Intrinsic Energy Partition in Fission

Outline

1. TIME DEPENDENT PAIRING EQUATIONS AND DISSIPATION
2. TIME DEPENDENT EQUATIONS WITH PARTICLE NUMBER PROJECTION
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THE TIME DEPENDENT PAIRING EQUATIONS

In a mean field approximation (even in the HF) the two-body collisions are incorporated in the equations of motion only to the extend to which they contribute to the mean field. In principle, the time dependent equations of motion treats the residual interactions exactly only if the mean field is allowed to break all symmetries. Such approaches lead to huge computational problems. Usually, the mean field is constrained to be at least axially symmetric. In this case, levels characterized by the same good quantum numbers cannot intersect, each individual wave function will belong to only one orbital, and the mechanism of level slippage is not allowed.

This behaviour leads to the unpleasant feature that a system even moving infinitely slowly could not end up in its ground state.

Solutions for the problem: for ex. in the HF approximation the equations of motion were extended to include collision terms (Stochastic time dependent approaches).

Inclusion of the pairing interaction: time dependent pairing equations (formally similar to the TDHFB) in the 1980's. (Schutte and Wilets, Z.Phys.A 280, 313, 1978; Koonin and Nix, PRC 13, 209,1976; Blocki and Flocard, NPA 273, 45, 1976).

An average value of the dissipation energy can be computed from the time dependent pairing equations.

DISSIPATION

The coupling of collective degrees of freedom with the microscopic ones causes dissipation and a modification of the adiabatic potential. The term dissipation usually refers to exchange of energy (either linear or angular momentum) by all kind of damping from collective motion to intrinsic heat. A measure of the dissipated energy can be obtained solving the time dependent pairing equations (that are similar to the Hartree-Fock-Bogoliubov ones):

$$i\hbar\frac{\partial_i\rho}{\partial t} = \kappa_i\Delta^* - \kappa_i^*\Delta,$$

$$i\hbar\frac{\partial\kappa_i}{\partial t} = (2\rho_i - 1)\Delta - 2\kappa_i(\epsilon_i - \lambda)$$

where $\rho_i = v_i^2$, $\kappa_i = u_i v_i^*$, and $\Delta = G\sum_i \kappa_i$

DEFINITION OF DISSIPATION

Energy with densities and pairing moment components obtained from the equations of motion - Lower energy state (BCS solutions):

$$E = 2\sum \rho_k \varepsilon_k - G\left|\sum \kappa_k\right|^2 - G\sum \rho_k^2$$

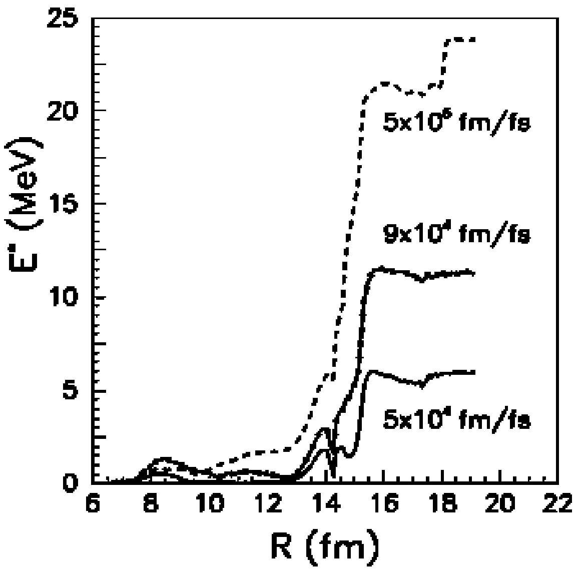
$$\Delta E = E - E_0$$

Where ρ are single particle densities and κ pairing moment components

Dissipation along the minimal action trajectory for different tunneling velocities velocities for the fission of ^{236}U in the partition $^{86}Se+^{150}Ce$.

The dissipation after the scission tends to increase when the tunneling velocity increases.

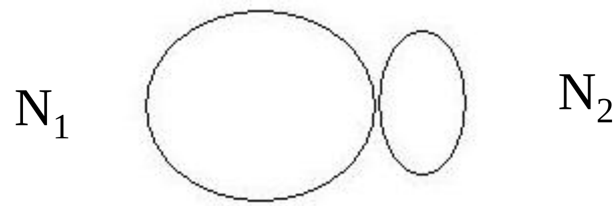
The dissipation increases especially in the final part of the process (when the second barrier is tunneled)



M. Mirea and al., NPA 735, 21 (2004).

A deep connection with the Landau-Zener transitions is included in the time dependent pairing equations: pairs undergo Landau-Zener transitions on virtual levels with coupling strengths given by the magnitude of the gap Δ.

TIME DEPENDENT PAIRING EQUATIONS WITH PROJECTION OF NUMBER OF PARTICLES



The number of nucleons N in the active level space before scission must be equal with the sum of numbers of nucleons N_1+N_2 in the two fragments in the same active level space. But the sum of BCS occupation probabilities of the levels of one fragment is not equal with its expected number of nucleons.

$N_0=N_1+N_2$

$\Sigma\rho_{k0}=N_0$ but $\Sigma\rho_{k1}\neq N_1$ $\Sigma\rho_{k2}\neq N_2$

N_1 and N_2 are not integers.

FORMALISM FOR ENERGY PARTITION IN NUCLEAR FRAGMENTS

The partition of dissipation energy between fragments can be evaluated with conditions that project the number of particles in each fragment.

In order to obtain the equations of motion we start from the variational principle taking the following energy functional as:

$$\mathcal{L} = \langle \varphi \mid H - i\hbar \frac{\partial}{\partial t} - \lambda (N_1 \hat{N}_2 - N_2 \hat{N}_1) \mid \varphi \rangle$$

The trial state is a many-body expanded as a BCS seniority zero w.f.

$$\mid \varphi \rangle = \sum_k \left(u_k + v_k a_k^{+} a_{\bar{k}}^{+} \right) \mid 0 \rangle$$

u and v are time dependent occupation and vacancy amplitudes, rspectively

The Hamiltonian with pairing residual interactions is

$$H(t) = \sum_{k>0} \epsilon_k (a_k^+ a_k + a_{\bar{k}}^+ a_{\bar{k}}) - G \sum_{k,i>0} a_k^+ a_{\bar{k}}^+ a_i a_{\bar{i}}$$

A supplementary condition is introduced through the Lagrange multiplier λ

$$\langle \varphi \mid (N_1 \hat{N}_2 - N_2 \hat{N}_1) \mid \varphi \rangle = 0$$

The particle number operators in the pairing active level space for the fragments are

$$\hat{N}_1 = \sum_{k_1} (a_{k_1} a_{k_1}^+ + a_{\bar{k}_1} a_{\bar{k}_1}^+),$$

$$\hat{N}_2 = \sum_{k_2} (a_{k_2} a_{k_2}^+ + a_{\bar{k}_2} a_{\bar{k}_2}^+)$$

N_1 and N_2 (integers) are expected number of particles of fragments.

After variation, the equations of motions read, eventually

$$
\begin{aligned}
i\hbar\dot{\rho}_{k_1} &= \kappa_{k_1}\Delta_1^* - \kappa_{k_1}^*\Delta_1, \\
i\hbar\dot{\rho}_{k_2} &= \kappa_{k_2}\Delta_2^* - \kappa_{k_2}^*\Delta_2, \\
i\hbar\dot{\kappa}_{k_1} &= \left(2\rho_{k_1} - 1\right)\Delta_1 - 2\kappa_{k_1}\left(\epsilon_{k_1} + \lambda N_2\right), \\
i\hbar\dot{\kappa}_{k_2} &= \left(2\rho_{k_2} - 1\right)\Delta_2 - 2\kappa_{k_2}\left(\epsilon_{k_2} - \lambda N_1\right)
\end{aligned}
$$

where $\rho_k = \mid v_k \mid^2$ are occupation probabilities, $\kappa_k = u_k^* v_k$ are pairing moment components, and $\Delta = G\sum_k \kappa_k$ is the pairing gap. $\Delta_1 = G_1\sum_{k_1}\kappa_{k_1} + G_{12}\sum_{k_2}\kappa_{k_2}$ and $\Delta_2 = G_{12}\sum_{k_1}\kappa_{k_1} + G_2\sum_{k_2}\kappa_{k_2}$ are the gaps for the two fragments.

These equations project the number of particles on the two fragments providing that we know where the single particle levels will be located before that the scission is produced.

After scission, the pairing G_{12} matrix element between states belonging to the different fragments is zero.

$$\begin{aligned} E &= 2\sum_k \epsilon_k \rho_k - G\left|\sum_k \kappa_k\right|^2 - G\sum_k \rho_k^2 \\ &\to 2\sum_{k_1} \epsilon_{k_1}\rho_{k_1} - G_1\left|\sum_{k_1}\kappa_{k_1}\right|^2 - G_1\sum_{k_1}\rho_{k_1}^2 \\ &\quad + 2\sum_{k_2}\epsilon_{k_2}\rho_{k_2} - G_2\left|\sum_{k_2}\kappa_{k_2}\right|^2 - G_2\sum_{k_2}\rho_{k_2}^2 \\ &= E_1 + E_2, \end{aligned}$$

When G_{12}=0, the flux of the single particle density from one fragment to another is forbidden. The number of particles in the two fragments are conserved.

MACROSCOPIC-MICROSCOPIC MODEL

The whole nuclear

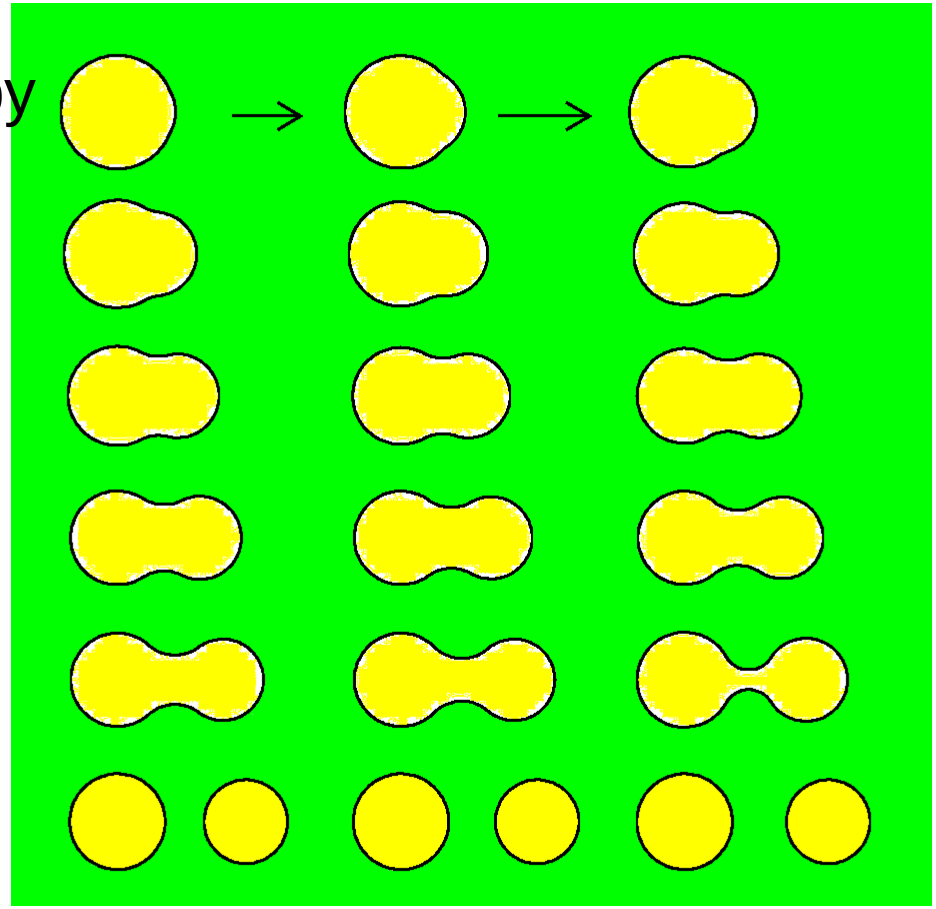
system is characterized by

some collective variables

which determine
approximately

the behavior of all other

intrinsic variables.



Nuclear shape parametrization

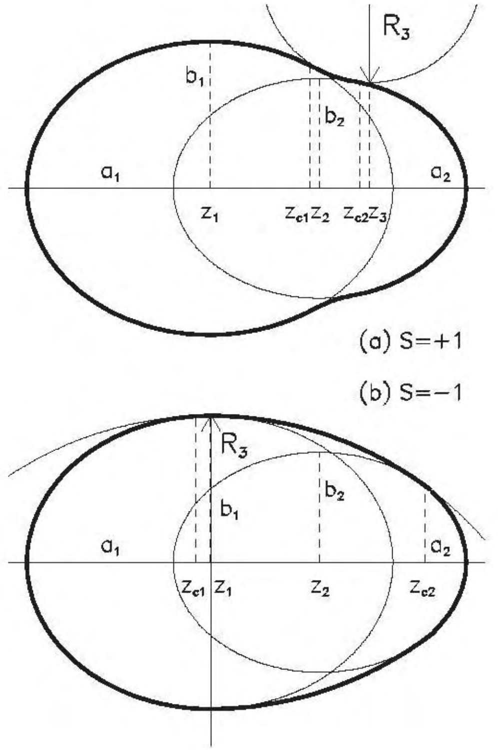
Most important degrees of freedom encountered in fission:

-elongation $R=Z_2-Z_1$

-necking-in $C=s/R_3$

-mass-asymmetry a_1/a_2

-fragments deformations



(a) Diamond-like (swollen) shapes

(b) Necked shapes

MINIMIZATION OF THE ACTION INTEGRAL AND FISSION TRAJECTORY

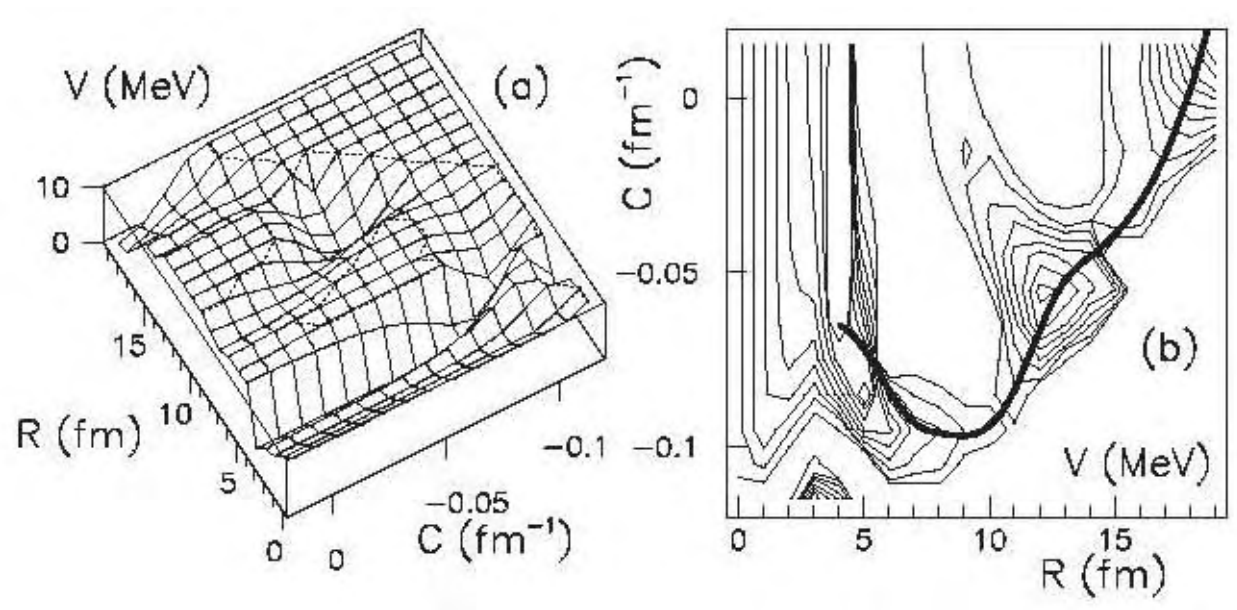
$P=\exp\{-(1/\hbar)\int[2B(E-E_0)]^{1/2}\,dR\}$ WKB integral

$E(R,C,R_2)$=potential energy (microscopic-macroscopic model)

E_0=ground-state energy

$B(R,C,R_2,dC/dR,dR_2/dR)$=inertial mass along the trajectory (cranking model)

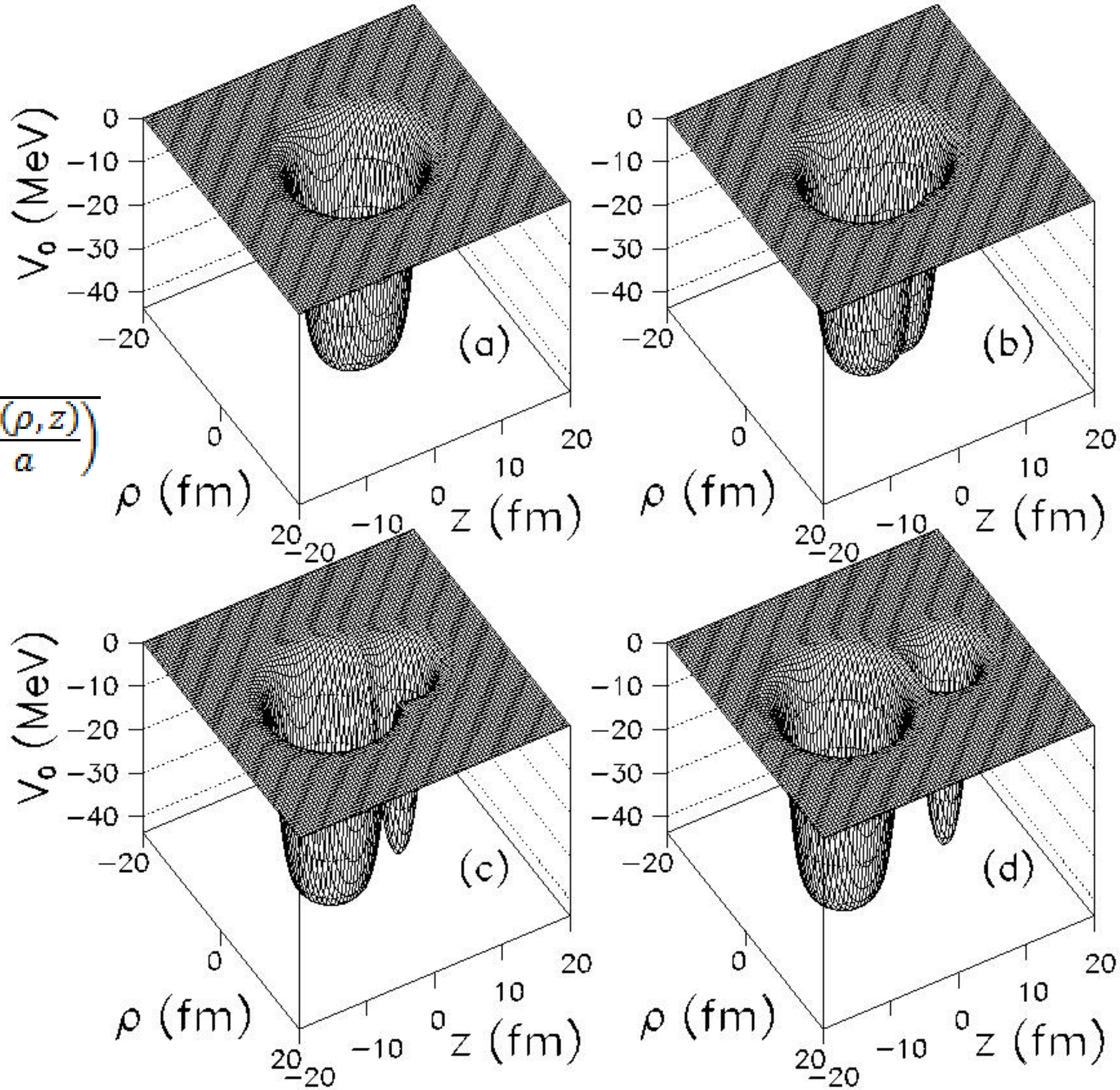
The functional P (from ground-state to exit point from the barrier) must be minimized in a configuration spacespanned by R,C,R_2. ➔ Optimum fission path in space.



Minimal values of the deformation energy in MeV as function of the neck coordinate C and the elongation R for ^{234}U. (b) Contours of the deformation energy. The lest action trajectory is superimposed.

Woods-Saxon mean field potential within the two center parametrization

$$V(\rho,z) = -\frac{V_c}{1+exp\left(\frac{D(\rho,z)}{a}\right)}$$



THE TWO CENTER MODEL

$$\left[-\frac{\hbar^2}{2m}\Delta + V_0(\rho,z) + V_{Ls}(\rho,z) + V_c(\rho,z)\right]\Psi(\rho,z,\varphi) = E\Psi(\rho,z,\varphi)$$

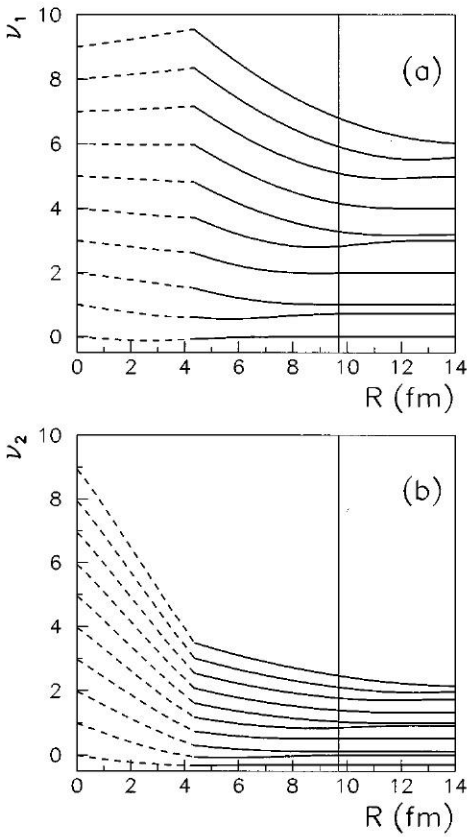
$$\Psi(\rho, z, \varphi) = Z(z)R(\rho)\Phi(\varphi),$$

with

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}}\exp(im\varphi),$$

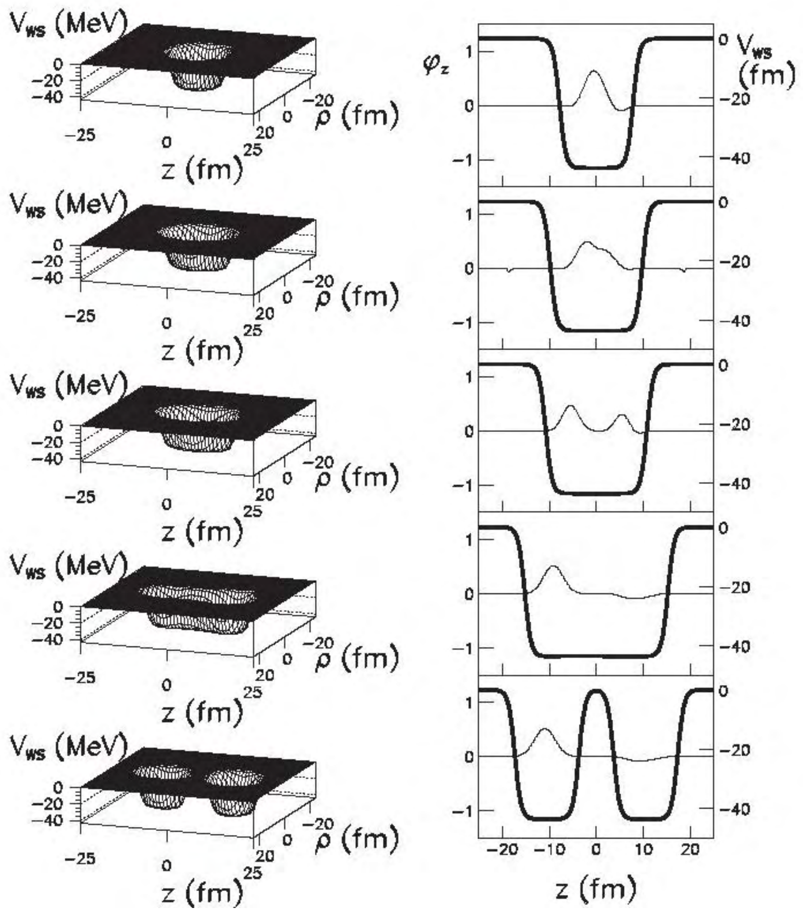
$$R_{nm}(\rho) = \sqrt{\frac{2n!}{(n+m)!}}\alpha_\rho \exp\left(-\frac{\alpha_\rho^2\rho^2}{2}\right)(\alpha_\rho\rho)^m L_n^m(\alpha_\rho^2\rho^2),$$

$$Z_\nu(z) = \begin{cases} C_{\nu_1}\exp\left(-\frac{\alpha_{z1}^2(z-c_1)^2}{2}\right)\mathbf{H}_{\nu_1}[-\alpha_{z1}(z+c_1)], \\ z<0, \\ C_{\nu_2}\exp\left(-\frac{\alpha_{z2}^2(z-c_2)^2}{2}\right)\mathbf{H}_{\nu_2}[\alpha_{z2}(z-c_2)], \\ z\geqslant 0, \end{cases}$$

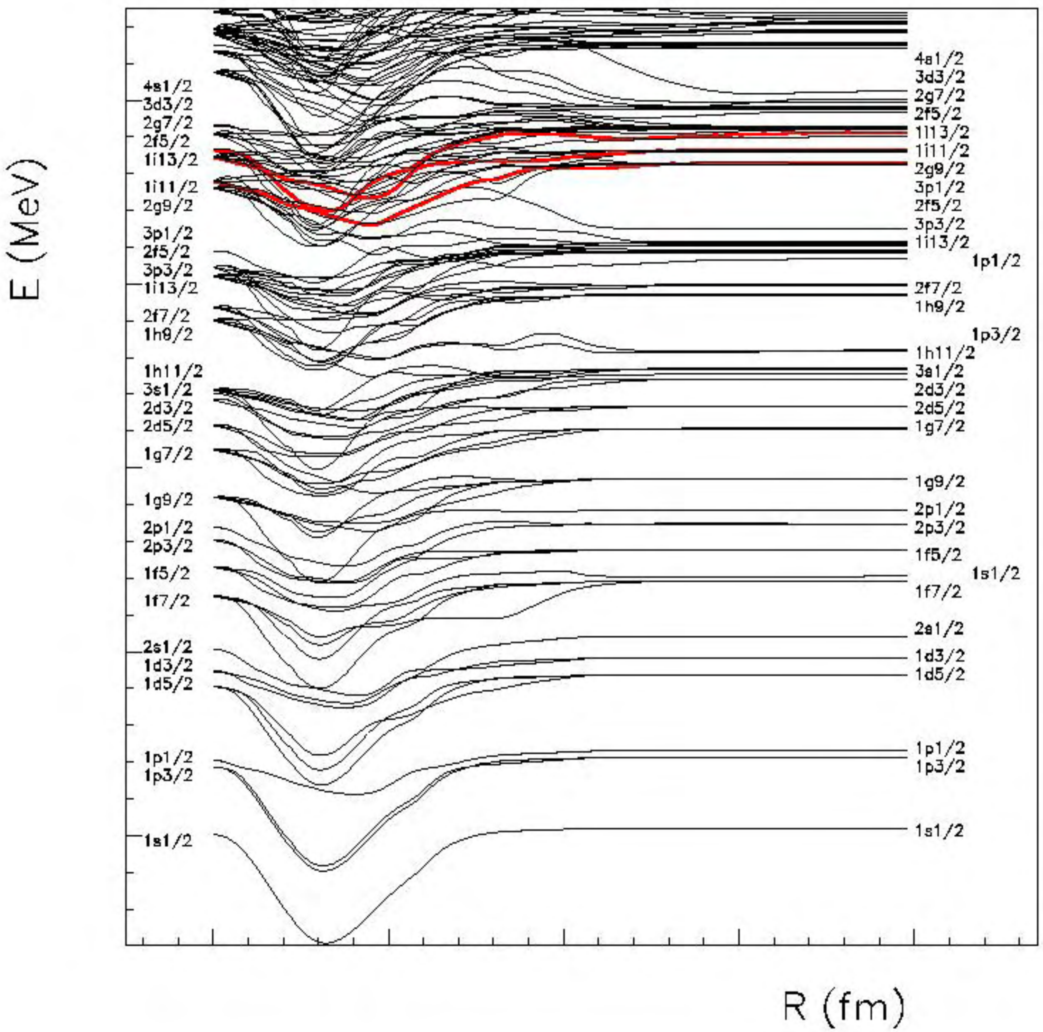


Orthogonal functions in ONE Hilbert space

DISENTANGLEMENT OF ASYMPTOTIC WAVE FUNCTIONS



EXAMPLE OF SINGLE PARTICLE LEVEL SCHEME



Solve a Woods-Saxon potential within the two-center semisymmetric eigenvector basis.

ENERGY PARTITION IN THE FISSION OF ^{234}U WITH ^{132}Sn AS HEAVY FRAGMENT

The previous time dependent equations are used to evaluate the energy partition in fission (M. Mirea PRC 83 (2011) 054608, PLB doi:10.1016/j.physletb.2012.09.023). This phenomena was recently investigated with a wide range of models:

- statistical K-H Schmidt and B Jurado PRL 104 (2010) 212501; PRC 83 (2011) 014607

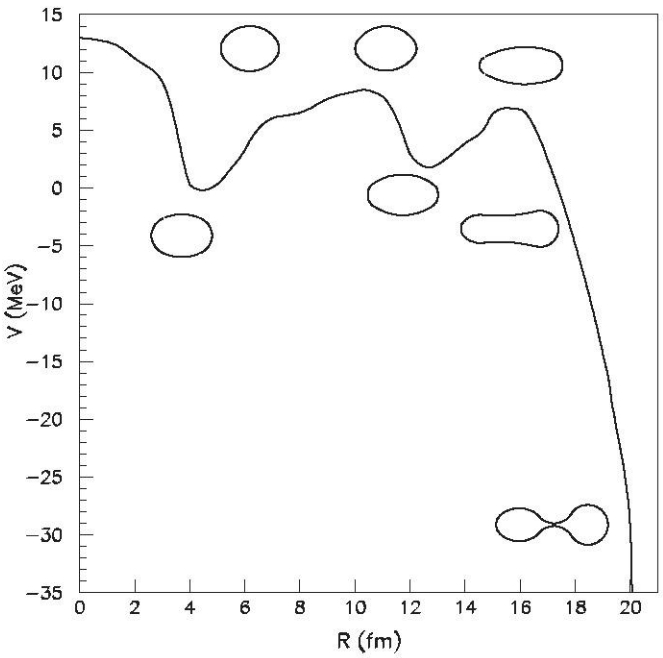
- phenomenological C Morariu, A Tudora, F J Hambsh, S Oberstedt and C Manailescu, JPG 39 (2012) 055103

- empirical C Yong-Jing, et al. IJMPE 21 (2012) 1250073

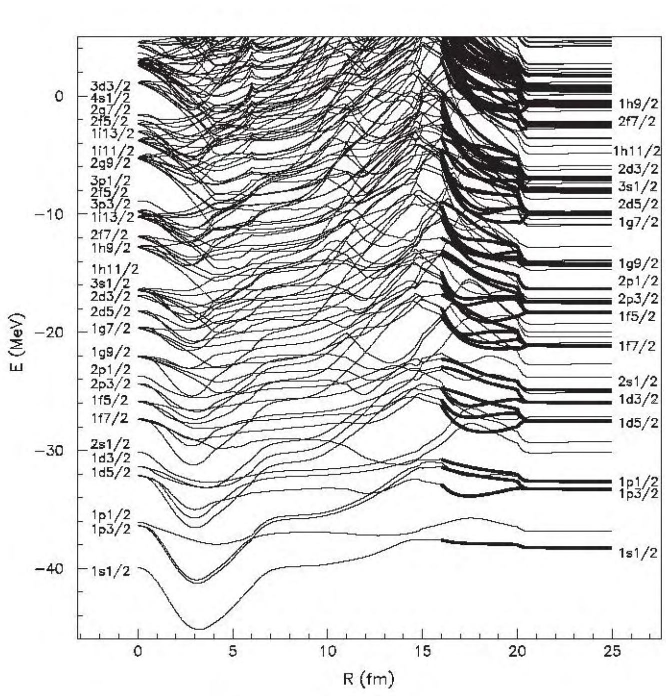
- Hartree-Fock W Younes and D Gogny, PRL (2011) 132501

- single particle in sudden approximation N Carjan, F J Hambsch, M Rizea and O Serot, PRC 85 (2012) 044601

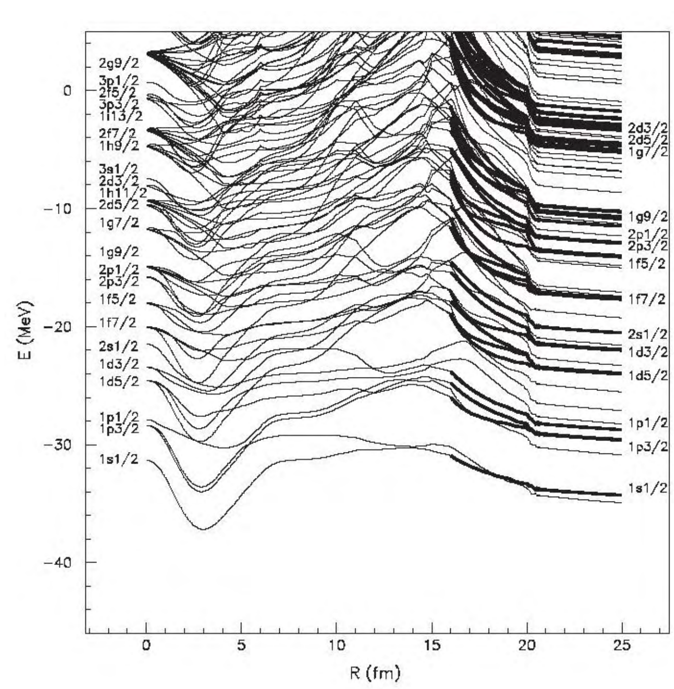
Calculation of the dissipated energy in the reaction $^{234}U \rightarrow {}^{102}Zr + {}^{132}Te$



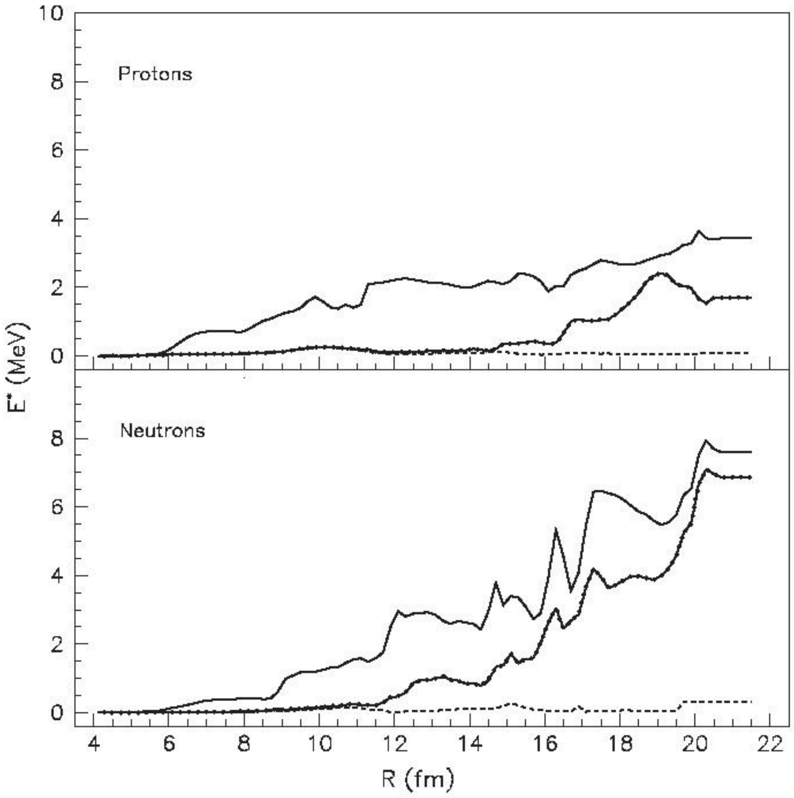
The levels of the heavy fragment can be identified before that the scission is produced



Neutron single particle energies

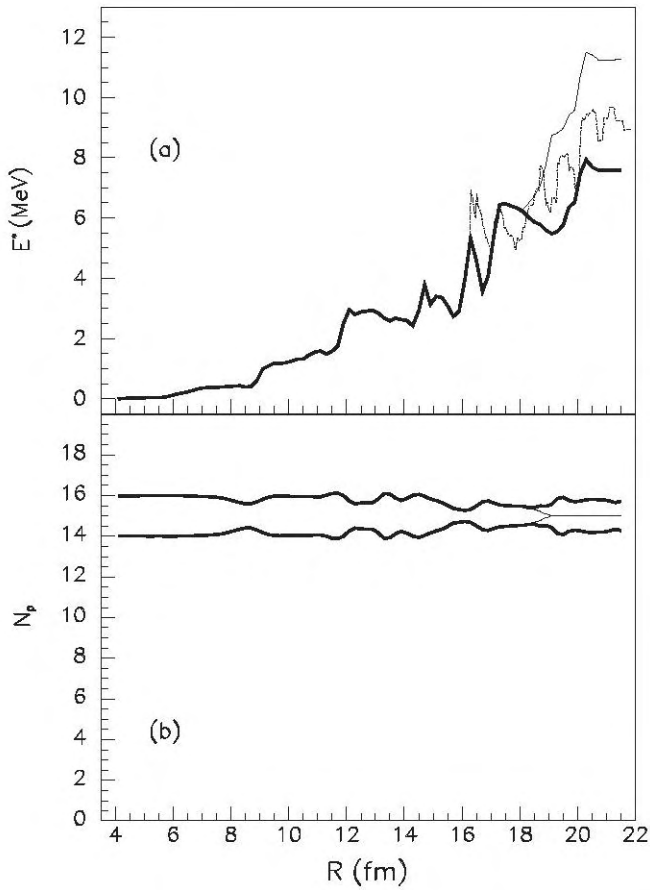


Proton single particle energies



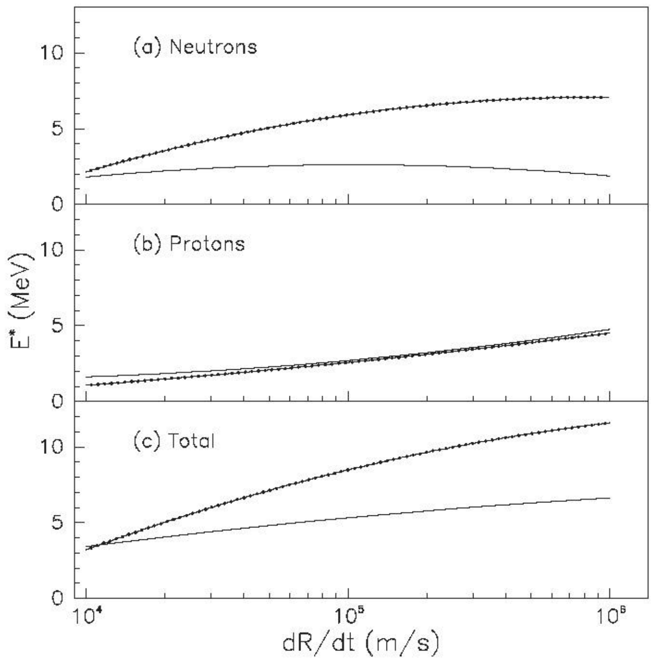
Dissipation energy as function of the distance between the centers of the fragments for three different values of the internuclear velocity: 10^4, 10^5, and 10^6 fm/fs

(no projection condition).



Dissipation energy for neutrons as function of the distance between the centers of the fragments for the internuclear velocity 10^6 fm/fs (projection condition).

Number of neutron pairs that are considered to be located in the two fragments.



Dissipation energy of the fragments as function of the internuclear velocity.

For dR/dt=10^6 fm/fs:

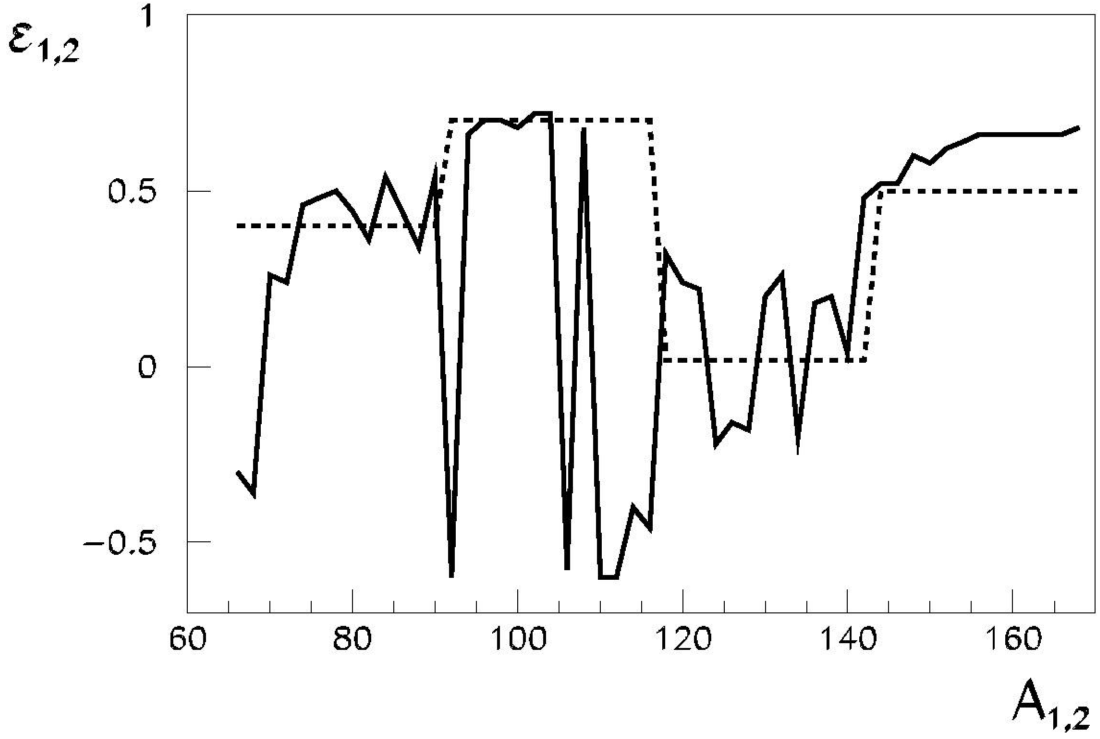
Heavy fragments Te E*=5 MeV

Light fragments Zr E*=12 MeV

Wide range in the mass distribution

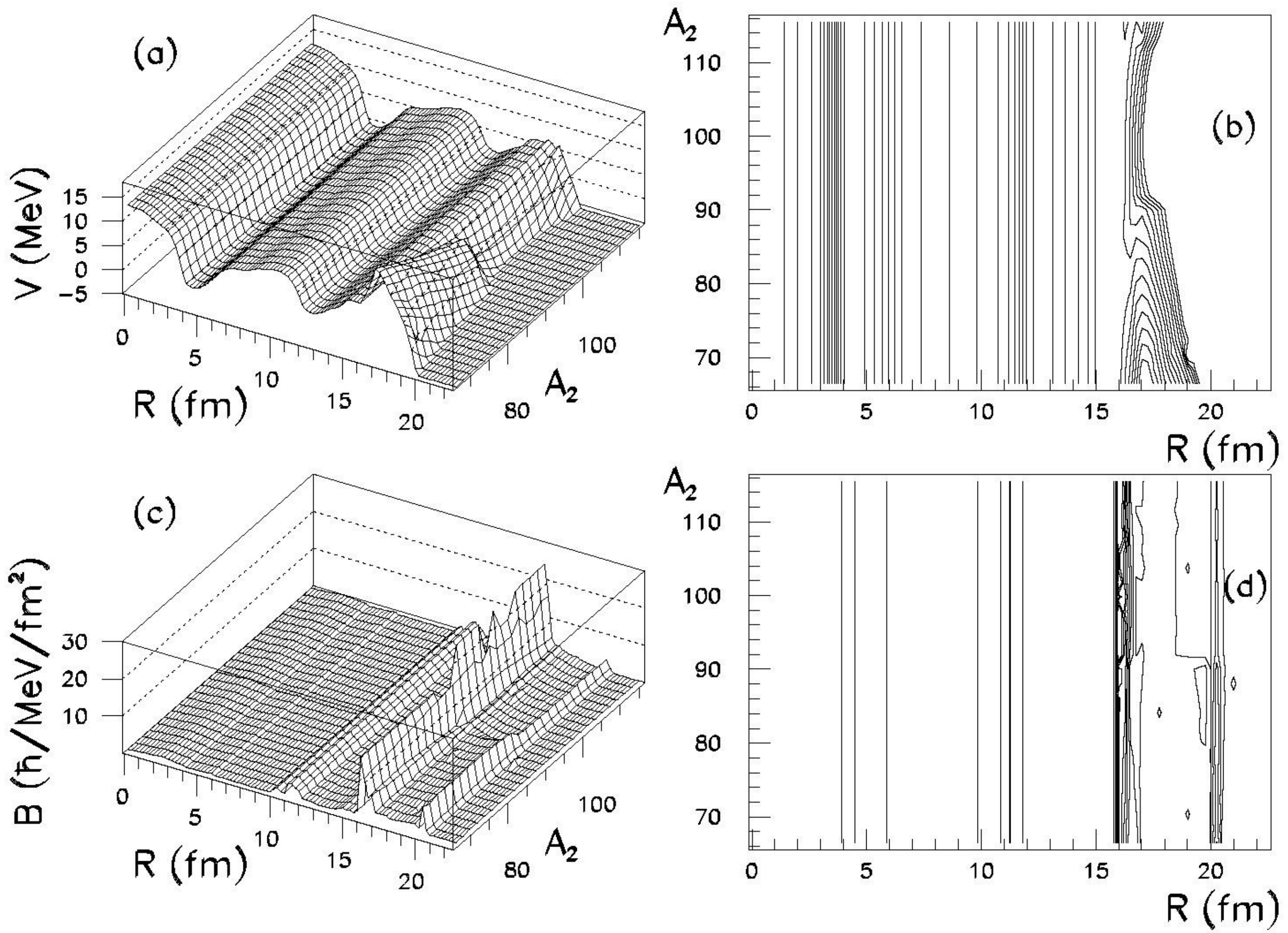
$^{66,68,70,72}Ni$, $^{74,76}Zn$, $^{78,80}Ge$, $^{82,84,86}Se$, $^{88,90,92}Kr$, $^{94,96}Sr$, $^{98,100,102}Zr$, $^{104,106,108}Mo$, $^{110,112}Ru$, $^{114,116,118,120}Pd$, $^{122,124}Cd$, $^{126,128,130}Sn$, $^{132,134,136}Te$, $^{138,140}Xe$, $^{142,144,146}Ba$, $^{148,150,152}Ce$, $^{154,156}Nd$, $^{158,160}Sm$, $^{162,164,166,168}Gd$

Ground state deformations of the fragments (eccentricities).

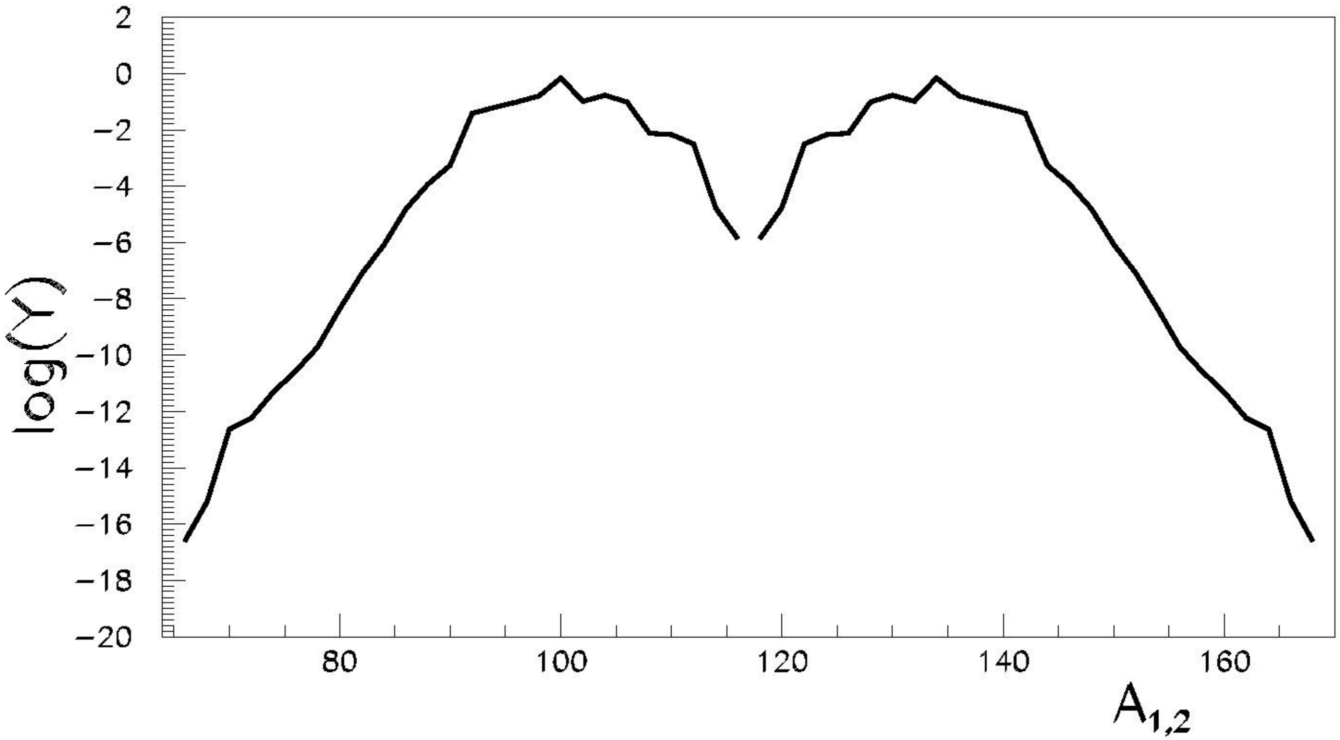


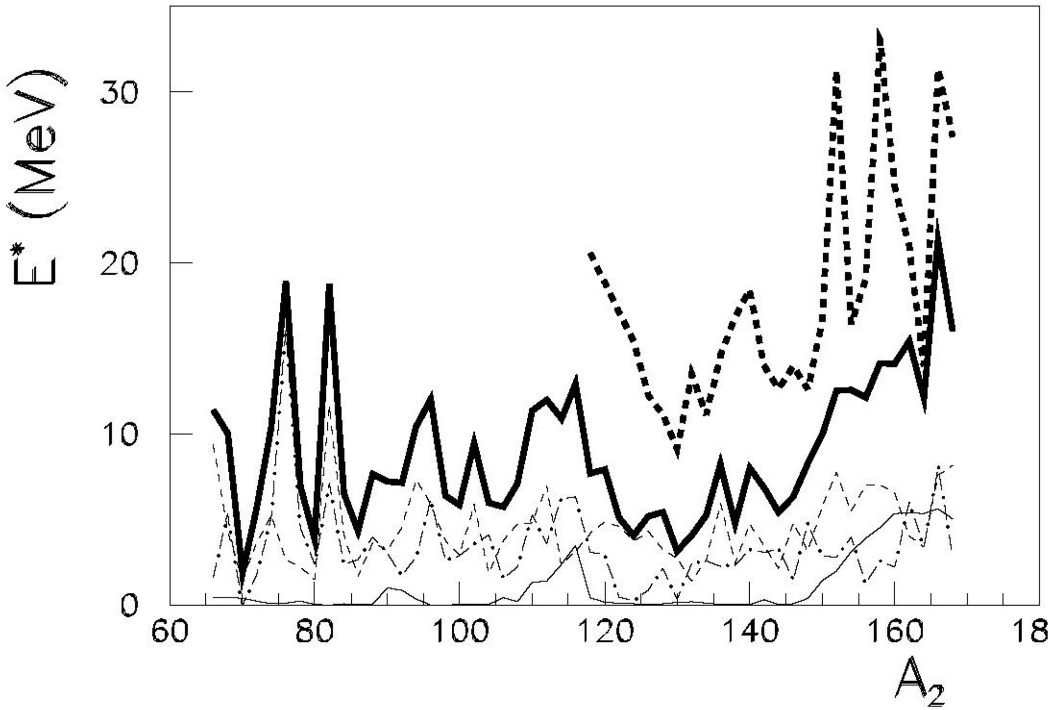
The difference between the energy of the emerging fragments and their ground state deformation energy is considered as a collective excitation. .

The potential energy and the semi-adiabatic cranking inertia as function of the light fragment mass



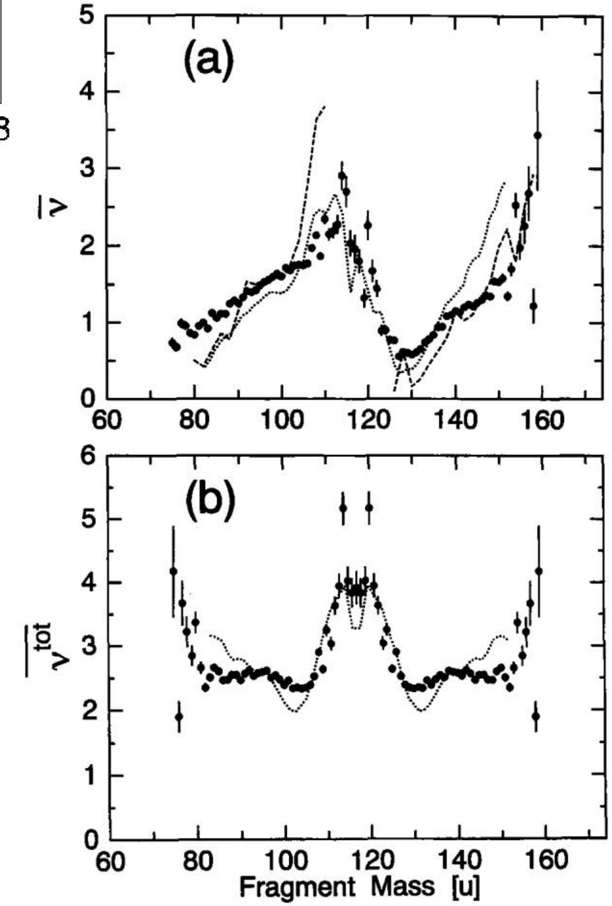
Normalized yield as function of the mass number





Dissipated energy, collective excitation, total excitation of the fragments as function of their mass numbers

K. Nishio and al., J. Sci. Tech. 35 (1998) 631



RESUME

It is a first microscopic description of the energy partition in a wide range of fission channels that succeed to reproduce the main behavior of the neutron multiplicities. Concluding, it is important to stress that the internal energy at scission is not a free energy which may be distributed in any way between the two fragments. The energy flow depends on the shapes at scission. The shapes at scission are directed by a dynamical trajectory. This trajectory depends on the internal structure of the system through the shell effects. Once the scission is obtained, the nucleons must be distributed onto the microscopic levels of the two fragments. The internal excitation is produced by this rearrangement of nucleons. But in the same time, the single particle energies distribution depends on the deformations of the fragments. Therefore, an subtle interplay exists in permanence between the intrinsic energy and the excitation energy due to deformations. A shift of the final deformations from the best configuration not only produces collective excitations, but also a variation of the dissipated energy.

THANK YOU