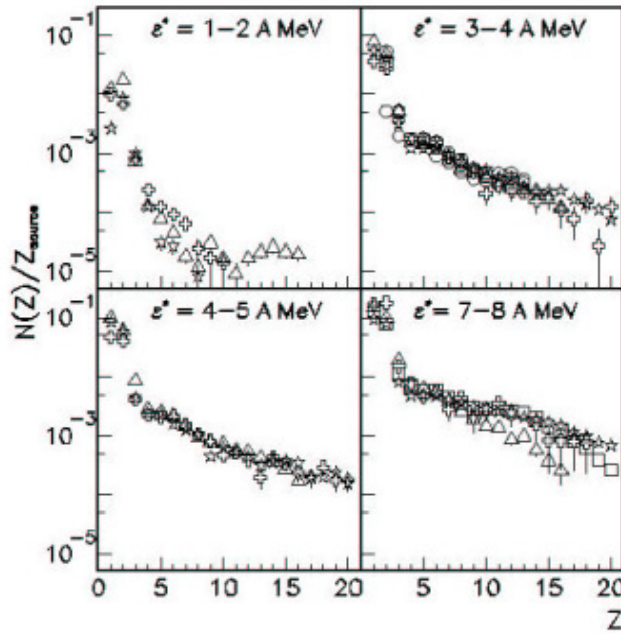


Fig. 9. Mass distribution for various excitation energy ranges obtained in several experiments involving very different entrance channels: stars: Au+Au central collisions from MULTICS data [2]; crosses: peripheral collisions with MULTICS [37]; hexagons: FASA data [35]; squares: 32MeV/u Xe+Sn INDRRA data [10] ; triangles: ISIS data [11]. This figure has been prepared by M. D'Agostino [21, 40].

In the case of fragmentation reactions the Hauser-Feshbach theory cannot be applied. Indeed this theory only treats two-body channels, and light (p,n,d,t,He) particle emission. In order to understand such complex reactions, it is important to understand the effect of temperature on the structure of the nucleus. The same is true to understand the structure and behavior of the hottest and denser astrophysical objects, core-collapse supernova and proto-neutron stars.

This subject is addressed in the next section, in the framework of the simplest modelization of nuclear structure, namely the independent particle model.

2. Independent particles at finite temperature

In the framework of the independent particle approach, the energy of a system of nucleons can be written as the sum of the single-particle energies :

$$E = \sum_{q=n,p} \sum_{i=1}^{N_q} e_i^q n_i^q \quad \text{with} \quad e_i^q = \frac{\langle \hat{p}^2 \rangle_i}{2m_q} + U_i^q, \quad (2.1)$$

where U_i^q is the single particle potential, and $n_i^q = 0, 1$ gives the (fermionic) occupation of the single-particle states. The orbitals filling rules for ground states imply that the system is described by a Slater determinant Ψ_0 where the lowest energy states are occupied (*hole states*), while the others (*particle states*) are empty.

If the system is at high excitation energy, a very huge number of particle-hole excitations (indeed: a continuum of states) are possible, with the unique constraint of energy and angular momentum conservation. The system will then be described by a *mixed state*:

$$\Psi = \sum_K c_K \Psi_K, \quad (2.2)$$

corresponding to different ensembles of occupation numbers of the single-particle states. We want to compute the mean value $\langle n_i^q \rangle$ of these occupations, as a function of the nucleus excitation energy.

This is a standard well-known problem in quantum statistical mechanics. The evaluation of the occupations, as well as of the whole nuclear thermodynamics, is based on the calculation of the *partition sum*:

$$\begin{aligned} Z_0 &= \text{Tr} \exp(\alpha_p \hat{Z}_0 + \alpha_n \hat{N}_0 - \beta \hat{W}) \\ &= \sum_l \exp(\alpha_p Z_l + \alpha_n N_l - \beta E_l) = \sum_{n_1^q} \sum_{n_2^q} \dots \exp \sum_{i,q} n_i^q (\alpha_q - \beta e_i^q) \\ &= \prod_{i,q} \sum_{n_i^q} \exp n_i^q (\alpha_q - \beta e_i^q) = \prod_{i,q} (1 + \exp - \beta (e_i^q - \mu_q)) \\ \ln Z_0 &= \sum_{i,q} \ln (1 + \exp - \beta (e_i^q - \mu_q)) \end{aligned} \quad (2.3)$$

All the observables can be calculated from the knowledge of the partition sum using standard statistical mechanics tools. In particular the particle numbers are given by:

$$\begin{aligned} \langle N \rangle_\beta &= \frac{\partial \ln Z_0}{\partial \alpha_n} = \sum_e g_e^n n_e^n \\ \langle Z \rangle_\beta &= \frac{\partial \ln Z_0}{\partial \alpha_p} = \sum_e g_e^p n_e^p \end{aligned}, \quad (2.4)$$

where g is the degeneracy of the state, and the energy distribution of the single-particle states follows a Fermi distribution at finite temperature :

$$n_q(e) = [1 + \exp \beta (e_q - \mu_q)]^{-1} \quad (2.5)$$

The average one-body energy is simply given by :

$$\langle E_0 \rangle_\beta = -\frac{\partial \ln Z_0}{\partial \beta} = \sum_{e,q} n_q(e) e_q \quad (2.6)$$

In principle the observables calculation demands the knowledge of the single-particle states, that is the diagonalization of the shell model Hamiltonian. The calculation is fully analytical in the limiting case of nuclear matter. Let us suppose a huge number of particles:

$$\begin{aligned} \frac{N}{V} &\xrightarrow{N,V \rightarrow \infty} \rho_n \\ \frac{Z}{V} &\xrightarrow{Z,V \rightarrow \infty} \rho_p \end{aligned} \quad (2.7)$$

We can apply the continuum limit to the density of states :

$$\sum_i n_i \rightarrow \int d^3 p \frac{d^3 n}{d^3 p} = gV \int \frac{d^3 p}{h^3} n(\vec{p}) \quad . \quad (2.8)$$

The single-particle occupations read :

$$n_q(\vec{p}) = \left[1 + \exp \beta \left(\frac{p^2}{2m_q} - \tilde{\mu}_q \right) \right]^{-1} \quad . \quad (2.9)$$

At first sight the system looks equivalent to a free non-interacting Fermi gas. This is however only a superficial resemblance. Indeed the chemical potential is shifted because of the mean-field

$$U_q = U_q(\rho_n, \rho_p):$$

$$\mu_q \rightarrow \tilde{\mu}_q = \mu_q - U_q \quad (2.10)$$

If this latter is self-consistently derived from the single-particle orbitals, eq.(2.9) is a self-consistency problem which, as we will see in detail, leads to thermodynamic properties deeply different from a free Fermi gas.

The average single-particle energy is given by equation (2.6):

$$\langle e_q \rangle_\beta = \frac{g_q}{\rho_q h^3} \int d^3 p n_q(\vec{p}) \left(\frac{p^2}{2m_q} + U_q \right) = \langle e_{kq} \rangle_\beta + U_q \quad , \quad (2.11)$$

where $g_q=2s+1=2$ represents the spin degeneracy. We can see that only the kinetic part of the average single-particle energy depends explicitly on the temperature.

The partition sum reads :

$$\begin{aligned} \ln Z_0 &= V \sum_{q=n,p} \frac{g_q}{h^3} \int dp 4\pi p^2 \ln \left(1 + \exp -\beta \left(\frac{p^2}{2m_q} - \tilde{\mu}_q \right) \right) \\ &= \frac{2}{3} V \sum_q \frac{g_q}{h^3} \int d^3 p n_q(\bar{p}) \frac{p^2}{2m_q} = \frac{2}{3} \langle E_K \rangle_\beta \end{aligned} \quad (2.12)$$

where $\langle E_K \rangle_\beta$ is the total kinetic energy.

The thermodynamic definition of the pressure $p_0 = \frac{1}{\beta} \frac{\partial \ln Z_0}{\partial V} = \frac{1}{\beta} \frac{\ln Z_0}{V}$ allows finding back the ideal gas result :

$$p_0 = \frac{2}{3} \varepsilon_k, \quad (2.13)$$

where $\varepsilon_k = \langle E_K \rangle_\beta / V$ is the kinetic energy density.

If the nuclear field depends on the density as it is the case in the framework of the self-consistent mean-field theory, it also contributes to the pressure. Eq.(2.13) is modified to :

$$p = p_0 - \frac{\partial \langle E^{pot} \rangle}{\partial V} = p_0 + \rho^2 \frac{\partial (\varepsilon_p / \rho)}{\partial \rho} \quad (2.14)$$

with $\rho = \rho_n + \rho_p$.

We also recall the relation between mean field and potential energy density ε_p : $U_q = \frac{\partial \varepsilon_p}{\partial \rho_q}$.

In order to calculate energy and pressure in this finite temperature problem, we have to deduce the relation between particle number(s) and chemical potential(s). This needs the evaluation of integrals with the functional form:

$$I = \int_0^\infty dx \frac{f(x)}{1 + \exp \frac{x-m}{T}} \quad (2.15)$$

A calculation at an arbitrary temperature demands a numerical integration. However the low and high temperature limits are analytical.

We analyze these limiting behaviors in the next sections.

3. Zero temperature limit

At zero temperature the Fermi function is a Heavyside step function. The observables read :

$$\begin{aligned}\rho_q &= \frac{16}{3h^3} \pi m_q \sqrt{2m_q} \tilde{\mu}_q^{3/2} \\ \varepsilon_k &= \frac{16}{5h^3} \pi \sum_{q=n,p} m_q \sqrt{2m_q} \tilde{\mu}_q^{5/2} \\ p &= \frac{2}{5} \sum_{q=n,p} \rho_q \tilde{\mu}_q + \rho^2 \frac{\partial(\varepsilon_p / \rho)}{\partial \rho}\end{aligned}\quad (3.1)$$

We can recognize the results of an ideal fully degenerate Fermi gas, with the important difference that the energies have to be calculated from the bottom of the mean field. In particular we can define the *Fermi energy* as the zero temperature chemical potential :

$$\mu_q = U_q + \frac{\hbar^2}{2m_q} (6\pi^2 \rho_q)^{2/3} = U_q + \varepsilon_{Fq} \quad (3.2)$$

4. Low temperature limit

In order to calculate the observables in the low temperature limit, it is useful to employ the following development :

$$\int_0^\infty \frac{dx f(x)}{1 + \exp(x - m)/T} = \int_0^m dx f(x) + \frac{\pi^2}{6} T^2 \left. \frac{df}{dx} \right|_m + O(T^4) \quad (4.1)$$

A temperature development for chemical potentials and energies can be deduced :

$$\begin{aligned}\tilde{\mu}_q &= \mu_q - U_{HF}^{(q)} = \varepsilon_{Fq} \left(1 - \frac{\pi^2}{12} \frac{T^2}{\varepsilon_{Fq}^2} \right) \\ \langle E_k \rangle_\beta &= \frac{3}{5} N \varepsilon_{Fn} \left(1 + \frac{5\pi^2}{12} \frac{T^2}{\varepsilon_{Fn}^2} \right) + \frac{3}{5} Z \varepsilon_{Fp} \left(1 + \frac{5\pi^2}{12} \frac{T^2}{\varepsilon_{Fp}^2} \right)\end{aligned}\quad (4.2)$$

The following notation is usually employed

$$\langle E_k \rangle_\beta = \frac{3}{5} (N \varepsilon_{Fn} + Z \varepsilon_{Fp}) + A a(\rho_n, \rho_p) T^2 \quad (4.3)$$

where the little-a parameter

$$a(\rho_n, \rho_p) = \frac{\pi^2}{4} \left(\frac{1+\delta}{2\varepsilon_{Fn}} + \frac{1-\delta}{2\varepsilon_{Fp}} \right) \quad (4.4)$$

Is called level density parameter, and we have used $\rho\delta = \rho_n - \rho_p$.

The great interest of this parameter is that its knowledge allows reconstructing the full energy dependence of the density of states in the low temperature limit, as we now show.

We define the excitation energy as the extra energy with respect to the ground state:

$$E^* = \langle E \rangle_T - \langle E \rangle_{T=0} \quad (4.5)$$

In the hypothesis that the mean field at finite temperature is the same as in the ground state, the excitation energy is given by Eq. (4.3), $E^* = \langle E_k \rangle_T$. We remark that this hypothesis is exact in the thermodynamic limit, see Eq.(2.11).

The level density at the excitation energy E^* is defined by Eq. (1.2). The logarithme of this quantity represents the statistical entropy within a constant :

$$\ln \rho(N, Z, E^*) = S_{N,Z}(E^*) + C \quad (4.6)$$

This latter is linked to the temperature by the fundamental statistical mechanics relation :

$$\frac{1}{T} = \frac{dS_{N,Z}}{dE^*} \Rightarrow S_{N,Z}(E^*) = \int dE^* \beta(E^*) \quad (4.7)$$

The approximation (4.3) can be inversed to express the temperature as a function of the excitation energy, as well as the entropy :

$$T = \sqrt{\frac{E^*}{Aa}} \Rightarrow S = 2\sqrt{AaE^*} \quad (4.8)$$

We deduce the expression of the level density as a function of the excitation energy :

$$\rho(N, Z, E) = C \exp 2\sqrt{Aa(E - E_{GS})} \quad , \quad (4.9)$$

where $E_{GS} = \langle E \rangle_{T=0}$ is the ground state energy.

We have already met this expression in the framework of the Hauser-Feshbach theory in the previous chapter. The independent particle modelization allows giving a simple expression (eq.(4.4)) for the little- a parameter.

A comparison with evaporation data reveals that this prediction ($a \sim 1/16$ for stable nuclei of mass ~ 100) is false of a about a factor 2 : realistic little- a parameters are of the order of $a \sim 1/8$ in the excitation energy domain where the low temperature approximation we have applied is justified. This disagreement can be understood from the fact that we made the hypothesis that the mean field is not influenced by the excitation of the nucleus. In a more realistic description, the effect of the energy deposit inside the nucleus does not only lead to particle-hole excitations (also called single particle excitations), but also to modifications of the wave functions which lead to a rearrangement of the nuclear densities (vibrations, deformations, ..., globally known under the name of collective excitations). Since the mean field is a functional of the nuclear density, this implies that Eq.(4.3) cannot be applied to calculate the excitation energy, if the nuclear density is modified by the excitation. These collective states must be summed to the single particle states, which increases the nuclear entropy with respect to our prediction based on single particle excitations only.

Turning the argument around, it is very interesting to observe that the formalism we have developed is perfectly adequate to explain both the functional form and the order of magnitude

of the level density. Indeed this is surprising, considering that we have explicitly used the thermodynamic limit, which is certainly not verified in atomic nuclei.

We can intuitively understand this result considering that the thermodynamic limit is necessary to obtain Eq.(2.8). However, this equation can also be seen as a quasi-classical approximation

$$\sum_i n_i \rightarrow g \int \frac{d^3 r d^3 p}{h^3} n(\mathbf{p}) = gV \int \frac{d^3 p}{h^3} n(\mathbf{p}) \quad , \quad (4.10)$$

which has some sense speaking of high energy continuum states.

5. High temperature limit

At high temperature the single-particle distribution is dispersed over a huge number of states, and the Fermi distribution can be approximated by the Boltzmann distribution. The Fermi integrals are given by gaussian integrals which can all be analytically calculated :

$$\begin{aligned} \tilde{\mu}_q &= -T \ln \frac{g_q}{\rho_q h^3} (2\pi m_q T)^{3/2} \\ \varepsilon_k &= \frac{3}{2} \rho T \\ \rho &= \frac{2}{3} \varepsilon_k - \varepsilon_{pot} + \rho \frac{\partial \varepsilon_{pot}}{\partial \rho} \end{aligned} \quad (5.1)$$

If for simplicity we consider the symmetric case $\rho_n = \rho_p$, a functional study of the equation of state $p(\rho, T)$ reveals that for temperatures $0 < T < T_c$ (where the T_c value depends on the interaction) isothermes present an inversed curvature region, corresponding to a region of negative compressibility (spinodal region), similar to the Van der Waals equation of states of real fluids. A representative calculation done with two different realistic versions of the mean-field theory, is presented in the following figure. This behavior indicates an instability of the system with respect to phase separation, as we are going to show in the next chapter: nuclear matter presents a first and second order phase transition (*nuclear liquid-gas phase transition*).
sente une transition de phase du premier et deuxième ordre (*transition liquide-gaz nucléaire*).

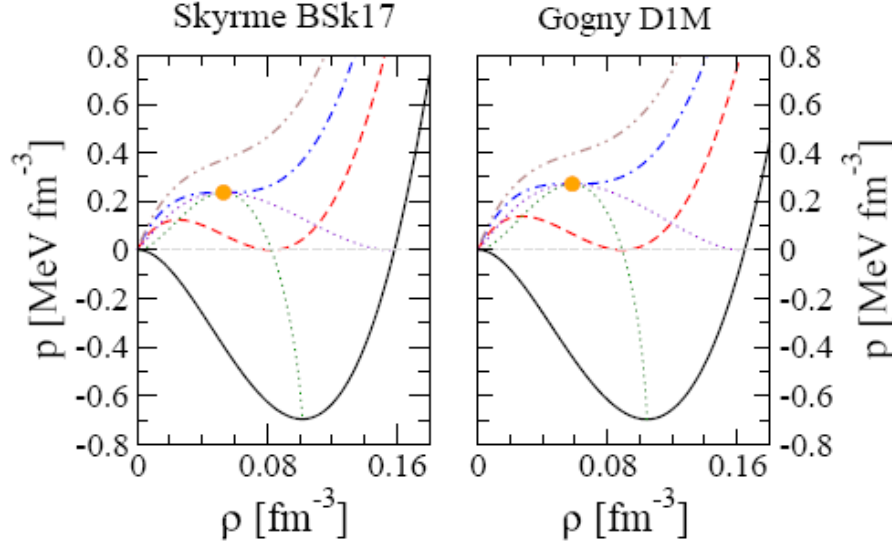


Figure 1: Pressure isotherms for different temperatures: $T = 0$ (solid line), $T = T_f$ (dashed line), $T = T_c$ (dash-dotted line) and $T = 18$ MeV (dash-double-dotted line). The dotted lines represent the corresponding spinodal and coexistence regions. The left panel has been obtained with the BSk17 interaction, while the right panel shows results for the Gogny D1M force.

The isotherm corresponding to a completely positive pressure function is called flashing temperature. Specifically, the flashing point satisfies the two simultaneous conditions :

$$p = \partial p / \partial \rho = 0 . \quad (5.2)$$

For an isolated system as an atomic nucleus, in the absence of an external gas which can stabilize it, this corresponds to the maximal temperature that the nucleus can sustain as a self-bound object. This temperature is the thermodynamic limit of the so-called *limiting temperature*, defined as the maximal temperature attainable in the lab before the nucleus vaporizes in a gas of nucleons. The search of the numerical value of this temperature is one of the aims of multi-fragmentation reactions.

Bibliography

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Exercices

1. Consider the Fermi gas model at a finite temperature T . calculate, at the second order in T , the value of the chemical potential and the mean energy. It will be useful to use the development :

$$\int_0^\infty def(e)(1 + \exp((e - \mu)/T))^{-1} = \int_0^\mu def(e) + \frac{\pi^2}{6} T^2 \left. \frac{\partial f}{\partial e} \right|_\mu + O(T^4)$$

How do these functions behave in the low density limit ? Comment the result.