Frontiers in Nuclear and Hadronic Physics

School

GGI Institute for theoretical physics

Arcetri (Florence), Italy, February 24-March 7 2014

Thermal Properties of Nuclear Systems

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8h CM

1- The theory of compound nucleus decay

1. Finite temperature, why ?

The two basic foundations of modern theoretical physics, namely quantum mechanics and statistical mechanics, rarely interact. We are used to think that quantum mechanics is the correct approach to describe the Hamiltonian, reversible, microscopic world from the Angstrom scale downwards, while statistical mechanics allows introducing the thermodynamic variables describing the macroscopic, classical, irreversible, entropic thermal world of our everyday experience.
This superficial view is not correct. It is well known that superconductivity and Bose condensation are macroscopic realizations of purely quantum phenomena. In an analogous way, many different aspects of nuclear structure and reactions can only be described through statistical tools.
In these lessons, we will briefly review some selected thermal phenomena taking place in nuclear physics.
In undergraduate courses on thermal physics, the concept of temperature – the basic concept of any thermal theory – is only associated to macroscopic objects, because an infinite (that is: comparable to the Avogadro number) number of degrees of freedom is needed to define a thermal bath or thermostat and demonstrate the fluctuation-dissipation theorem which is needed to justify the lack of energy conservation and the entropy increase that characterizes the thermal world. Atomic nuclei are isolated objects constituted of a very limited number of effective degrees of freedom (protons and neutrons). All the possible nuclear reactions obey strict conservation laws of energy, baryonic number and angular momentum and satisfy the basic principle of microscopic reversibility. In this context, it might therefore appear awkward to speak of a nuclear temperature.
However different nuclear phenomena exist where a temperature is a perfectly well defined theoretical concept. Schematically we can define two different situations in nuclear physics where thermal concepts apply, and will develop different applications for both situations in the following chapters.

a. Isolated nuclei as thermal objects

Temperature, and all related thermal quantities as pressure, enthalpy, free energy, chemical potential, etc., naturally emerges in quantum statistical mechanics when the system is complex enough that the exact quantum microstate cannot be known exactly. This is notably the case for isolated nuclei in the laboratory, when they are excited by a nuclear reaction into the continuum which characterizes the excitation spectrum of any quantum system well above the particle separation energy (of the order of 10 MeV, for the nuclear case). In such a situation, the spectroscopic knowledge (E,J^{π}) is not sufficient to characterize the state and it is more relevant to reason in terms of *level density*

$$\rho(E,J)=\sum_K \delta(E-E_K)\delta(J-J_K) \ , \tag{1.1}$$

where the sum runs over the excited states of the nucleus.
The system, or at least the knowledge that we have of the system, is therefore not described by a pure quantum state, but by a linear combination of the different states, or *mixed state*:

$$\left|\Psi\right\rangle = \sum_K c_K \left|\Psi_K\right\rangle \ , \qquad (1.2)$$

It is useful to introduce the projector over occupied states, or *density matrix*:

$$\hat{D} = \sum_K \left|\Psi_K\right\rangle p_K \left\langle\Psi_K\right| \ , \qquad (1.3)$$

This operator allows defining the *information entropy:*

$$S = -Tr\hat{D}\ln\hat{D} = \sum_K p_K \ln p_K \ . \qquad (1.4)$$

A maximization of S under the constraint of the energy of the system, which is supposed to be known, leads to

$$\delta\left(S - \beta Tr\hat{D}\hat{H}\right) = 0 \quad \Rightarrow \quad p_K = Z_\beta^{-1}\exp -\beta E_K \ . \qquad (1.5)$$

The β parameter measuring the average energy of the incompletely known complex isolated quantum system plays the role of an inverse temperature. The formalism leads to exactly the same equations as for a system in contact with a thermal bath, but the associated temperature has a very different physical meaning. $T=\beta^{-1}$ is a measurement of the energy variation of the density of states, as we now show. The statistical mechanics relation between the observable E and its associated Lagrange multiplier reads:

$$\beta = \frac{\partial S}{\partial\left\langle E\right\rangle}, \quad \left\langle E\right\rangle = Tr\hat{D}\hat{H}, \ , \qquad (1.6)$$

where the canonical entropy is the Legendre transform of the partition sum

$$S = \ln Z_\beta + \beta\left\langle E\right\rangle. \ , \qquad (1.7)$$

Using the definition of the partition sum, and performing a saddle point approximation, we get:

$$Z_\beta = \sum_K \exp -\beta E_K = \int dE\rho(E)\exp -\beta E \cong \exp\left[\ln\rho(\left\langle E\right\rangle) - \beta\left\langle E\right\rangle\right] \ , \qquad (1.8)$$

leading to:

$$\beta = \frac{d}{dE}\ln\rho(E)\Big|_{\left\langle E\right\rangle} \ , \qquad (1.9)$$

where ρ(E) is summed over the different angular momenta.

b. Nuclei in a thermal bath

A more trivial situation where finite nuclei can be associated to a well defined temperature value, is given by the case in which they are found in an external hot environment. This occurs in different astrophysical sites in the cosmos. In particular, all elements heavier than Fe in our solar system and elsewhere are synthetized through nuclear reactions taking place at high density and temperature. During this *explosive nucleosynthesis* process, the temperature of the nuclei is simply given by the temperature of the (macroscopic) environment. The different possible sites associated to these various phenomena (surface of massive stars in the pre-supernova regime, neutrino-driven wind in core-collapse supernova, binary systems producing X-ray bursts, neutron star mergers) are characterized by an explosive dynamics, which however takes place on time scales (10^{-9} sec or slower) much longer than the typical equilibrium times of the strong interaction ($\sim 10^{-13}$ sec). In this situation we can safely assume that the nuclear system is in thermodynamic equilibrium, meaning that the temperature of the environment can be equalized to the nuclear temperature defined by eq.(1.9).

2. The Hauser-Feshbach theory of compound nucleus decay

Historically, the first application of statistical mechanics to nuclear physics is the theory of Compound Nucleus (CN), which we briefly review in this chapter. It is interesting to observe that this is the oldest theory of nuclear physics (Niels Bohr, 1936) preceding the independent particle model. This shows that from the beginning of nuclear physics if was recognized that the complexity of the quantum many-body problem would lead to statistical concepts.
In nuclear reaction theory, the cross section associated to the transition from a binary channel α=(a,A) to a channel β=(b+B) is associated to the square of a transition amplitude. The well known DWBA for instance gives:

$$d\sigma_{\alpha\beta} = \sum_J \frac{2J+1}{(2j_a+1)(2j_A+1)} \left| f_\beta^J(\theta,\phi) \right|^2 , \tag{2.1}$$

$$f_\beta^J(\theta,\phi) = -\frac{1}{4\pi} \int d\vec{r}_\alpha d\vec{r}_\beta \, \chi_\beta^{(-)*}\left(\vec{k}_\beta,\vec{r}_\beta\right) \langle \beta | \hat{V} | \alpha \rangle \chi_\alpha^{(+)}\left(\vec{k}_\alpha,\vec{r}_\alpha\right) , \tag{2.2}$$

where $\chi_\alpha^{(+)}\left(\vec{k}_\alpha,\vec{r}\right)$ is the relative motion wave function, $\chi^{(-)}\left(\vec{k},\vec{r}\right) = \chi^{(+)*}\left(-\vec{k},\vec{r}\right)$ is its temporal inverse, and $\left\langle \beta \middle| \hat{V} \middle| \alpha \right\rangle$ is the matrix element of the potential responsible for the transition. In the case of a reaction at high beam energy, many different doorway states are energetically accessible during the interaction. We could in principle describe such a process as a multi-step reaction, considering all the possible successive interaction steps from the entrance to the exit channel:

$$f_{\alpha\beta} \propto \langle \beta | \hat{V} | \gamma \rangle \langle \gamma | \hat{V} | \gamma' \rangle \langle \gamma' | \hat{V} | \gamma'' \rangle \ldots \langle \gamma'''''' | \hat{V} | \alpha \rangle \tag{2.3}$$

If the number of open channels is important, the final result will have little to do with the superposition of entrance and exit channels $\left\langle \beta \middle| \hat{V} \middle| \alpha \right\rangle$, but will rather depend on the total number of matrix elements, that is on the total number of available states. In turn, this number will solely depend on the good quantum numbers, that is on the available energy and angular momentum. A modelization where the probability of a process depends on the available energy via the number of accessible states, is by definition a statistical modelization. In nuclear physics, such a theory is known under the name of the theory of CN decay.

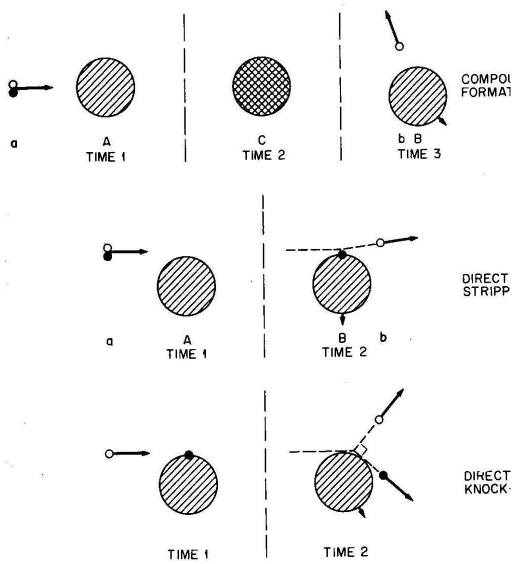
The starting point is the hypothesis of *statistical independence* between the entrance and exit channel. Schematically we can write:

$$a + A \to C^*\left(E^*, J^\pi\right) \to b + B . \tag{2.4}$$

In terms of cross section, the probability of exciting the intermediate state or compound nucleus, and the probability of decay of this state into the exit channel, are factorized (*Bohr's independence hypothesis*, see picture):

$$\sigma_{\alpha\beta} = \sigma_\alpha^C(E,J)G_\beta^C(E,J) = \sigma_\alpha^C(E,J)\frac{\Gamma_\beta}{\Gamma}, \tag{2.5}$$

where $\Gamma = \hbar/\tau = \hbar dP/dt = \sum_\beta \Gamma_\beta$ is the state width, and decay probability towards the specific channel β is given by $\Gamma_\beta/\hbar = dP/dt(C^* \to \beta)$.



2.28 Illustrating schematically the two limiting kinds of nuclear reacti
ıs formation and decay, and direct reactions. The latter are represented l
and knock-out occurring in the nuclear surface

This factorization implies that the decay probability can only depend on the good quantum numbers of the compound nucleus, that is on the physical quantities conserved by the reaction (total energy, total angular momentum). The Bohr's independence hypothesis can never be proved, but it has to be a-posteriori verified. One has to select a given reaction channel produced with two different entrance channels, which correspond to the same value of energy and angular momentum

$$a + A \to C^*\left(E, J\right) \to b + B \quad ; \quad d + D \to C^*\left(E, J\right) \to b + B . \tag{2.6}$$

If the independence hypothesis is correct, we must have:

$$\frac{\sigma_{\alpha\beta}}{\sigma_{\delta\beta}} = \frac{\sigma_{\alpha}^{C}}{\sigma_{\delta}^{C}} = cst \tag{2.7}$$

This means that the ratio of cross sections must not depend on the kinematical characteristics of the b particle in the exit channel. Two examples of validation of the hypothesis of statistical independence are presented in the following pictures.

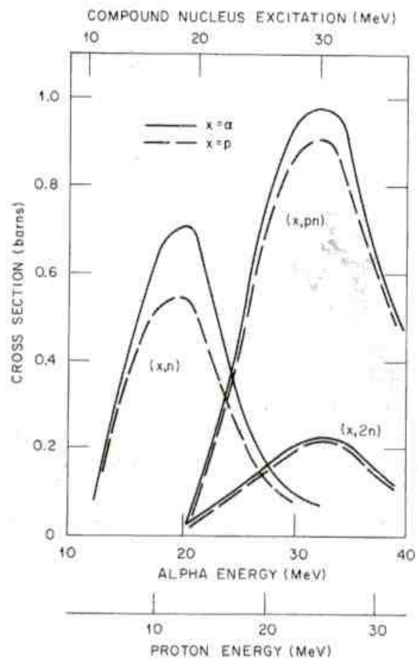
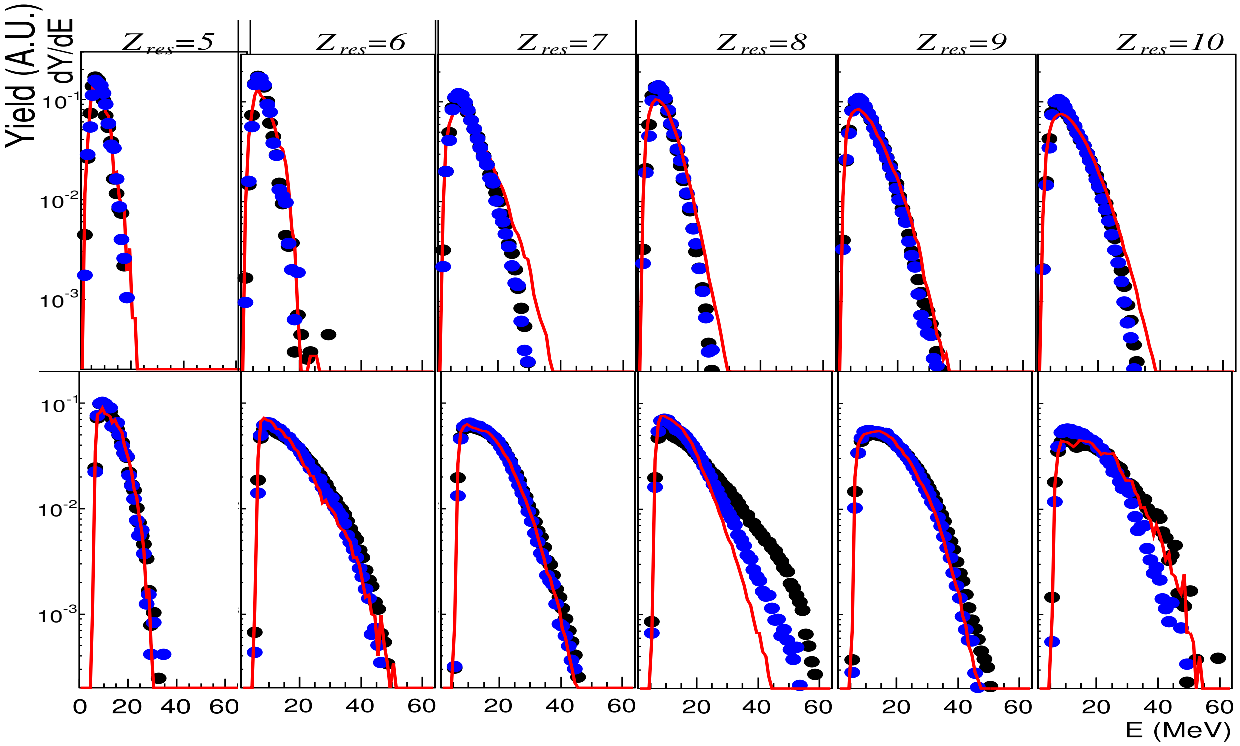


Figure 2.29 Experimental evidence for the independence of formation and decay in a compound nucleus reaction. The same compound nucleus ^{64}Zn, with the same excitation energy, is formed in two different ways, but the excitation curves are very similar. (After Goshal,
2 1950)



Proton (upper part) and alpha (lower part) energy spectra measured in the 95 MeV $^{12}C+^{12}C$ (black symbols) and 80 MeV $^{14}N+^{10}B$ (blue symbols) fusion reactions, in coincidence with a residue of atomic number between Z=5 et Z=10 (from left to right). The Hauser-Feshbach predictions are shown as full red lines. The two reactions lead to the formation of the same ^{24}Mg compound at the same excitation energy 2.6 A.MeV.
(L.Morelli, GARFIELD collaboration, 2013)

Equation (2.5) means that the description of CN reactions passes through an independent evaluation of the CN formation cross section (or *fusion* cross section), and the decay probability of the CN.

The basic equation is *principle of detailed balance*, which reflects the fundamental principle of microscopic reversibility of all quantum elementary processes. This principle can be written as:

$$\frac{dP}{dt}\left(\beta \to C^*\right) N_\beta\left(b,B\right) = \frac{dP}{dt}\left(C^* \to \beta\right) N_C\left(C^*\right). \tag{2.8}$$

The number of accessible states for the CN is given by:

$$N_C\left(E^*,J\right) = \rho_C\left(E^*,J\right) dE^*, \tag{2.9}$$

where ρ_C is the compound density of states. The number of states of the exit channel is the product of the number of states of the two bodies:

$$N_\beta\left(b,B\right) = N_B\left(B\right) n_b\left(e_b, j_b\right) = \rho_B\left(E_B^*, J_B\right)\left(2j_b+1\right) V \int \frac{d^3k_b}{\left(2\pi\right)^3}, \tag{2.10}$$

V in order to count the plane wave continuum states which otherwise would diverge.
The CN decay probability is defined as a function of the partial decay width :

$$\frac{dP}{dt}\left(C^{*}\to\beta\right)=\int d^{3}k_{\beta}\frac{dP}{dt}\left(C^{*}\to\beta,k_{\beta}\right)=\frac{\Gamma_{\beta}}{\hbar}\ . \tag{2.11}$$

The probability of the inverse process is linked to the fusion cross section by:

$$\frac{dP}{dt}\left(\beta\to C^{*}\right)=\frac{dV_{fus}\,/\,dt}{V}=\frac{\sigma_{\beta}^{C^{*}}v_{\beta}}{V}\ . \tag{2.12}$$

This cross section is expressed as a function of transmission coefficients as :

$$\sigma_{\beta}^{C}\left(e_{\beta},J_{B}\right)=\frac{\pi}{k_{\beta}^{2}}\frac{1}{2j_{b}+1}T_{LS}^{J} \tag{2.13}$$

In the realistic applications of the CN decay theory, these coefficients are calculated in the framework of diffusion theory from the probability that a partial wave L is absorbed by a complex potential which takes the name of *optical potential* and which is either determined phenomenologically, or calculated microscopically.
In the classical collision theory, if we consider that all impact parameters up to a limiting value (*grazing*) lead to the absorption of the projectile by the target, the fusion cross section simply results:

$$\sigma_{\beta}^{C}\left(e_{\beta},J_{B}\right)=\frac{\pi}{k_{\beta}^{2}}\sum_{L=0}^{L_{grazing}}\left(2L+1\right), \tag{2.14}$$

corresponding to a simple definition of the transmission coefficients as $T_{LS}^{J}=T_{L}=\left(2L+1\right)\theta\left(L-L_{grazing}\right)$. An even simpler estimation of this expression consists in employing a geometrical absorption cross section, which reads for a neutron :

$$\sigma_{\beta}^{C}=\pi R_{b+B}^{2}\,, \tag{2.15}$$

And for a charged particle :

$$\sigma_{\beta}^{C}=\pi R_{b+B}^{2}\left(1-\frac{B_{coul}}{e_{\beta}}\right), \tag{2.16}$$

where B_{coul} is the Coulomb barrier between b et B.

Using the conservation laws

$$\begin{aligned} &E^* = Q + e_\beta + \frac{\hbar^2}{2\mu_\beta} L(L+1) + E_B^*, \\ &\vec{J}_B + \vec{j}_b = \vec{S} \quad ; \quad \vec{J} = \vec{L} + \vec{S}, \end{aligned} \tag{2.17}$$

and considering all the allowed angular momentum couplings we get:

$$\frac{\Gamma_\beta}{\hbar} \rho_C\left(E^*, J\right) dE^* = \sum_{J_B, L, S} \int_0^{E^*-Q-E_L} de_\beta \frac{\sigma_\beta^C\left(e_\beta, J_B\right) v_\beta}{V} \frac{d^3 p_\beta}{h^3} \left(2 j_b + 1\right) \rho_B\left(E_B^*, J_B\right) dE_B^*, \tag{2.18}$$

where $E_L = \frac{\hbar^2}{2\mu_\beta} L(L+1)$ is the rotational energy of the relative motion . After some easy algebra we finally get :

$$\Gamma_\beta^J = \int_0^\infty de_\beta \frac{dn}{de_\beta} = \frac{1}{2\pi} \sum_{J_B, L, S} \int_0^{E^*-Q-E_L} de_\beta T_{LS}^{J_B} \frac{\rho_B\left(E^* - Q - E_L - e_\beta, J_B\right)}{\rho_C\left(E^*, J\right)} \tag{2.19}$$

This formalism is known under the name of *Hauser-Feshbach theory*, and has shown a remarkable predictive power over the decades.

To derive this expression we have used many statistical concepts but we have not explicitly included the notion of nuclear temperature. However this can be made naturally appear, as we now show. The experimental nuclear densities of states are typically exponential functions, very well described by the following functional form

$$\rho_C(N, Z, E) = \frac{1}{2\pi\sqrt{\Sigma}} \exp 2\sqrt{aE} \tag{2.20}$$

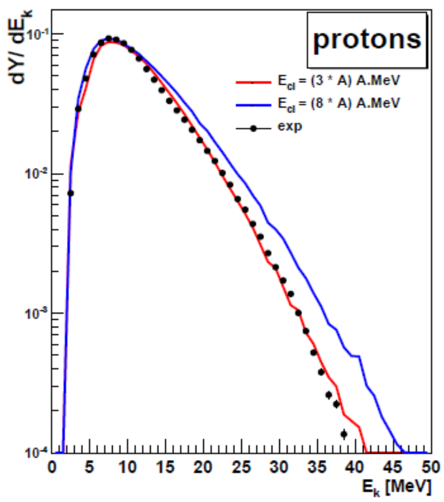
where Σ is a normalization, the parameter a is called *level density* parameter and depends on the values of N,Z,E, and to account for pairing effects the excitation energy has to be corrected as $E=E^*-\Delta$, where this backshift parameter has a different sign for odd-odd and odd-even nuclei. We will come back on this function in the next chapter.
Neglecting for the sake of simplicity the dependence on angular momentum we can write

$$\begin{aligned} \ln\rho\left(E - dE, N - dN, Z - dZ\right) &\cong \ln\rho\left(E, N, Z\right) - dE \left.\frac{\partial \ln\rho}{\partial E}\right|_{E,N,Z} - dN \left.\frac{\partial \ln\rho}{\partial N}\right|_{E,N,Z} - dZ \left.\frac{\partial \ln\rho}{\partial Z}\right|_{E,N,Z} \\ &= \ln\rho\left(E, N, Z\right) - \frac{dE}{T} + \mu_n \frac{dN}{T} + \mu_p \frac{dZ}{T}, \end{aligned} \tag{2.21}$$

where we have introduced the thermodynamic definition of temperature and chemical potential derived in section 1. Replacing in eq.(2.19) we get

$$\frac{dn}{de_\beta} \propto \exp - \frac{e_\beta + Q}{T} \exp \frac{\mu_n n + \mu_p z}{T} \tag{2.22}$$

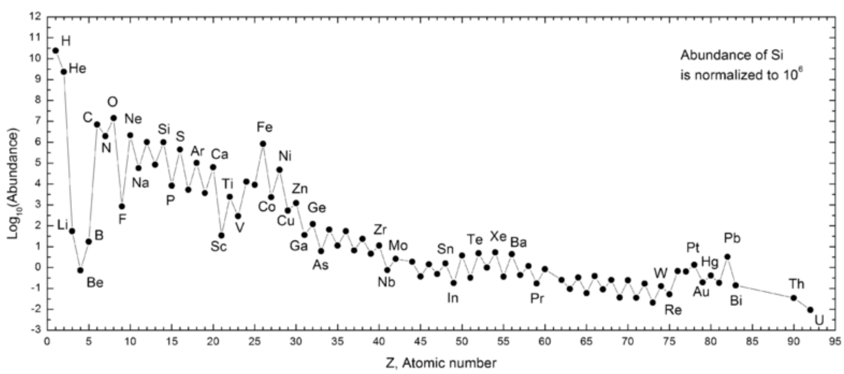
This simplified version of the Hauser-Feshbach theory is known under the name of Weisskopf theory. It shows that the particle spectra emitted by the compound nucleus mechanism are expected to be exponential function, their slope giving the nuclear temperature. An example of the Maxwellian shape of emitted particles, and of the predictive power of the HF theory, is given in the picture below.



Proton spectrum measured in 95 MeV $^{12}C+^{12}C$ fusion reactions, with a complete detection in charge of all the reaction products with the detection system GARFIELD +RCo. The two curves represent HF calculations with two different prescriptions for the high excitation energy level density. G.Baiocco, PhD thesis, 2012.

3. *Application to nucleosynthesis*

The Hauser-Feshbach theory of compound nucleus decay has a large number of applications, ranging from fission studies to surrogate reactions, from the synthesis of new elements to level density measurements… In this section we briefly review the astrophysical application of the nucleosynthesis of heavy elements. All elements of the universe are synthetized by means of fusion reactions. The different isotopes of Fe and Ni being the most bound nuclei in terms of energy per particle, endothermic stellar fusion reactions cannot synthetize any element heavier than iron, and the production of heavy elements has to proceed via *explosive nucleosynthesis.* The measured abundances of the different elements in the solar system is shown in the figure below.



Solar system abundances of the different elements.

Though different nucleosynthesis processes (s, r, rp) are known to contribute to these heavy elements abundances, the localization of these processes and the detailed abundances are still not understood. As a general statement, stable isotopes of elements heavier than Fe tend to be neutron rich. The synthesis of such elements thus requires the process of neutron capture. The evolution in time of the abundance of a species A is governed by rate equations, or *master equations*:

$$\frac{dN_A}{dt} = \sum_B N_B(t) \frac{dP_{B\to A}}{dt} - N_A(t) \frac{dP_{A\to B}}{dt}, \tag{3.1}$$

where the sum runs over all the possible nuclear species. Let us specify the reaction probabilities dP/dt to the case of neutron capture for an element Z in a finite temperature environment :

$$\frac{1}{V}\frac{dN_A}{dt} = \rho_n \left(N_{A-1}(t) \frac{\langle \sigma_{nA} v_v \rangle}{V} - N_A(t) \frac{\langle \sigma_{nA+1} v_v \rangle}{V} \right). \tag{3.2}$$

The neutron capture cross section for a neutron of velocity v_n (or momentum $k_n = \mu_{nA} v_n / \hbar$, or energy $e_n = \hbar^2 k_n^2 / \mu_{nA}$) is given by the HF theory:

$$\sigma_{nA}(e_n) = \frac{\pi}{2k_n^2} \sum_{L,S,J} T_{LS}^J, \tag{3.3}$$

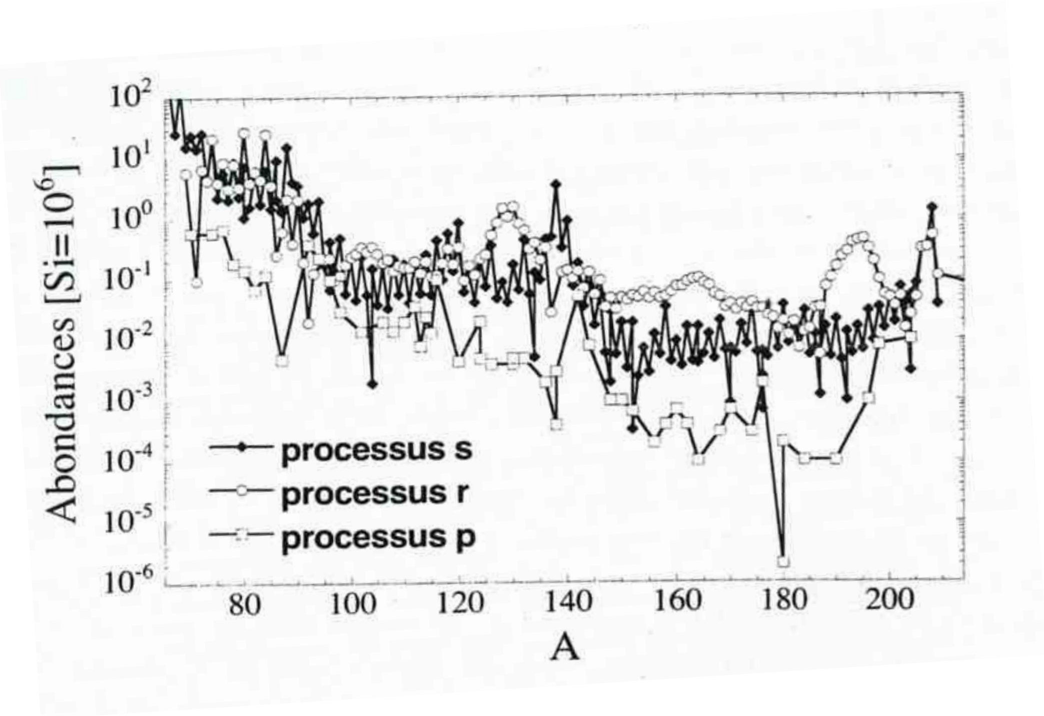
and the average in Eq.(2.22) is a thermal average:

$$\langle \sigma_{nA} v_v \rangle = \frac{\int d^3k_n \sigma_{nA} v_v e^{-e_n/T}}{\int d^3k_n e^{-e_n/T}} \cong 4\pi R_A^2 \sqrt{\frac{T}{2\pi\mu_{nA}}}. \tag{3.4}$$

where the last equality is obtained using the simplified expression (2.15) for the absorption cross section. The neutron capture process is in competition with beta-decay. The beta-decay rate is then added as a coupled Master equation that has to be solved together with eq.(2.23). Other secondary processes take place, and the nucleosynthesis calculations consist in the numerical solution of a very complex network of coupled rate equations. Limiting to the competition between neutron capture and beta decay, we can consider two limiting cases: if the reaction rate is comparable or smaller than the inverse of the isotope half-life with respect to beta decay, $\langle \sigma_{nA} v_v \rangle \approx \tau^{-1}$, the nucleosynthesis will proceed along the stability valley. If on the contrary $\langle \sigma_{nA} v_v \rangle >> \tau^{-1}$, very exotic neutron-rich nuclei can be formed, which will sebsequently decay over long times towards the stable isotopes. As we can see from Eqs.(2.23),(2.25), this second scenario will apply if the surrounding medium is very hot and neutron rich.

The first nucleosynthesis scenario is called the s-process, and it is believed to occur starting from Fe in very massive stars ($M>8M_o$) in their pre-supernova stage. The second scenario is called the r-process. The site of this process is still largely unknown, two possible candidates being the neutrino driven wind which favors the explosion of core-collapse supernova, and/or the merging of the binary system constituted by two neutron stars.

As we can see from the figure, both processes are considered to contribute in an important way to the synthesis of heavy elements, as well as another process we have not mentioned yet, the rp-process. This latter, linked to the production of exotic proton-rich nuclei and triggered by proton capture in a hot and dense environment, is not entirely understood either. One of the most probable scenario is given by the X-ray bursts associated to the rapid rotation of binaries constituted of a white dwarf and a neutron star.



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Exercices

1. We wish to describe proton and neutron emission from a (N,Z) compound in the framework of the Weisskopf theory of compound nucleus decay.

   a. Show that the ratio between proton and neutron spectra can be written in the CN reference frame : $R(e)=\left(1-\frac{B_C}{e}\right)\exp\frac{Q_n-Q_p}{T}$, where e is the particle energy , B_C the Coulomb barrier of the nucleus (N,Z-1), T the CN temperature, Q_b the mass balance associated to the emission of particle b. Detail the approximations needed to obtain this expression.
   b. Compute the ratio R for a kinetic energy e=20 MeV, with a temperature of the mitting source T=3 MeV or T=10 MeV, for the stable and double magic nucleus ^{40}Ca.
   c. Compare the rsult obtained at point b with the same calculation, done this time for the exotic compound nucleus , ^{50}Ca (mean life : 13,9s).
   d. Conclude: what is the effect of the Coulomb barrier ? Of the temperature ? Of the exoticity of the source ?

   For the calculation of Coulomb barriers, we will make the hypothesis that all nuclei are spherical and have a radius $R \approx 4\,fm$.

Some mass excess (http://www.nndc.bnl.gov) **:**

$\Delta(^{40}\mathrm{Ca})$=-34.85 MeV
$\Delta(^{39}\mathrm{Ca})$=-27.28 MeV
$\Delta(^{39}\mathrm{K})$ =-33.81 MeV
$\Delta(^{50}\mathrm{Ca})$=-39.57 MeV
$\Delta(^{49}\mathrm{Ca})$=-41.29 MeV
$\Delta(^{49}\mathrm{K})$ =-30.32 MeV