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Nuclear dynamics within the Energy Density Functional formalism

Applications to pairing vibrations and
nearly symmetric, heavy ions fusion

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Introduction

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Energy density functional formalism :

- *Approximate solution of the Time-dependent Schroedinger equation*
- *Microscopic approach*
- *Consistency between structure and dynamics*
- *Few parameters (Skyrme), large pannel of applications (structure, collective excitations, heavy ions collisions...)*

Outline :

- *Pairing in nuclear dynamics :
Pairing vibrations study within the TDHFB formalism*
- *Heavy ions collisions :
Fusion of nearly symmetric heavy ions (TDHF)*

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I. Pairing in nuclear dynamics

Pairing vibrations

(Time-Dependent Hartree-Fock-Bogolyubov formalism)

B. A., C. Simenel and Ph. Chomaz, nucl-th:0808.3507 (2008)

Introduction : pairing in nuclear physics

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- Structure :
 - Odd-even mass staggering
 - Inertia of deformed nuclei...

- Dynamics ? :
 - Superfluid effects on dynamics
 - Nuclear Josephson Effect in heavy ions collisions
 - Pair transfers on pairing collective states
 - « Pairing vibrations »

Introduction : Pairing vibrations

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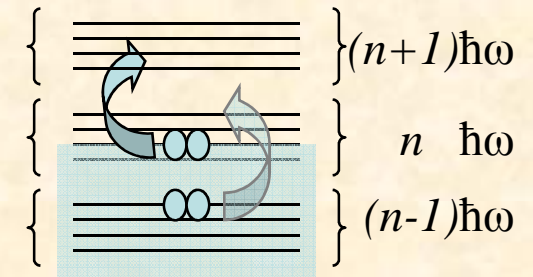
- **Pairing correlations** → « pairing vibrations » $L=0^+$

- Low energy modes

- « **Giant Pairing Vibrations (GPV)** »
(analogous to giant resonances)

- No experimental confirmation

- Probes : Pair transfer reactions



$$\hat{F} = \int (a_{r,\uparrow}^+ a_{r,\downarrow}^+ + a_{r,\downarrow} a_{r,\uparrow}) d^3 r$$

- Tool : **TDHFB formalism**^{nucl}

Bès and Broglia, Nucl Phys. 80, 289 (1966)

- **Results**

- Oxygen isotopes (comparison with QRPA) *Khan et al., PRC 69, 014314 (2004)*

- Calcium isotopes

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- Evolution of the generalized density matrix $\mathcal{R}(t)$

$$\mathcal{R}(t) = \begin{pmatrix} \rho(t) & \kappa(t) \\ -\kappa^*(t) & 1 - \rho^*(t) \end{pmatrix}$$

$$\rho_{ij}(t) = \langle a_j^+ a_i \rangle_{\psi(t)}$$

$$\kappa_{ij}(t) = \langle a_j a_i \rangle_{\psi(t)}$$

$$\kappa_{ij}^*(t) = \langle a_i^+ a_j^+ \rangle_{\psi(t)}$$

Ψ quasiparticle vacuum at each time t :

$$\beta_i(t) = \sum_j (U_{ji}(t)a_j^+ + V_{ji}(t)a_j)$$

$$\forall i, \quad \beta_i(t)|\psi(t)\rangle = 0$$

TDHFB formalism

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- Evolution of the generalized density matrix $\mathcal{R}(t)$

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$$\rho_{ij}(t) = \langle a_j^+ a_i \rangle_{\psi(t)}$$

$$\kappa_{ij}(t) = \langle a_j a_i \rangle_{\psi(t)}$$

$$\kappa_{ij}^*(t) = \langle a_i^+ a_j^+ \rangle_{\psi(t)}$$

- Energy functional $E[\mathcal{R}(t)]$
- Variational method on the action \rightarrow **TDHFB equations**

$$i\hbar \frac{\partial}{\partial t} \mathcal{R} = [\mathcal{H}, \mathcal{R}] \quad \mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \quad h_{ij} = \frac{\delta E}{\delta \rho_{ji}}, \quad \Delta_{ij} = \frac{\delta E}{\delta \kappa_{ij}^*}$$

\mathcal{H} Bogoliubov Hamiltonien

TDHFB formalism

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- Implementation of TDHFB assuming spherical symmetry
- Energy density functional $E[\mathcal{R}]$
 - ph channel : **Sly4 parameterization**
Chabanat et al., NPA 635, 231-256 (1998)
 - pp (hh) channel : **Local, density-dependent pairing
bulk+surface**

$$E_{pair}[\mathcal{R}] = \frac{V_0}{4} \int \left(1 - \frac{\rho(r)}{\rho_c} \right) \tilde{\rho}^*(r) \tilde{\rho}(r) d^3r \quad \tilde{\rho}(r) = \sum_{\sigma} -\sigma \kappa(r\sigma, r-\sigma)$$

Cut-off E_{qp} at 80 MeV, $\rho_c = 0.32 \text{ fm}^{-3}$, $V_0 = -275.25 \text{ MeV}$

TDHFB formalism

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- Spherical symmetry + energy defined only from local densities

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_{nlj}(r,t) \\ v_{nlj}(r,t) \end{pmatrix} = \begin{pmatrix} h_{lj}(r,t) & \tilde{h}(r,t) \\ \tilde{h}^*(r,t) & -h_{lj}^*(r,t) \end{pmatrix} \begin{pmatrix} u_{nlj}(r,t) \\ v_{nlj}(r,t) \end{pmatrix}$$

$$\tilde{h}(r\sigma, r'\sigma') = \frac{\delta E}{\delta \tilde{\rho}^*(r\sigma, r'\sigma')}$$

- Iterative solution :

$$\begin{pmatrix} u_{nlj}(t + \delta t) \\ v_{nlj}(t + \delta t) \end{pmatrix} = e^{\frac{i}{\hbar} \begin{pmatrix} h_{lj}(r, t + \frac{\delta t}{2}) & \tilde{h}(r, t + \frac{\delta t}{2}) \\ \tilde{h}^*(r, t + \frac{\delta t}{2}) & -h_{lj}^*(r, t + \frac{\delta t}{2}) \end{pmatrix} \delta t} \begin{pmatrix} u_{nlj}(t) \\ v_{nlj}(t) \end{pmatrix}$$

TDHFB formalism : Particle number

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- HFB states are NOT eigenstate of N
 - Fixed in average through a Lagrange constraint « $-\lambda N$ »

$$\begin{pmatrix} h_{lj}(r) - \lambda & \tilde{h}(r) \\ \tilde{h}^*(r) & -h_{lj}^*(r) + \lambda \end{pmatrix} \begin{pmatrix} u_{nlj}(r) \\ v_{nlj}(r) \end{pmatrix} = \begin{pmatrix} E_{nlj} & 0 \\ 0 & E_{nlj} \end{pmatrix} \begin{pmatrix} u_{nlj}(r) \\ v_{nlj}(r) \end{pmatrix}$$

- TDHFB : $\langle N \rangle(t) = \text{constant of motion}$

$$i\hbar \frac{\partial}{\partial t} \langle \hat{N} \rangle = \text{Tr}([h, \rho] + \kappa \Delta^* - \Delta \kappa^*) = 0$$

- What about λ ? If *stationnary evolution, dropping λ* :

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_{nlj}(r, t) \\ v_{nlj}(r, t) \end{pmatrix} = \begin{pmatrix} E_{nlj} + \lambda & 0 \\ 0 & E_{nlj} - \lambda \end{pmatrix} \begin{pmatrix} u_{nlj}(r, t) \\ v_{nlj}(r, t) \end{pmatrix}$$

TDHFB formalism : Phase evolution

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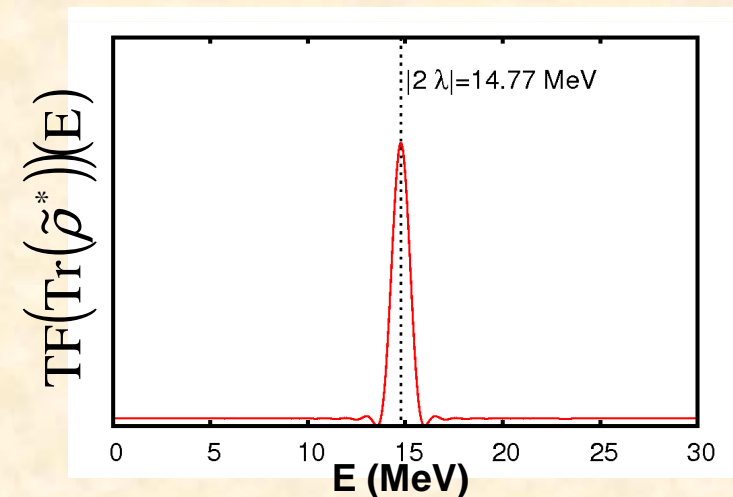
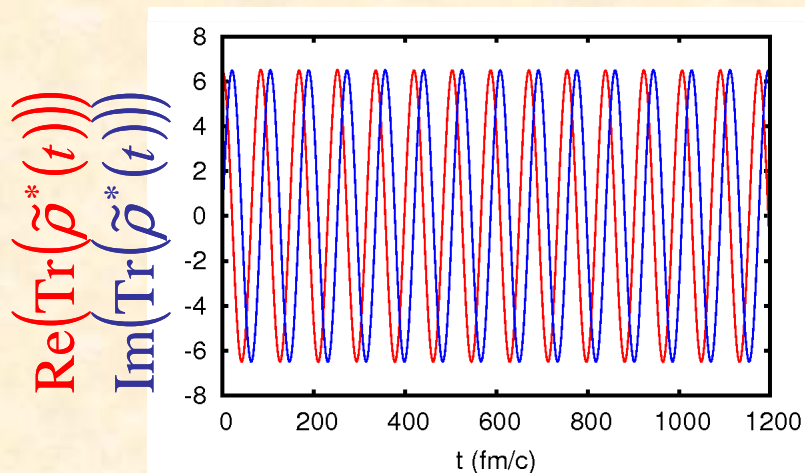
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→ Evolution of normal and anomalous densities

$$\rho(t) = \rho(0)$$

$$\tilde{\rho}^*(t) = \tilde{\rho}^*(0) \exp\left(\frac{2i\lambda t}{\hbar}\right)$$



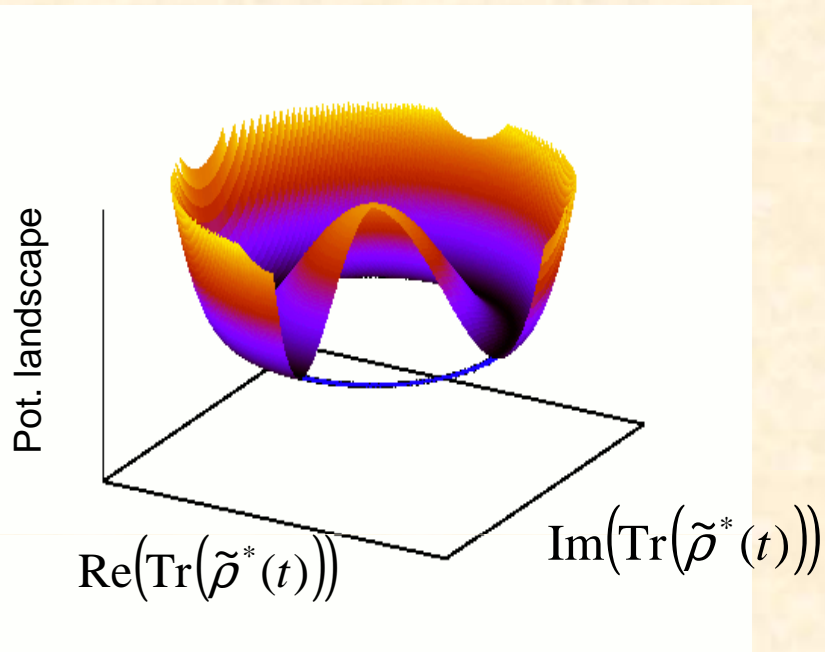
Example : ^{18}O ($|2\lambda| = 14.77$ MeV)

TDHFB formalism : Nambu-Goldstone mode

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$$\tilde{\rho}^*(t) = \tilde{\rho}^*(0) \exp\left(\frac{2i\lambda t}{\hbar}\right)$$

Nambu-Goldstone mode

→ Evolution the initial Lagrange constraint

$$i\hbar \frac{\partial}{\partial t} \mathcal{R} = [\mathcal{H}, \mathcal{R}] \quad \mathcal{H} = \begin{pmatrix} \mathbf{h} - \lambda & \Delta \\ -\Delta^* & -\mathbf{h}^* + \lambda \end{pmatrix}$$

TDHFB formalism : Linear response

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- **Perturbation at t=0**

$$i\hbar \frac{\partial}{\partial t} \mathcal{R} = [\mathcal{H}', \mathcal{R}] \quad \hat{H}' = \hat{H} + \varepsilon \delta(t) \hat{F}$$

$$\hat{F} = \int_{nucl} (a_{r,\uparrow}^+ a_{r,\downarrow}^+ + a_{r,\downarrow} a_{r,\uparrow}) d^3r$$

- **Fourier transform of** $\langle \hat{F} \rangle(t) = \int_{nucl} \text{Re}(\tilde{\rho}(r,t)) d^3r$

« Strength » function
$$S(E) = \sum_{\nu} |\langle 0 | \hat{F} | \nu \rangle|^2 \delta(E - E_{\nu})$$

Excitations in the next $A \pm 2$ nuclei
(with ground-state energies $\approx E_A \pm 2\lambda$)

Linear response : TDHFB \leftrightarrow QRPA

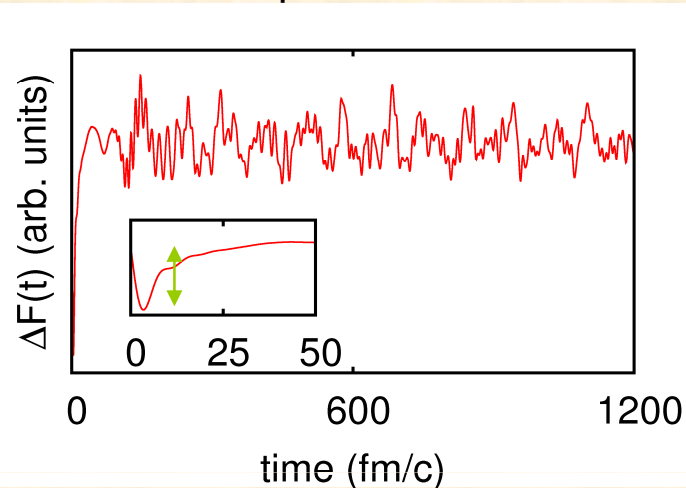
Example : the ^{18}O case

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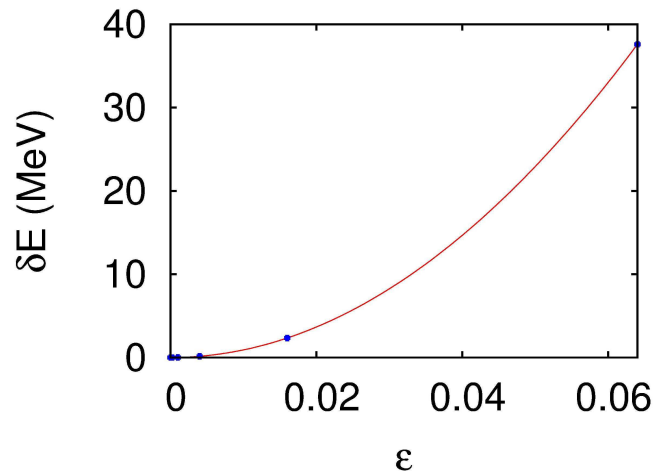
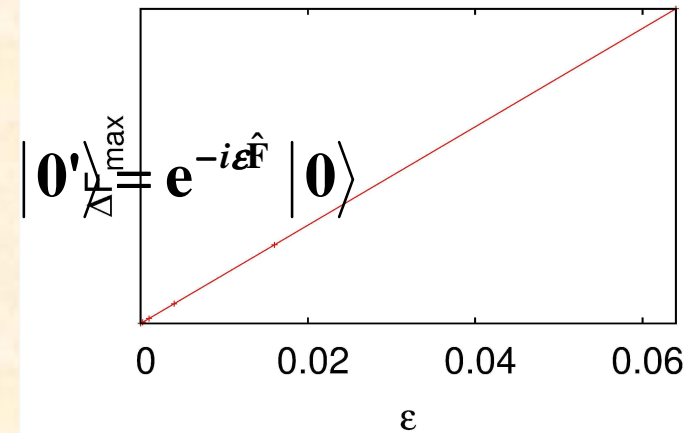


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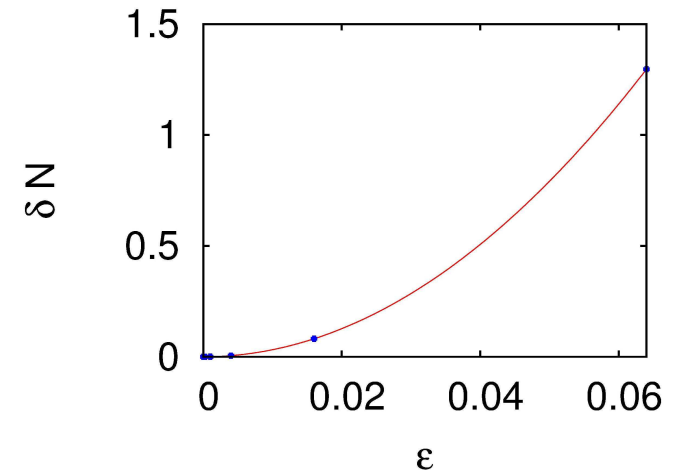
Small amplitude excitation



Width of the 1st oscillation



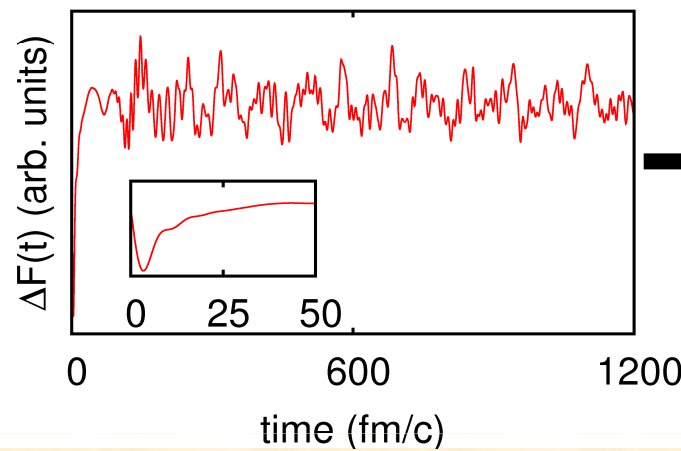
t=0



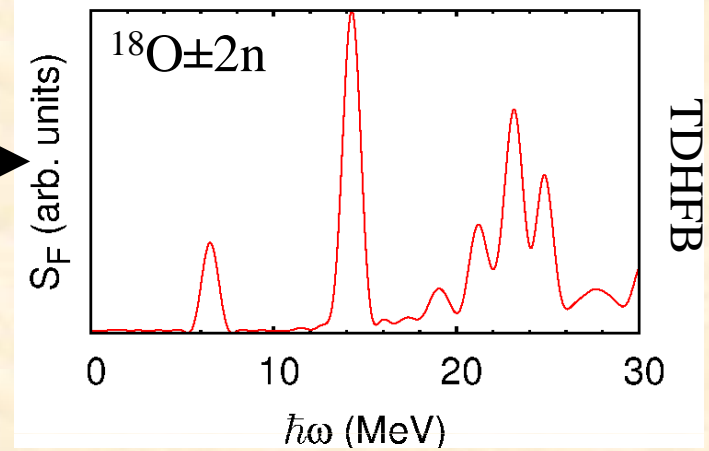
second order effects (> QRPA)

Example : the ^{18}O case

Small amplitude excitation



« Strength » function

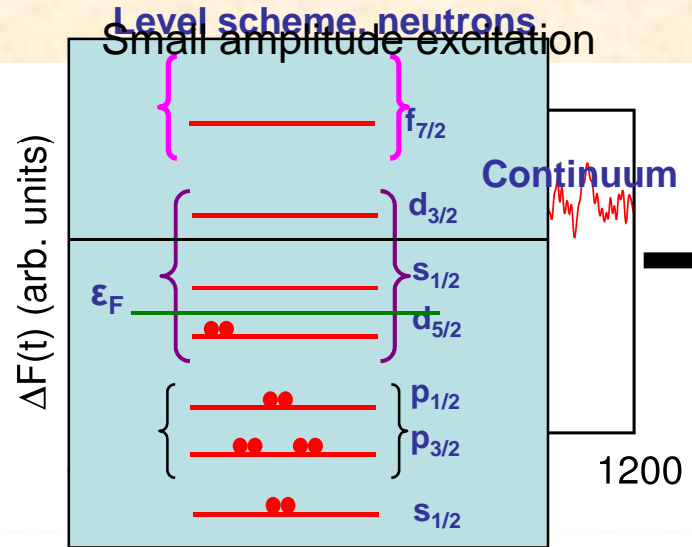


Example : the ^{18}O case

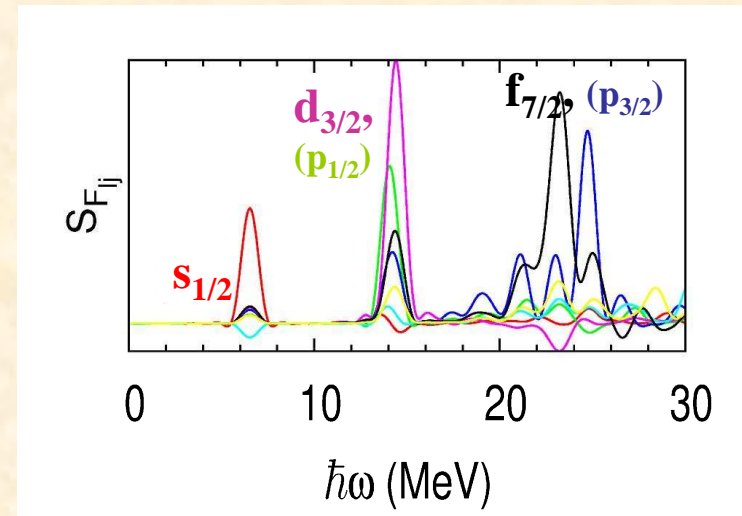
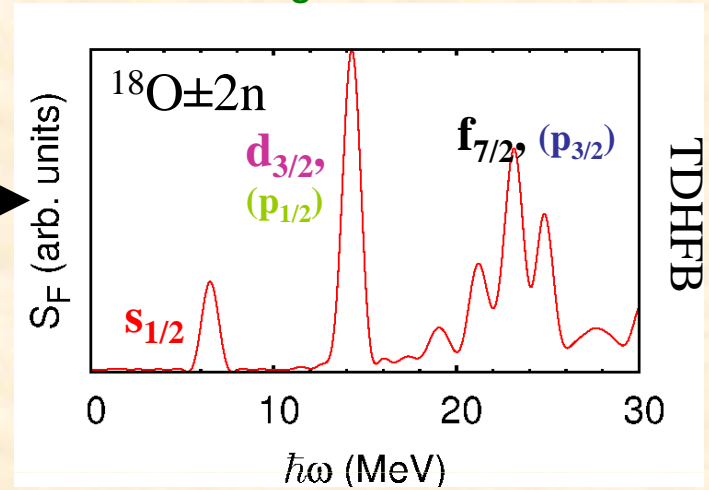
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« Strength » function

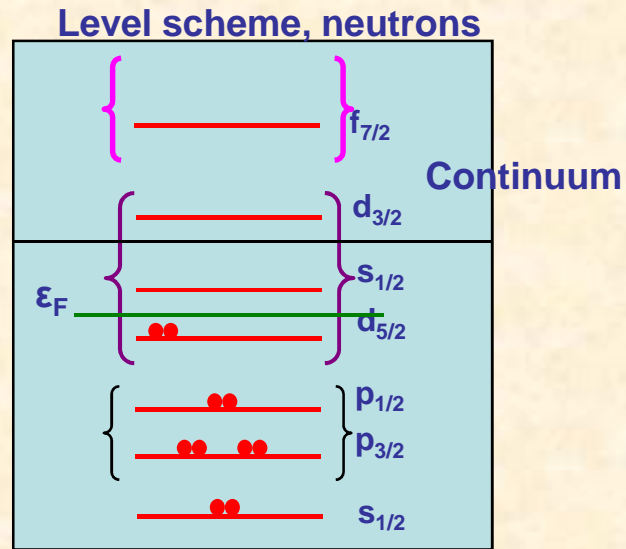


Example : the ^{18}O case

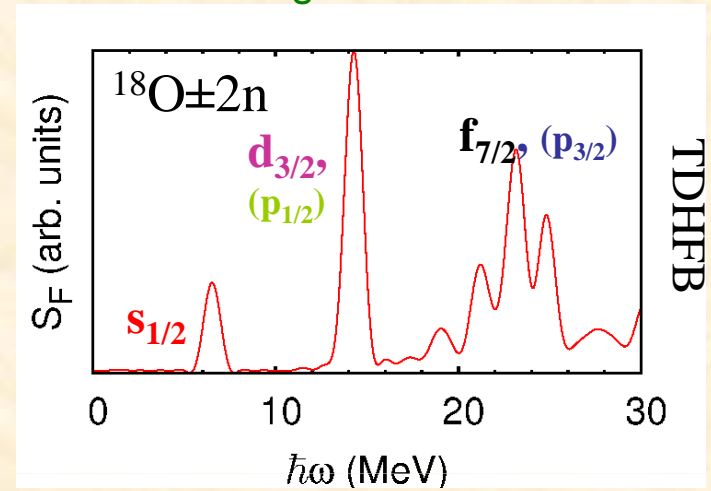
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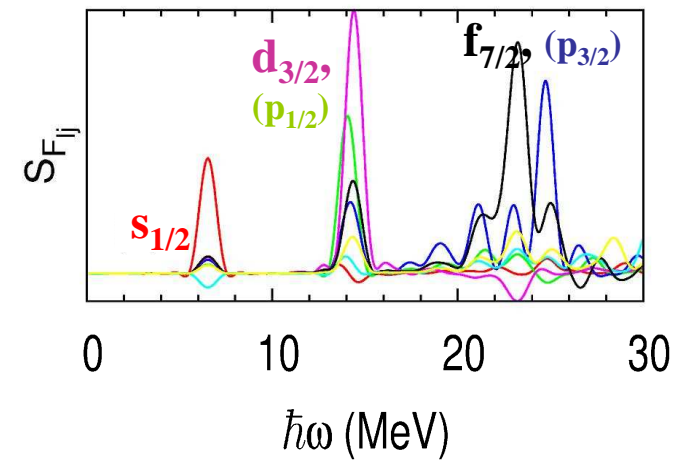


« Strength » function



Good agreement with QRPA

-Possible differences :
 \neq Pairing functional
 \neq implementation

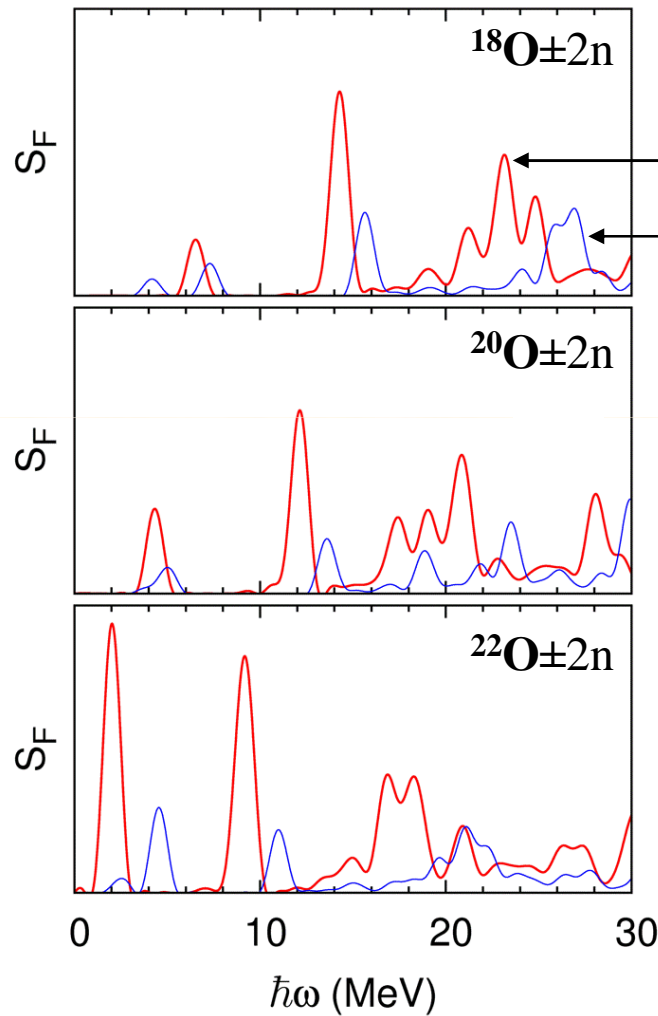


Results : Oxygen isotopes

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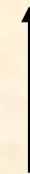
TDHFB response

HFB response (unperturbed spectrum)

Unperturbed spectrum :

$$S^{unpert}(E) = \sum_{\nu} \left| \langle 0 | \hat{F} | \mu\nu \rangle \right|^2 \delta(E - e_{\nu} - e_{\mu})$$

$$|\mu\nu\rangle = \beta_{\nu}^{+} \beta_{\mu}^{+} |\psi\rangle$$



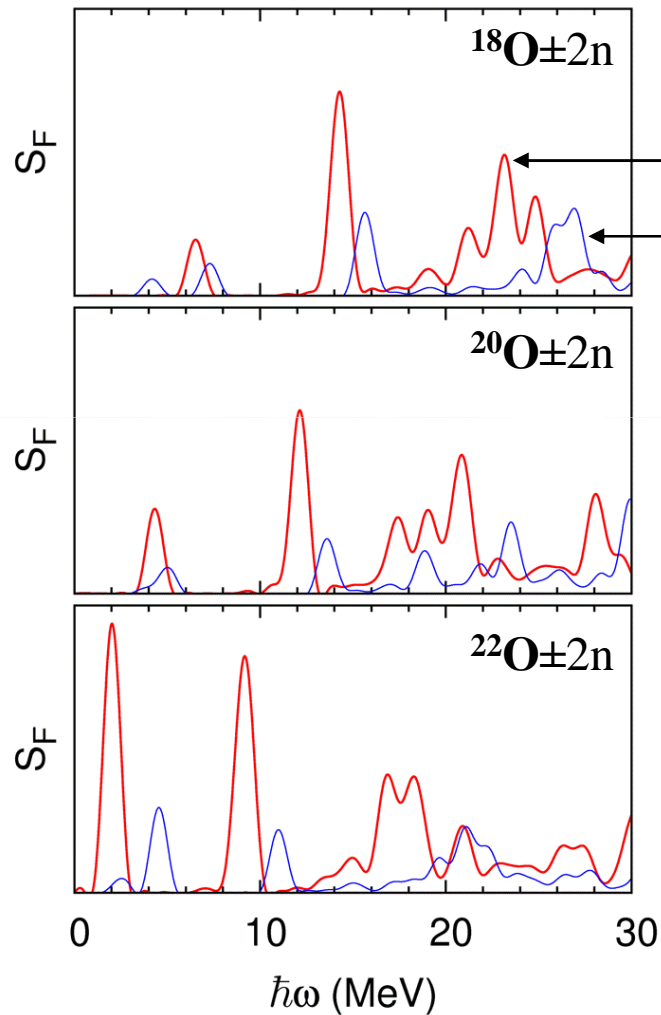
2qp excitations
(from the static ground state solution)

Results : Oxygen isotopes

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TDHFB response

HFB response (unperturbed spectrum)

- « residual interaction » effect

- $S_F(\hbar\omega)$ increases
dynamical pairing

- **collectivity**

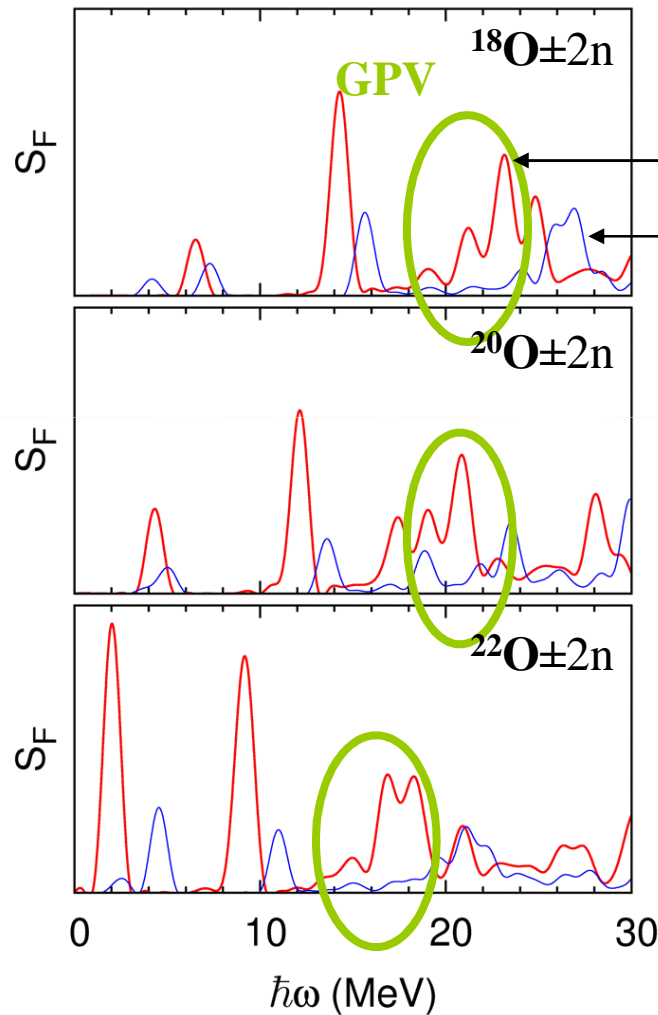
- Shift towards low energy
(attractive character of the pairing)

Results : Oxygen isotopes

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TDHF response

HFB response (unperturbed spectrum)

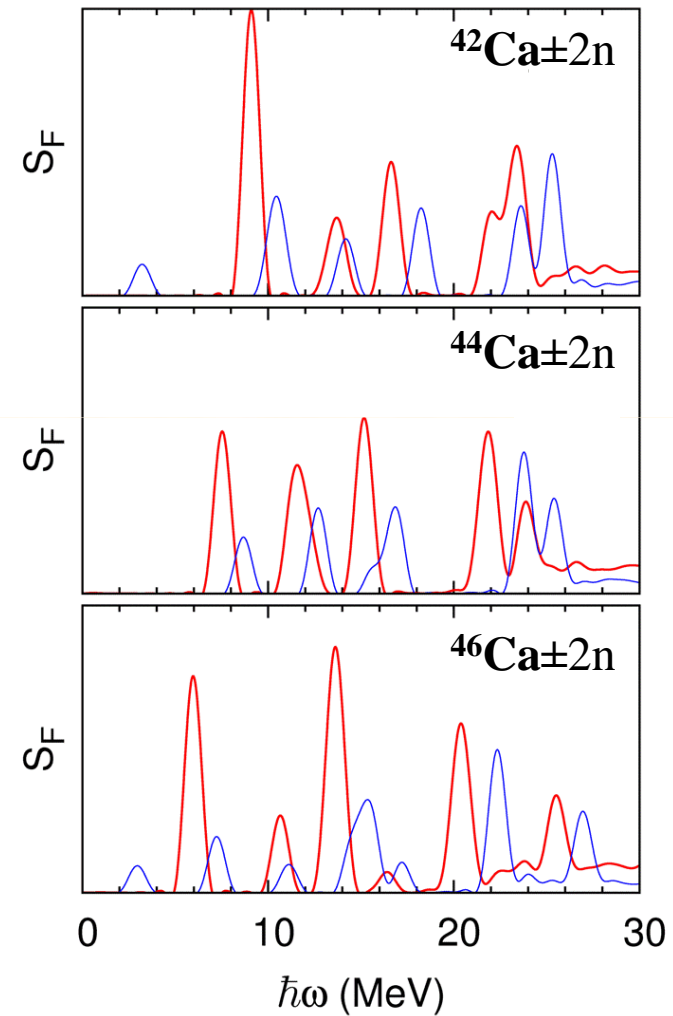
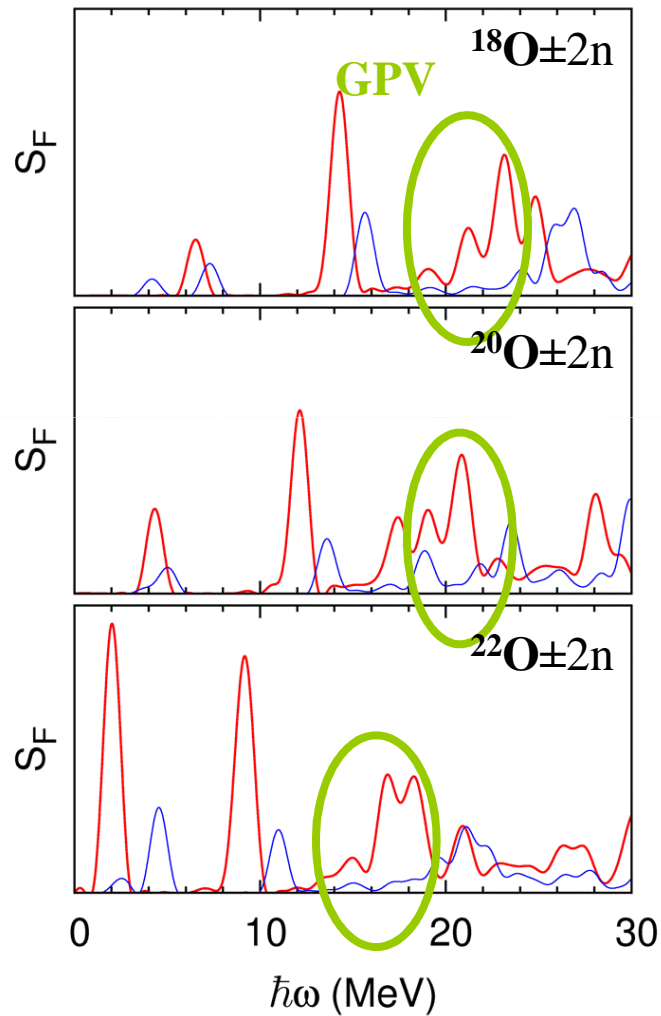
- « residual interaction » effect
 - $S_F(\hbar\omega)$ increases dynamical pairing
→ collectivity
 - Shift towards low energy (attractive character of the pairing)
- GPV +2n mainly $f_{7/2}$

Results : Oxygen and Calcium isotopes

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Conclusions : Pairing and Nuclear dynamics

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- Effect of the dynamical pairing correlations on pairing vibrations
Applications on Oxygen and Calcium isotopes
- Good comparison with QRPA (Oxygen isotopes)
- Presence of the GPV confirmed in Oxygen isotopes
- Not seen in Calcium isotopes

Outlook

- Heavier nuclei (Sn, Pb)
- Treatment of the continuum
- Application of TDHFB to nuclear reactions

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II. Heavy ions collisions

Fusion of heavy, nearly symmetric systems

(Time-Dependent Hartree-Fock formalism)

Time-Dependent Hartree-Fock formalism

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TDHF equations : evolution of the 1-body density

$$\rho_{ij} = \langle a_j^+ a_i \rangle_\Psi$$

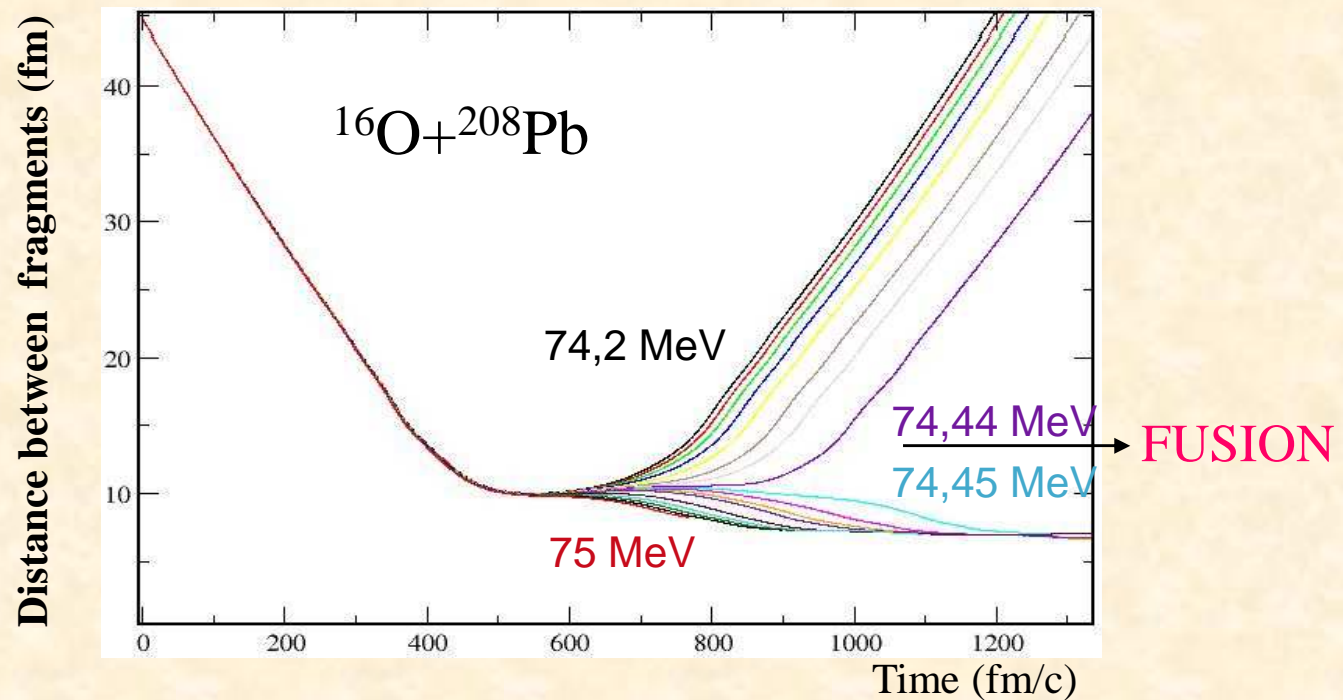
Ψ Slater determinant

$$i\hbar \frac{\partial}{\partial t} \rho = [h, \rho]$$

$$h = \frac{\delta E}{\delta \rho}$$

$E[\rho] : \text{Sly4d}$

Extracting fusion barriers from TDHF



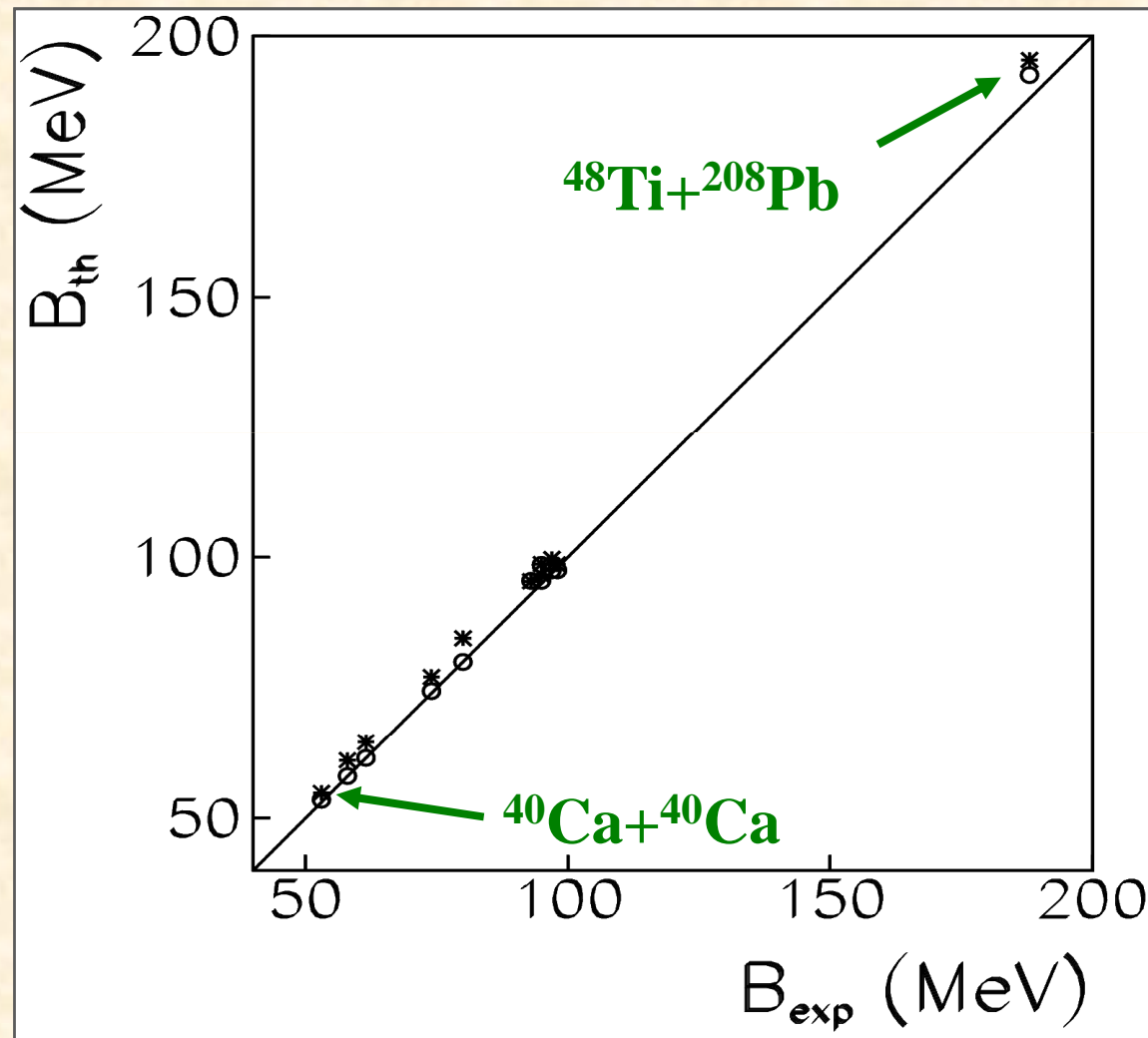
TDHF formalism : Comparison with experiments

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TDHF3D code : P. Bonche (Kim,Otsuka & Bonche, JPG 23, 1267 (1997))



C. Simenel and B.A., Int. J. Mod. Phys. E 17, 31 (2008)

Macroscopic vision of fusion

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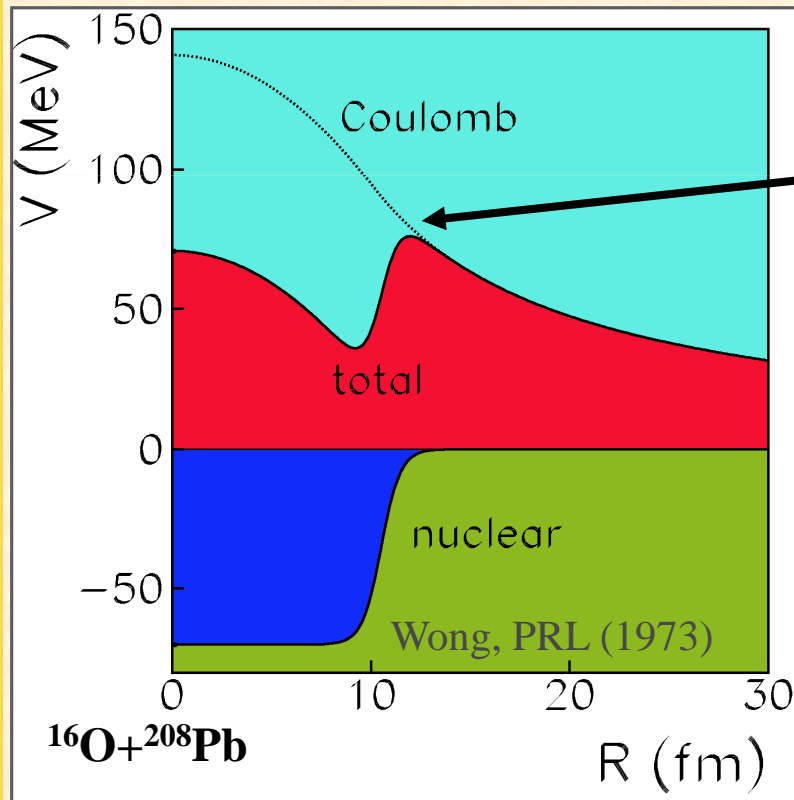
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« frozen » nuclear densities

$$V = V_{nucl} + V_{Coul}$$

Nucleus-nucleus potential



Fusion barrier V_b
(r_b, V_b)

Ex. : Bass, PRL 39 (1977)
Blocki, Ann. Phys. 105 (1982)

...

Towards symmetric systems

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Symmetric and heavy collision partners ($Z_1 Z_2 > 1600$):

→ Hindrance of fusion

Kinetic energy between fragments → Internal degrees of freedom

Compared to « frozen » models, the system needs an additional energy, an « extra push », to accomplish fusion

Models :

- *Extra-push, W.J. Swiatecki, Phys. Scr. 24, 113 (1981); NPA 376, 275 (1982)*
- *Dinuclear system, G.G. Adamian et al, NPA 618 (1997)*
- *Surface-Friction model, P. Fröbrich, Phys. Rep. 116, 337 (1984)*
- *Langevin based models...*

- *TDHF ?*

$^{90}\text{Zr} + ^{124}\text{Sn}$: trajectories

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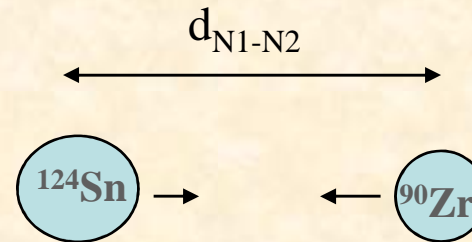


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TDHF results :

$^{124}\text{Sn} + ^{90}\text{Zr}$

head-on collision



« Frozen »

$B_{\text{HF}} = 218 \text{ MeV}$

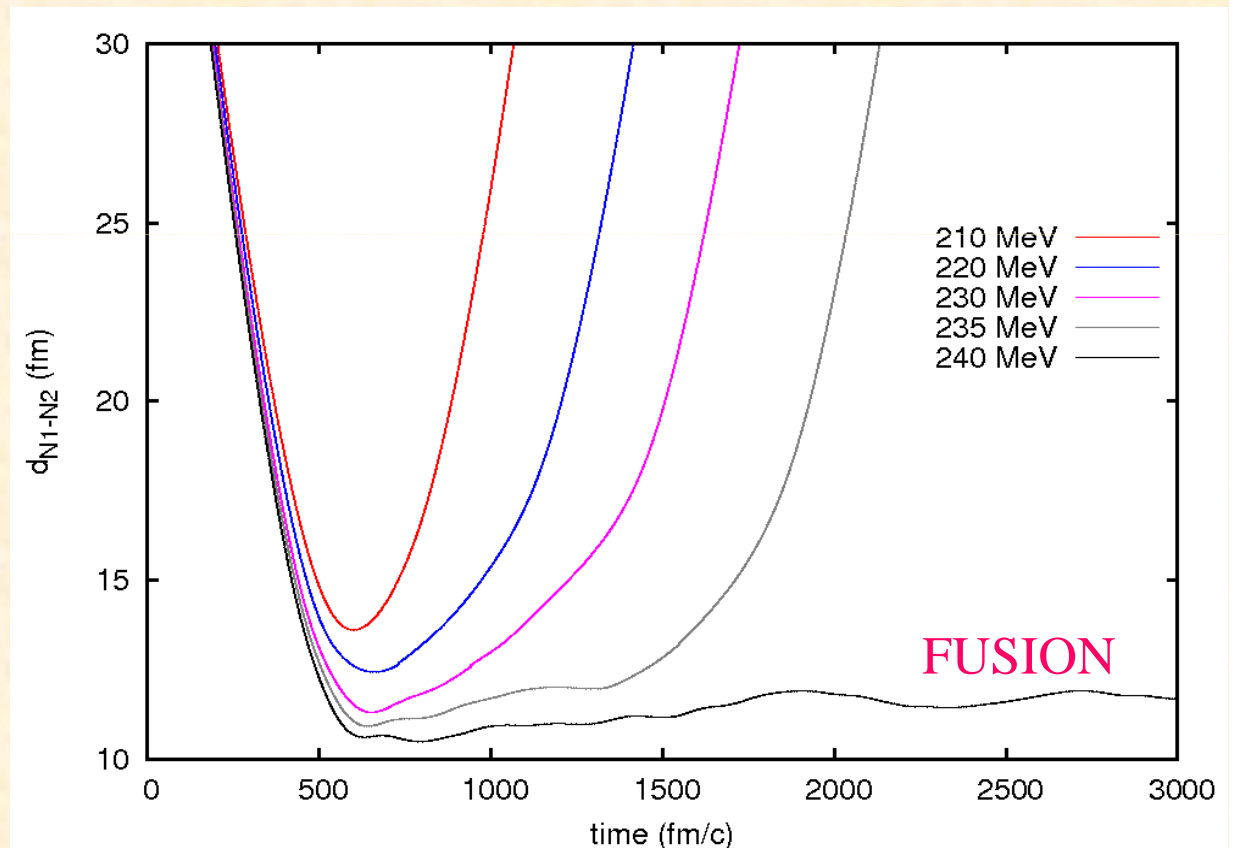
$B_{\text{Bass}} = 216 \text{ MeV}$

« Extra-push »

$B_{\text{Swiatecki}} = 230 \text{ MeV}$

Experiment

$B_{\text{exp}} = 237 \text{ MeV}$



$^{90}\text{Zr} + ^{124}\text{Sn}$: Evolution of the 1-body density

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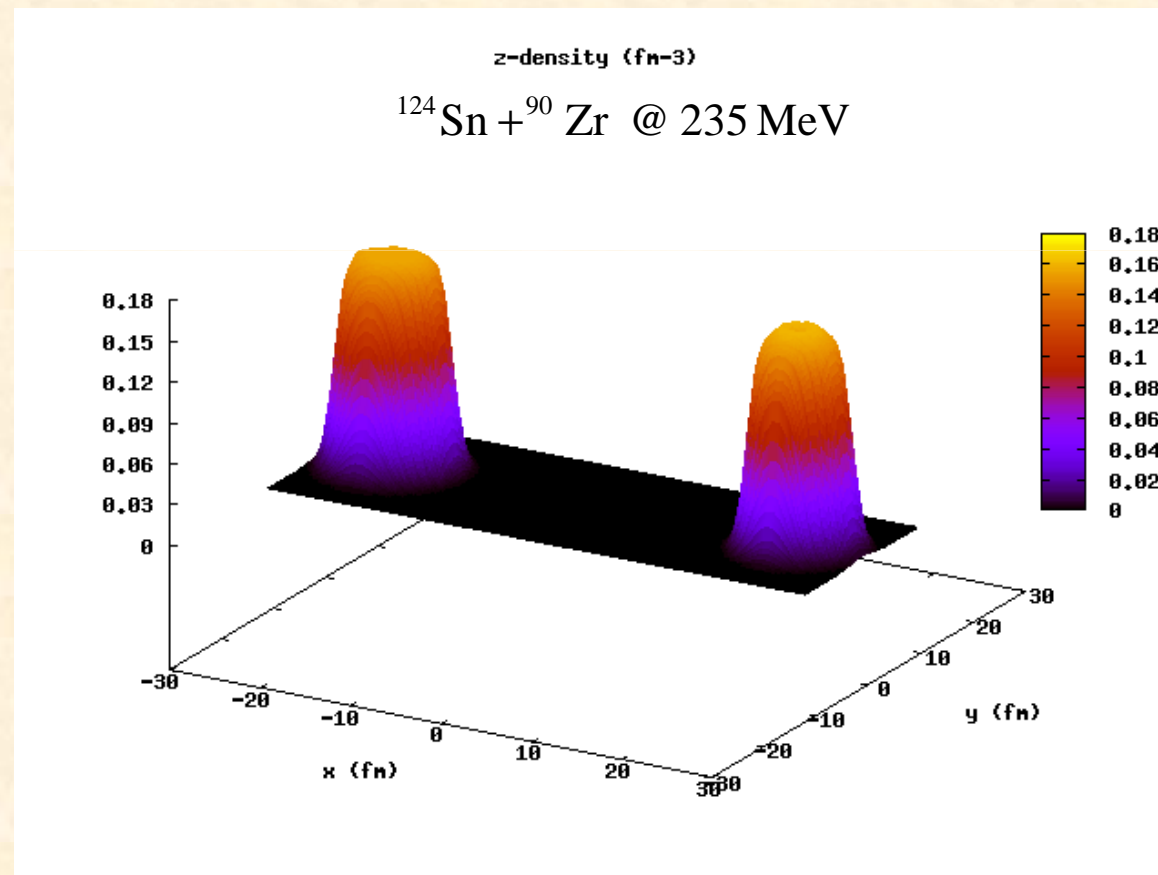
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TDHF results :

$^{124}\text{Sn} + ^{90}\text{Zr}$

@ 235 MeV center of mass, head-on collision

density in the reaction plane



$^{90}\text{Zr} + ^{124}\text{Sn}$: Evolution of the 1-body density

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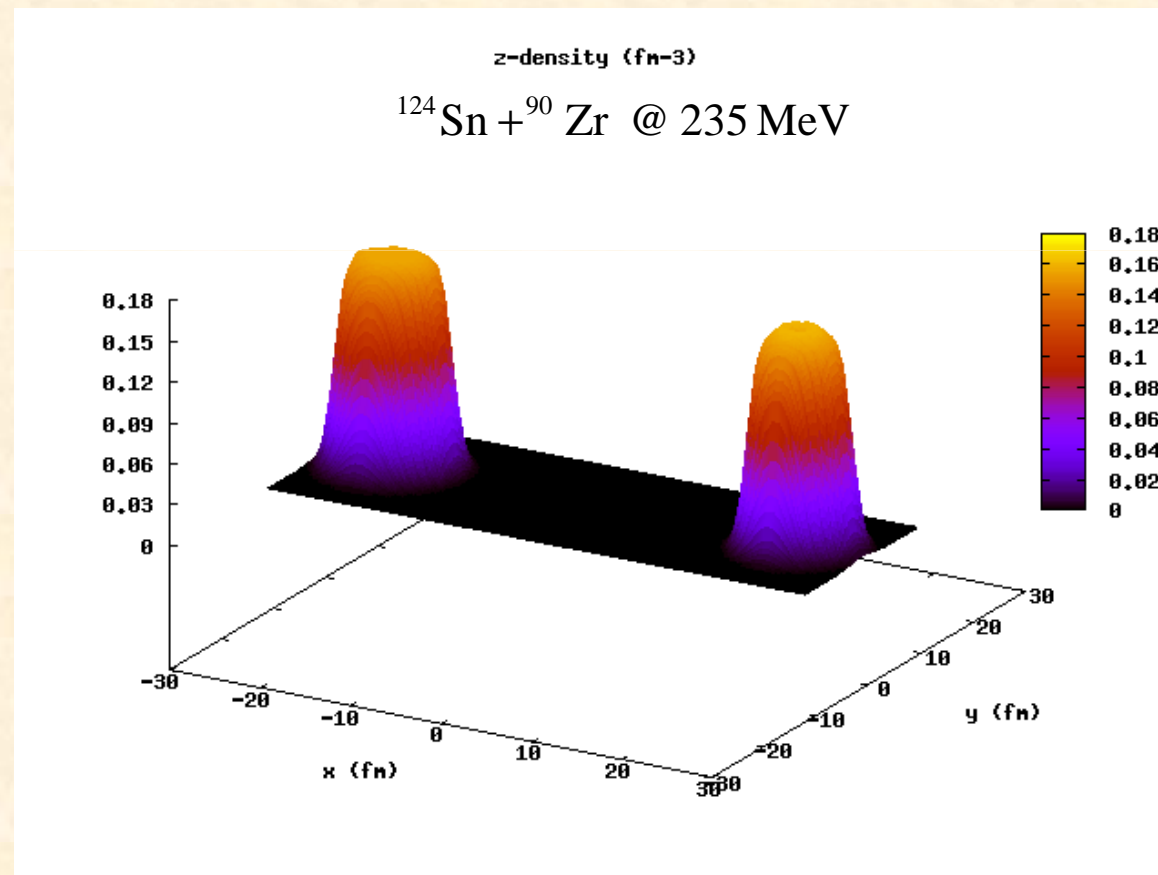
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TDHF results :

$^{124}\text{Sn} + ^{90}\text{Zr}$

@ 235 MeV center of mass, head-on collision

density in the reaction plane



$^{90}\text{Zr} + ^{124}\text{Sn}$: Density in the neck

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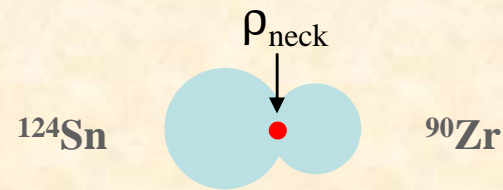
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TDHF results :

$^{90}\text{Zr} + ^{124}\text{Sn}$

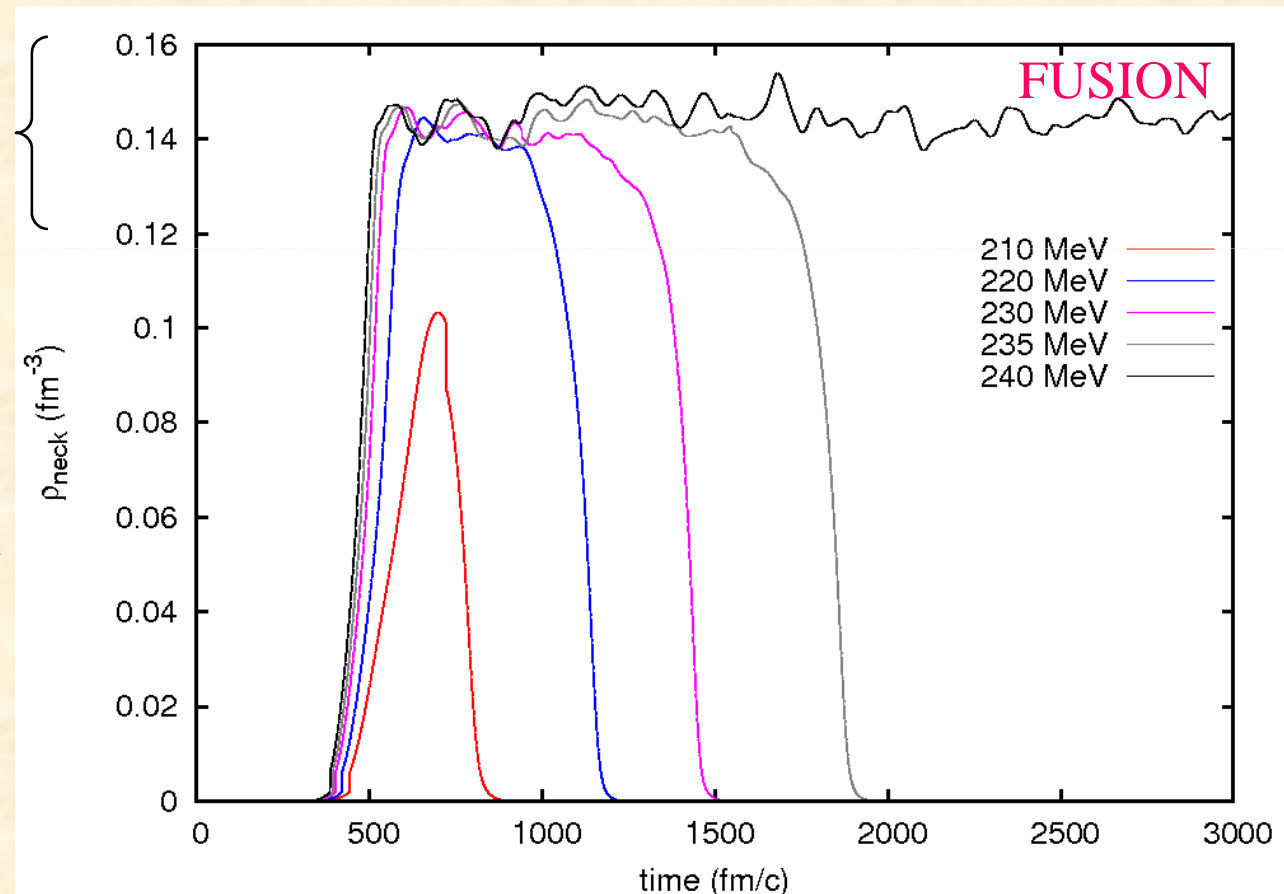
head-on collision



Strong and long overlap



Rearrangment of the
Internal degrees of
freedom
(isospin, surface,
etc...)



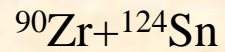
$^{90}\text{Zr} + ^{124}\text{Sn}$: Interaction time

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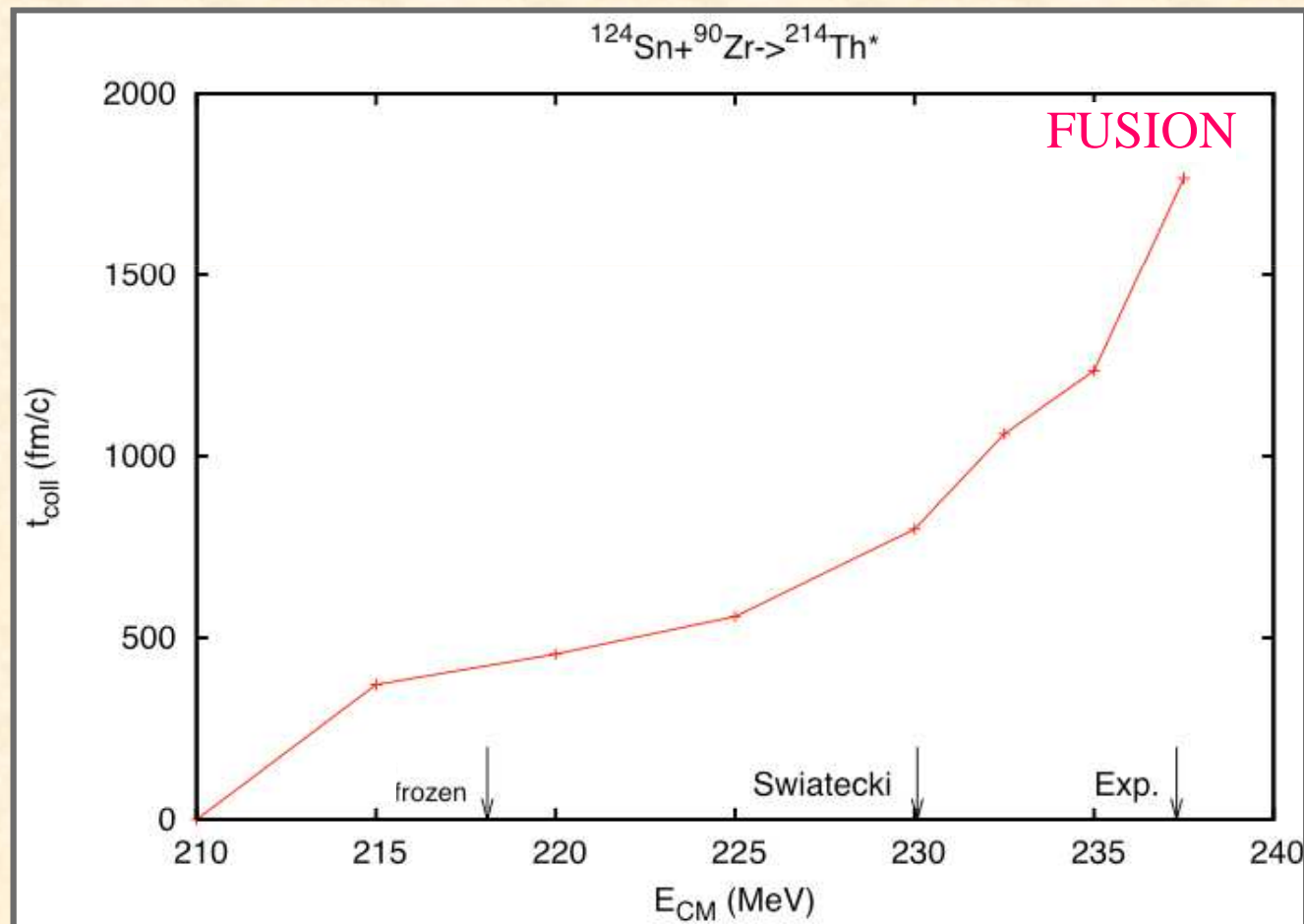
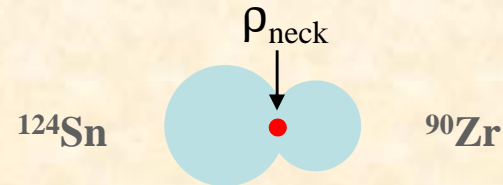
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TDHF results :



head-on collision



Conclusions : Heavy ions collisions

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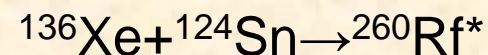
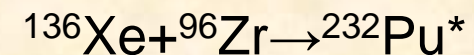


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- Reproduces well fusion barriers
(« extra-push » energy for free)
- Provides us a lot of informations through the 1-body density
(interaction time, isospin, masses, shape, etc...)

Outlook

- Study of the reaction mechanism
- Repeat these studies on experimental systems



E533 @ GANIL

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Acknowledgements and references

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Initial conditions for the TDHFB code :

K. Bennaceur, J. Dobaczewski, Comp. Phys. Com. 168, 96 (2005)

Pairing vibrations

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D.R. Bès and R.A. Broglia, Nucl. Phys. 80, 289 (1966)

E. Khan, N. Sandulescu, N. Van Giai, and M. Grasso, PRC 69, 014314 (2004)

3D TDHF (TDHF3D code, P. Bonche)

K.-H. Kim, T. Otsuka and P. Bonche, JPG 23, 1267 (1997)