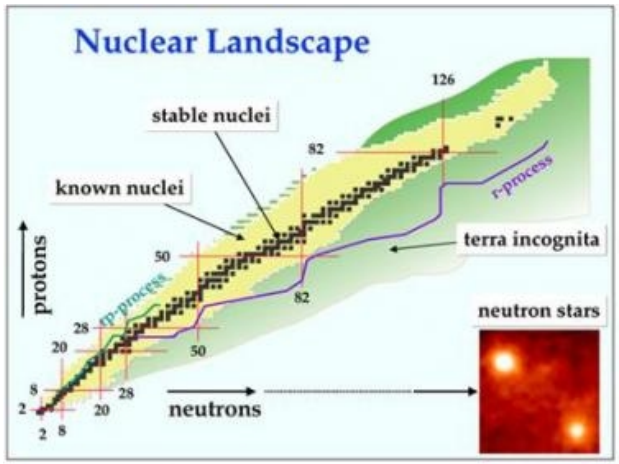
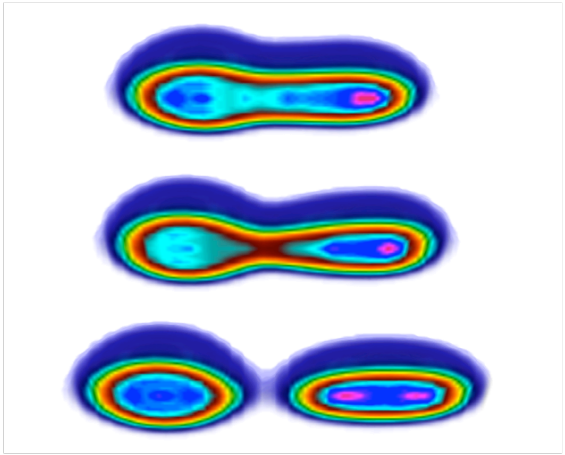
UNIVERSITY *of* WASHINGTON

General Exam
Density functional theory in nuclear many-body problems





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University of Washington
7/11/2017

Outline

- Introduction
- Density functional theory (DFT)
- Nuclear energy density functional
- Nuclear fission: overview
- Time-dependent density functional theory (TDDFT)
- Induced fission of ^{240}Pu with TDDFT.
- Summary and outlook

Introduction

The nucleus, consisting protons and neutrons, is a complex many-body system.

It has the following general properties:

- The nucleus is a saturating system, with a constant interior density of nucleons $n_0 \approx 0.16\ \mathrm{fm}^{-3}$ and it is hard to compress.
- The nucleus can be described approximately as a sphere with a well-defined surface with radius $R \approx r_0 A^{1/3}, \quad r_0 = 1.2\ \mathrm{fm}$, where A is the total number of nucleons.
- Nucleons (neutrons and protons) are held together by the short-range two-body and three-body nuclear force, while the Coulomb repulsion is also present between protons.

Liquid drop model

Initially, the nucleus was described within the liquid drop model (LDM).

- The mass of an atomic nucleus (N,Z) is given by (c=1)

$$m = Zm_p + Nm_n - E_B$$

where m_p and m_n are the rest mass of a proton and neutron and E_B is the **binding energy** of the nucleus.

- Bethe-Weizsäcker formula for the binding energy :

$$E_B(N,Z) = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \delta(A)$$

Bethe-Weizsäcker formula

- Volume term: since the nucleus is a saturating system, this energy is proportional to *A*

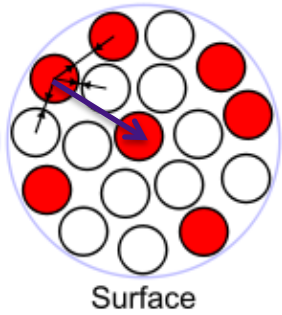
$$E_B(N,Z) = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \delta(A)$$

$$a_V = 15.68, a_S = 18.56, a_C = 0.717, a_A = 28.1 \quad [\text{MeV}]$$

$$\delta(A) = \begin{cases} 12A^{-1/2} & \text{even-even nuclei,} \\ 0 & \text{odd nuclei,} \\ -12A^{-1/2} & \text{odd-odd nuclei.} \end{cases}$$

- Surface term: The nucleons on the surface feel the attractive net force towards inside. One can relate this to the surface tension of the liquid drop.

$$a_S A^{2/3} = \sigma S, \quad \sigma = \frac{a_S}{4\pi r_0^2}$$



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- Coulomb term: it accounts the Coulomb repulsion of the protons.
- Assuming a uniformly distributed charged sphere, this energy is proportional to Z^2 and inversely proportional to the radius R ($\sim A^{1/3}$)

$$E_B(N,Z) = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \delta(A)$$

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$$\delta(A) = \begin{cases} 12A^{-1/2} & \text{even-even nuclei,} \\ 0 & \text{odd nuclei,} \\ -12A^{-1/2} & \text{odd-odd nuclei.} \end{cases}$$

- Symmetry term: results from the isospin dependent term in nuclear force and the Pauli principle (in the kinetic energy).

$$V_\tau \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$

$$E_B(N,Z) = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \delta(A)$$

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- Pairing term: the "*pairing effect*" and even-odd staggering of the binding energy will be discussed later

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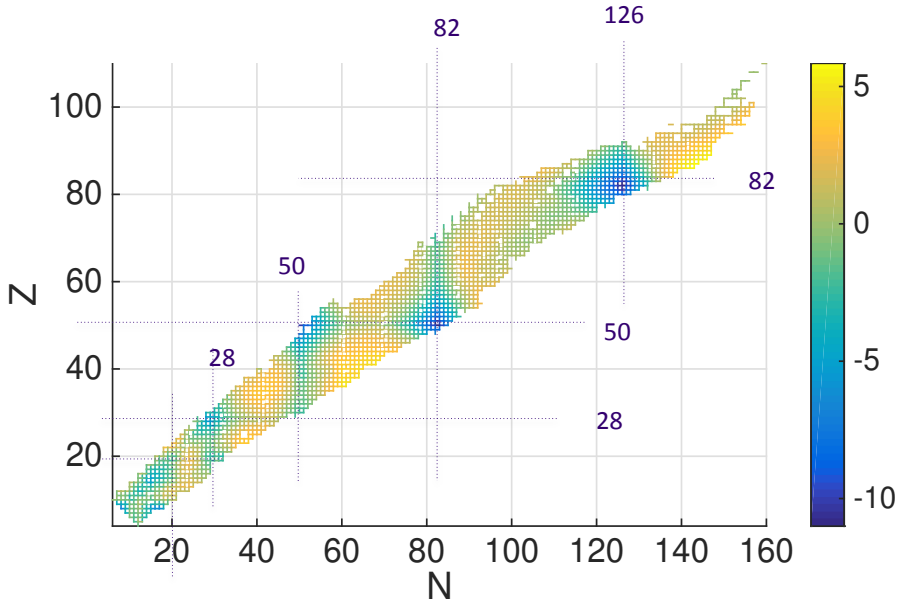
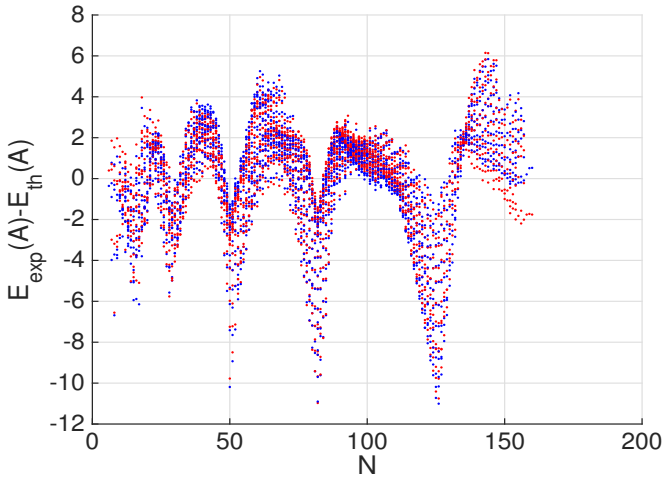
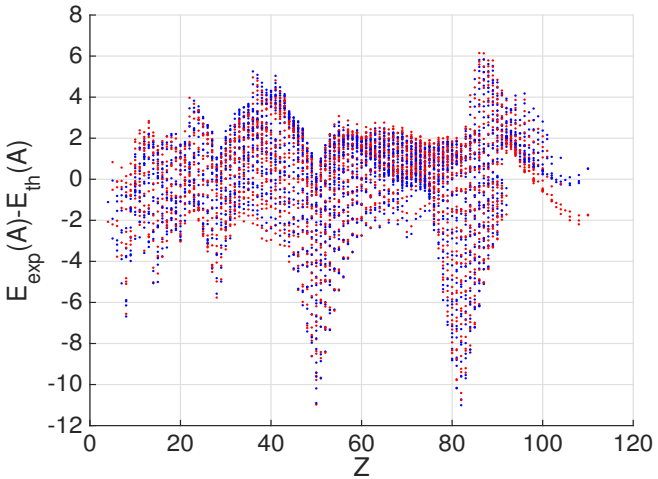
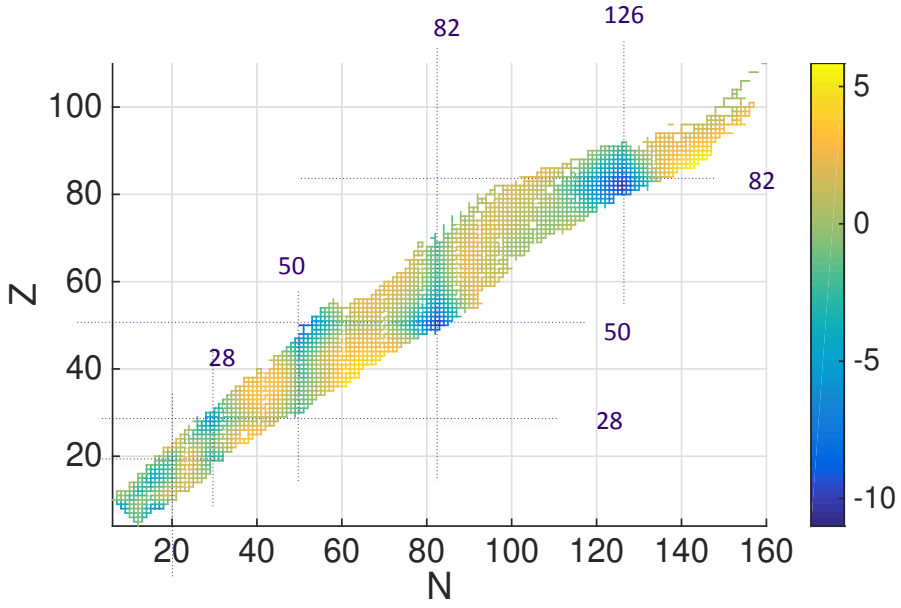


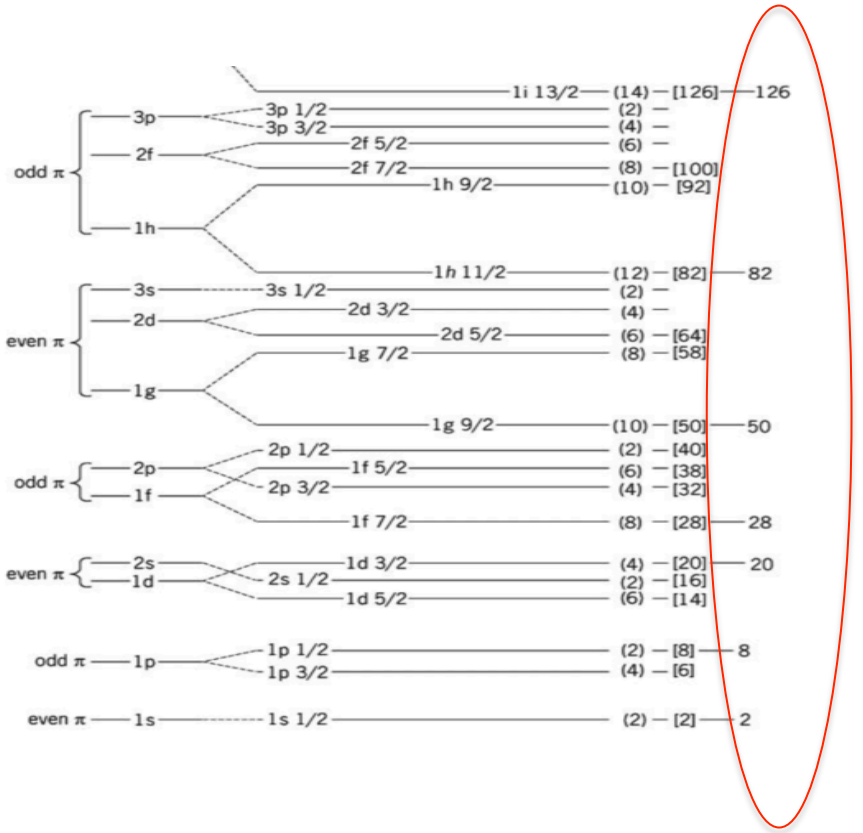
$E_{th}(N,Z) - E_{exp}(N,Z)$ (MeV)

rms : ~ 3 MeV









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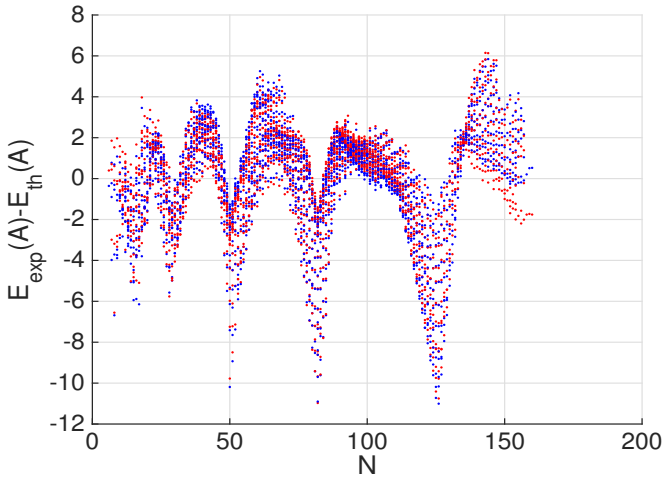

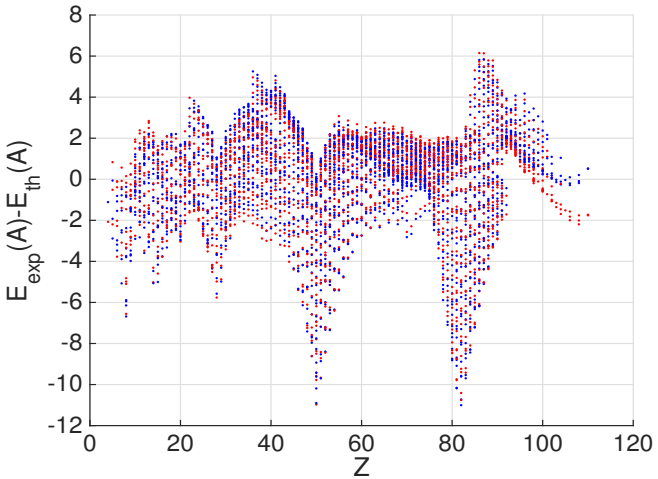

Microscopically a nucleus is described by the (static) many-body Schrödinger equation:

$$H\Psi(1,\cdots,A) = E\Psi(1,\cdots,A),$$

$$H = \overbrace{\sum_{i}^{A} -\frac{\hbar^2}{2m}\Delta_i}^{\hat{T}} + \overbrace{\sum_{i<j}^{A}\hat{V}_{ij} + \sum_{i<j<k}^{A}\hat{V}_{ijk}}^{\hat{W}} + \overbrace{\sum_{i}^{A}\hat{V}_{\mathrm{ext},i}}^{\hat{V}_{\mathrm{ext}}}$$

$(i) = (\mathbf{r}_i, s_i, t_i)$: spatial coordinates (x, y, z), spin (up and down), isospin (neutron and proton).

- A heavy nucleus, e.g. ^{240}Pu: $\Psi(1,\cdots,A)$ has 720 spatial coordinates and $2^{240} \approx 1.77 \times 10^{72}$ spin components.

- A direct solution of the many-body SE is not possible within current computing resources.

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Density functional theory (DFT)

$$H\Psi(1,\cdots,A) = E\Psi(1,\cdots,A),$$

$$H = \overbrace{\sum_{i}^{A} -\frac{\hbar^2}{2m}\Delta_i}^{\hat{T}} + \overbrace{\sum_{i<j}^{A}\hat{V}_{ij} + \sum_{i<j<k}^{A}\hat{V}_{ijk}}^{\hat{W}} + \overbrace{\sum_{i}^{A}\hat{V}_{\mathrm{ext},i}}^{\hat{V}_{\mathrm{ext}}}$$

Hohenberg and Kohn (HK) theorem:

$$\Psi(1,...,A) \Leftrightarrow \Psi[n] \Leftrightarrow V_{\mathrm{ext}}(\boldsymbol{r}) \Leftrightarrow n(\mathbf{r})$$

$$n(\boldsymbol{r}) = \langle\Psi|\sum_{s}\hat{\psi}_s^{\dagger}(\boldsymbol{r})\hat{\psi}_s(\boldsymbol{r})|\Psi\rangle$$

$$E_0 = \langle\Psi[n]|\hat{H}|\Psi[n]\rangle = \min_{n(\boldsymbol{r})}\int d^3r\,(\mathcal{E}[n(\boldsymbol{r})] + V_{\mathrm{ext}}(\boldsymbol{r})n(\boldsymbol{r}))$$

$\mathcal{E}[n(\boldsymbol{r})] = \langle\Psi|\hat{T}+\hat{W}|\Psi\rangle$ is independent of $V_{\mathrm{ext}}(\boldsymbol{r})$

Density functional theory (DFT)

How to calculate $n(\mathbf{r})$?

$$E_0 = \langle \Psi[n] | \hat{H} | \Psi[n] \rangle = \min_{n(\boldsymbol{r})} \int d^3 r \left(\mathcal{E}[n(\boldsymbol{r})] + V_{\text{ext}}(\boldsymbol{r}) n(\boldsymbol{r}) \right)$$

exchange correlation

$$\mathcal{E}[n(\boldsymbol{r})] = T[n] + \mathcal{E}_{\text{xc}}[n] + \cdots$$

local

$$\int \delta n(\boldsymbol{r}) \left\{ \frac{\delta T[n]}{\delta n(\boldsymbol{r})} + \frac{\delta \mathcal{E}_{\text{xc}}[n]}{\delta n(\boldsymbol{r})} + V(\boldsymbol{r}) \right\} = 0$$

non-local

For inhomogeneous system:

$$\mathcal{E}_{\text{xc}}[n] = n(\boldsymbol{r}) \varepsilon_{\text{xc}}(n(\boldsymbol{r}))$$

Local density approximation (LDA)

$$T[n] = \frac{3\hbar^2}{10m} (3\pi^2)^{2/3} n^{5/3} + \cdots$$

Thomas-Fermi (TF) approximation, but it cannot correctly describe the surface.

Density functional theory (DFT)

How to calculate $n(\mathbf{r})$?

$$E_0 = \langle \Psi[n] | \hat{H} | \Psi[n] \rangle = \min_{n(\boldsymbol{r})} \int d^3 r \left(\mathcal{E}[n(\boldsymbol{r})] + V_{\text{ext}}(\boldsymbol{r}) n(\boldsymbol{r}) \right)$$

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For inhomogeneous system:

$$\mathcal{E}_{\text{xc}}[n] = n(\boldsymbol{r}) \varepsilon_{\text{xc}}(n(\boldsymbol{r}))$$

Local density approximation (LDA)

$$T[n] = \frac{3\hbar^2}{10m} (3\pi^2)^{2/3} n^{5/3} + \frac{\hbar^2}{2m} \left[\frac{1}{36} \frac{(\nabla \rho)^2}{\rho} + \frac{1}{3} \nabla^2 \rho \right] + \mathcal{O}[(\nabla \rho)^4]$$

Extended Thomas-Fermi (ETF) approximation, can describe the surface, still cannot describe the quantum oscillations brought by the shell structure.

Density functional theory (DFT)

Kohn and Sham (KS) theorem:

For any interacting system, there exists a non-interacting system that has the same ground state density.

$$H\Psi = E\Psi$$

$$n(\boldsymbol{r}) = \langle\Psi| \sum_s \hat{\psi}_s^\dagger(\boldsymbol{r})\hat{\psi}_s(\boldsymbol{r})|\Psi\rangle$$

KS equation (neglecting spins)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r}) + V_{\text{ext}}(\boldsymbol{r})\right]\phi_i(\mathbf{r}) = \epsilon_i\phi_i(\mathbf{r})$$

$$n_{KS}(\boldsymbol{r}) = \sum_i |\phi_i(\boldsymbol{r})|^2$$

$$n(\boldsymbol{r}) = n_{KS}(\boldsymbol{r})$$

Normal densities:

$$E_0 = \langle \Psi | \hat{H} | \Psi \rangle = \min_{n(\boldsymbol{r})} \int d^3r \left(\mathcal{E}[n(\boldsymbol{r})] + V_{\text{ext}}(\boldsymbol{r}) n(\boldsymbol{r}) \right)$$

For nucleus, the universal functional $\mathcal{E}[n(\boldsymbol{r})]$ should also contains the following one-body local densities. (for neutrons and protons respectively)

- Kinetic energy density: $E_{\text{kin}} = \langle \Psi | \hat{T} | \Psi \rangle = \int d^3r \frac{\hbar^2}{2m} \tau(\boldsymbol{r})$

$$\tau(\boldsymbol{r}) = \sum_{k,s} |\boldsymbol{\nabla} \phi_k(\boldsymbol{r}, s, \sigma)|^2$$

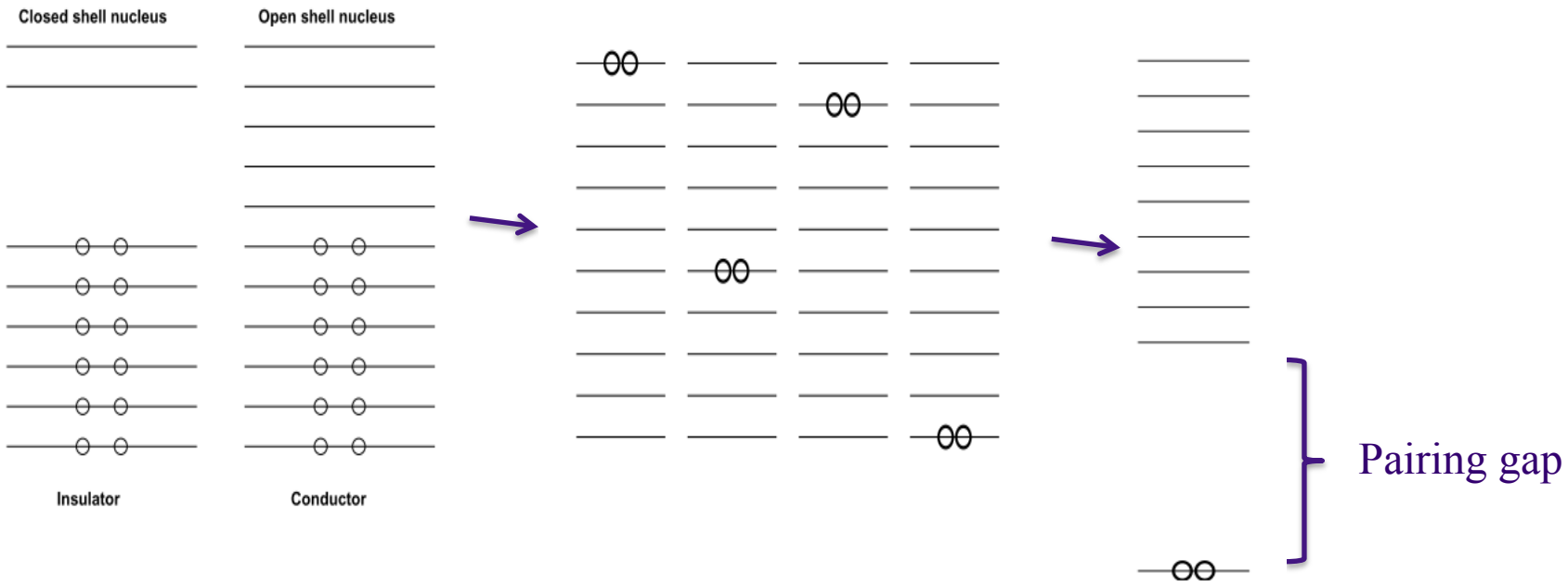
- The nucleus has spin-orbit interaction, spin-orbit density is needed :

$$\boldsymbol{J}(\boldsymbol{r}) = (-i) \sum_{k,s,s'} \phi_k^*(\boldsymbol{r}, s, \sigma) \left[\boldsymbol{\nabla} \phi_k(\boldsymbol{r}, s, \sigma) \times \boldsymbol{\sigma}_{ss'} \right]$$

- To describe the surface of nucleus, $\boldsymbol{\nabla} n(\boldsymbol{r})$ is also needed.

Pairing correlations

- Analogous to the BCS theory in superconductivity, for open shell nucleus, nucleons near the Fermi surface with opposite momentum and spin form “Cooper pairs” (m, -m).



Quasi-particle wavefunctions

- The single particle wavefunctions (wf.) are extended to 4-component quasi-particle wfs.

$$\phi_k(\boldsymbol{r}) \Rightarrow [u_{k\uparrow}(\boldsymbol{r}), u_{k\downarrow}(\boldsymbol{r}), v_{k\uparrow}(\boldsymbol{r}), v_{k\downarrow}(\boldsymbol{r})]^T$$

- The order parameter, the "anomalous density" which signals the presence of "Cooper pairs":

$$\nu(r) = \sum_k v^*_{k\uparrow}(\boldsymbol{r}) u_{k\downarrow}(\boldsymbol{r}) \quad \leftrightarrow \quad \nu(\boldsymbol{r}) \sim \langle \Psi | \hat{\psi}_\uparrow(\boldsymbol{r}) \hat{\psi}_\downarrow(\boldsymbol{r}) | \Psi \rangle$$

And all the normal local densities are rewritten as:

$$n(\boldsymbol{r}) = \sum_{k,s} v^*_{k,s}(\boldsymbol{r}) v_{k,s}(\boldsymbol{r}),$$

$$\tau(\boldsymbol{r}) = \sum_{k,s} \boldsymbol{\nabla} v^*_{k,s}(\boldsymbol{r}) \cdot \boldsymbol{\nabla} v_{k,s}(\boldsymbol{r}),$$

$$\boldsymbol{J}(\boldsymbol{r}) = -i \sum_{k,s,s'} v^*_{k,s}(\boldsymbol{r}) \left[\boldsymbol{\nabla} v_{k,s}(\boldsymbol{r}) \times \boldsymbol{\sigma}_{s,s'} \right]$$

- The total energy of a nucleus is a functional of various one-body local densities (for neutron and proton respectively)

$$E = \int d^3r \mathcal{E}[n(\boldsymbol{r}), \tau(\boldsymbol{r}), \boldsymbol{J}(\boldsymbol{r}), \boldsymbol{\nabla} n(\boldsymbol{r}), \nu(\boldsymbol{r})]$$

- Kohn-Sham equation is extended to 4-component Hartree-Fock-Bogoliubov (HFB) type equation:

$$\begin{pmatrix} h_{\uparrow\uparrow} - \mu & h_{\uparrow\downarrow} & 0 & \Delta \\ h_{\downarrow\uparrow} & h_{\downarrow\downarrow} - \mu & -\Delta & 0 \\ 0 & -\Delta^* & -h^*_{\uparrow\uparrow} + \mu & -h^*_{\uparrow\downarrow} \\ \Delta^* & 0 & -h^*_{\downarrow\uparrow} & -h^*_{\downarrow\downarrow} + \mu \end{pmatrix} \begin{pmatrix} u_{k\uparrow} \\ u_{k\downarrow} \\ v_{k\uparrow} \\ v_{k\downarrow} \end{pmatrix} = E_k \begin{pmatrix} u_{k\uparrow} \\ u_{k\downarrow} \\ v_{k\uparrow} \\ v_{k\downarrow} \end{pmatrix}$$

$h(\boldsymbol{r})$ is the single particle Hamiltonian, and $\Delta(\boldsymbol{r})$ is the pairing potential.

$$hv_{k\uparrow} = \frac{\delta E}{\delta v^*_{k\uparrow}}, \quad \Delta v_{k\uparrow} = \frac{\delta E}{\delta u^*_{k\uparrow}}$$

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Nuclear energy density functional (NEDF)

DFT proves that there exists a universal EDF for any fermion systems.

However, it does not provide a recipe for the construction of this EDF.

- In nuclear physics accurate EDFs are typically constructed phenomenologically.
- There exists more than 300 NEDFs at present, which depend on a large number of fitting parameters (typically 14 and sometimes even more).
- However, among these parameters, only some parameters or their combinations are uncorrelated, which makes it difficult to study the relations between parameters and various nuclear properties.

- We have developed a qualitatively new NEDF, which contains only 7 uncorrelated parameters.
  (A. Bulgac, M. M. Forbes, S. Jin, N. Schunck, R. Navarro Perez, to be updated)

Our Strategy:

$$E_B(N,Z) = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \delta(A)$$

$$\downarrow$$

$$E = \int d^3r \mathcal{E}[n(\boldsymbol{r}), \tau(\boldsymbol{r}), \boldsymbol{J}(\boldsymbol{r}), \boldsymbol{\nabla} n(\boldsymbol{r}), \nu(\boldsymbol{r})]$$

We will describe a NEDF to account for all the contributions in the liquid drop formula.

Form of NEDF

kinetic Coulomb interaction

$$\mathcal{E}[n(\boldsymbol{r}), \tau(\boldsymbol{r}), \boldsymbol{J}(\boldsymbol{r}), \boldsymbol{\nabla} n(\boldsymbol{r}), \nu(\boldsymbol{r})] = \mathcal{E}_{\mathrm{kin}} + \mathcal{E}_{\mathrm{C}} + \mathcal{E}_{\mathrm{int}}$$

Kinetic energy and Coulomb energy are well motivated (no free parameters):

$$\mathcal{E}_{\mathrm{kin}} = \frac{\hbar^2}{2m}(\tau_n + \tau_p), \quad m = \frac{m_n + m_p}{2}$$

$$\mathcal{E}_{\mathrm{C}} = \frac{1}{2}\int d^3r' \frac{e^2 n_p(\boldsymbol{r}) n_p(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} - \frac{3e^2}{4}\left(\frac{n_p(\boldsymbol{r})}{3\pi}\right)^{4/3}$$

Form of NEDF

$$\mathcal{E}[n(\boldsymbol{r}), \tau(\boldsymbol{r}), \boldsymbol{J}(\boldsymbol{r}), \boldsymbol{\nabla} n(\boldsymbol{r}), \nu(\boldsymbol{r})] = \mathcal{E}_{\mathrm{kin}} + \mathcal{E}_{\mathrm{C}} + \mathcal{E}_{\mathrm{int}}$$

kinetic Coulomb interaction

Interaction energy consists of 4 terms:

$$\mathcal{E}_{\mathrm{int}} = \mathcal{E}_{\mathrm{homo}} + \mathcal{E}_{\mathrm{grad}} + \mathcal{E}_{\mathrm{so}} + \mathcal{E}_{\mathrm{pair}}$$

homogeneous

gradient

spin-orbit

pairing

$$\mathcal{E}_{\rm int} = \mathcal{E}_{\rm homo} + \mathcal{E}_{\rm grad} + \mathcal{E}_{\rm so} + \mathcal{E}_{\rm pair}$$

homogeneous

gradient

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pairing

Homogeneous term:

$$\mathcal{E}_{\rm homo} = \sum_{j=0}^{2} (a_j n^{5/3} + b_j n^2 + c_j n^{7/3}) \beta^{2j}$$

$$n = n_n + n_p, \quad \beta = \frac{n_n - n_p}{n_n + n_p}$$

Among the 9 parameters $a_j, b_j, c_j, \quad j = 0, 1, 2$, only 4 of them are independent, which describe the following bulk properties of the nucleus:

- saturation density:

  $n_0 \approx 0.16 \text{ fm}^{-3}$

- binding energy per nucleon in (symmetric) nuclear matter:

  $E_0/A \sim a_V \approx 16 \text{ MeV}$

  } b_0, c_0

- symmetry energy

  $S \sim a_A \approx 30 \text{ MeV}$

- slope of symmetry energy (controls the neutron skin thickness)

  $L = 30 \sim 60 \text{ MeV}$ $\qquad \Delta r = r_n - r_p$

  } b_1, c_1

$$\mathcal{E}_{\rm int} = \mathcal{E}_{\rm homo} + \mathcal{E}_{\rm grad} + \mathcal{E}_{\rm so} + \mathcal{E}_{\rm pair}$$

homogeneous

spin-orbit

gradient

pairing

Homogeneous term:

$$\mathcal{E}_{\rm homo} = \sum_{j=0}^{2} (a_j n^{5/3} + b_j n^2 + c_j n^{7/3}) \beta^{2j}$$

$$n = n_n + n_p, \quad \beta = \frac{n_n - n_p}{n_n + n_p}$$

- $a_0, a_1 - b_1 n_0^{1/3}$ are proved to be insignificant in the fitting (will be illustrated later), fixed as 0.

- *j*=2 terms are fixed by the equation of state for homogeneous neutron matter (obtained from QMC calculation with chiral effective force).

$$a_n = a_0 + a_1 + a_2 = -32.6\,\text{MeV fm}^2,$$
$$b_n = b_0 + b_1 + b_2 = -115.4\,\text{MeV fm}^3,$$
$$c_n = c_0 + c_1 + c_2 = 109.1\,\text{MeV fm}^4.$$

G. Wlazłowski *et al.*, Phys. Rev. Lett. 113,182503 (2014)

homogeneous spin-orbit

$$\mathcal{E}_{\rm int} = \mathcal{E}_{\rm homo} + \mathcal{E}_{\rm grad} + \mathcal{E}_{\rm so} + \mathcal{E}_{\rm pair}$$

gradient pairing

Gradient term:

$$\mathcal{E}_{\rm grad} = \eta_s \sum_{q=n,p} \frac{\hbar^2}{2m} |\boldsymbol{\nabla} n_q|^2$$

One parameter , describe the surface tension of the nucleus.

One can also introduce a cross-term

$$\mathcal{E}_{\rm grad} = \eta_s \sum_{q=n,p} \frac{\hbar^2}{2m} |\boldsymbol{\nabla} n_q|^2 + \eta'_s \sum_{q=n,p} \frac{\hbar^2}{2m} \boldsymbol{\nabla} n_p \cdot \boldsymbol{\nabla} n_n$$

but it does not bring any significant improvement on the fit.

$$\mathcal{E}_{\rm int} = \mathcal{E}_{\rm homo} + \mathcal{E}_{\rm grad} + \mathcal{E}_{\rm so} + \mathcal{E}_{\rm pair}$$

homogeneous

gradient

spin-orbit

pairing

Spin-orbit term:

$$\mathcal{E}_{\rm so} = W_0 \boldsymbol{J} \cdot \boldsymbol{\nabla} n, \quad \boldsymbol{J} = \boldsymbol{J}_n + \boldsymbol{J}_p$$

- One parameter , describe the spin-orbit interaction of the nucleus.
- Important for the formation of shell structure in the nucleus

homogeneous spin-orbit

$$\mathcal{E}_{\rm int} = \mathcal{E}_{\rm homo} + \mathcal{E}_{\rm grad} + \mathcal{E}_{\rm so} + \mathcal{E}_{\rm pair}$$

gradient pairing

Pairing term:

$$\mathcal{E}_{\rm pair} = \sum_{q=n,p} g_{\rm eff}(\boldsymbol{r}) |\nu_q(\boldsymbol{r})|^2$$

Here we use a superfluid local density approximation (SLDA) to describe the pairing energy of nucleus. $g_{\rm eff}(\boldsymbol{r})$ is obtained from a renormalization of **one** bare coupling constant g_0

Fitting procedure:

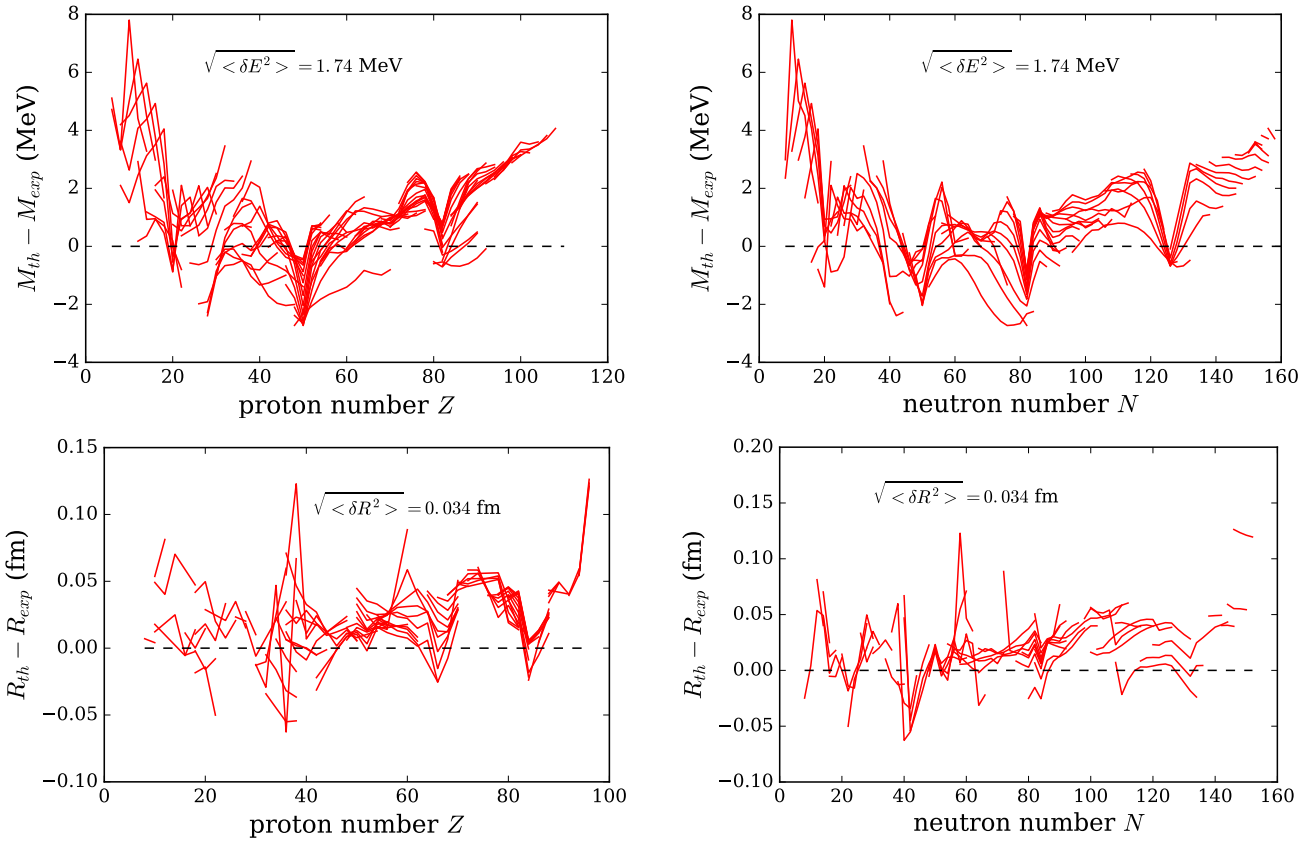
The values of the parameter set $b_0, c_0, b_1, c_1, \eta_s, W_0, g_0$

are obtained by minimizing

$$\chi^2_E = \sum \frac{|E_{\rm th}(N,Z) - E_{\rm exp}(N,Z)|^2}{N_E}$$

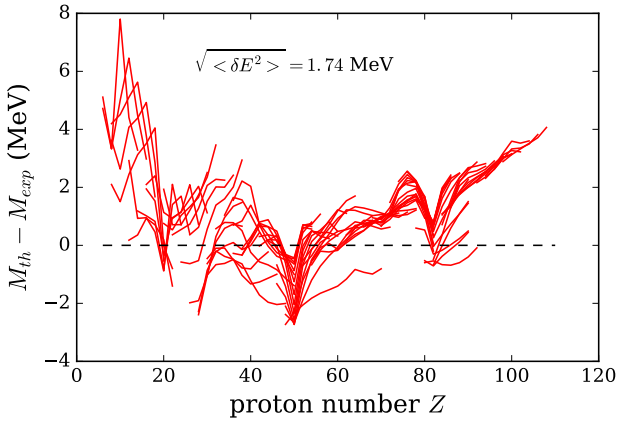
for 196 spherical nuclei in AME2012 dataset, and we name it "**SeaLL1**"

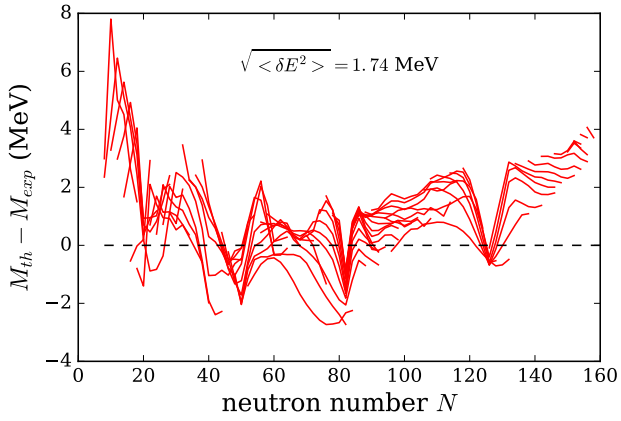
Masses and Radii

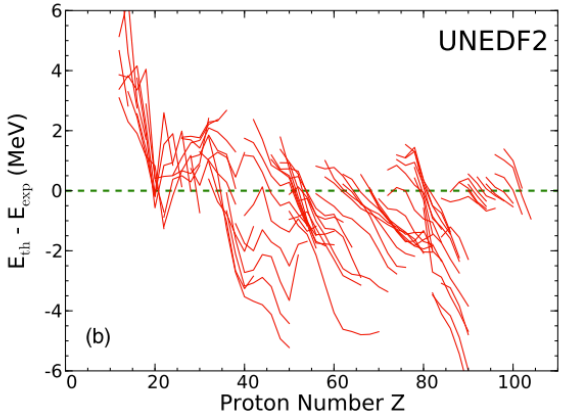


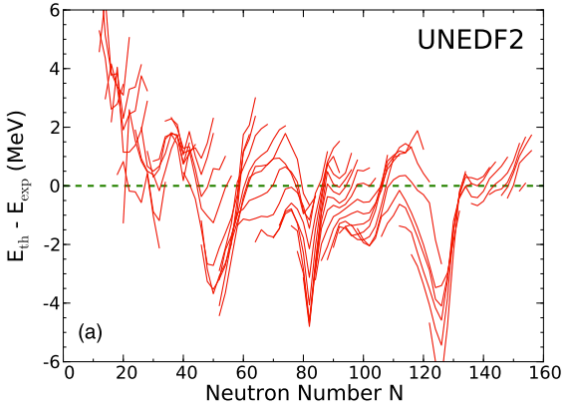
- $\chi_E = 1.74$ MeV for 606 measured even-even nuclei
- $\chi_r = 0.034$ fm for 345 measured even-even nuclei

Masses and Radii







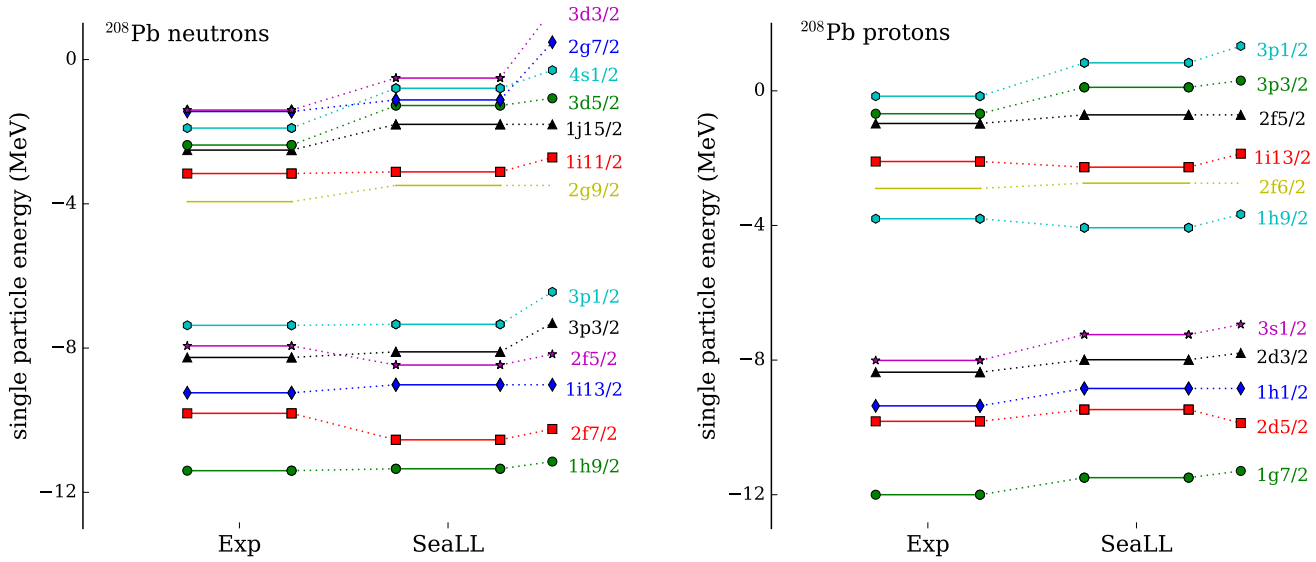


UNEDF2,
13 parameters ,
χ_E = 1.95 MeV

- χ_E = 1.74 MeV for 606 measured even-even nuclei
- χ_r = 0.034 fm for 345 measured even-even nuclei

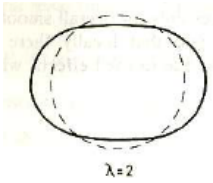
As good as any other competing EDFs!

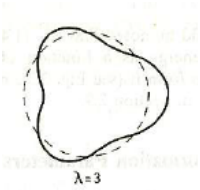
Energy spectrum



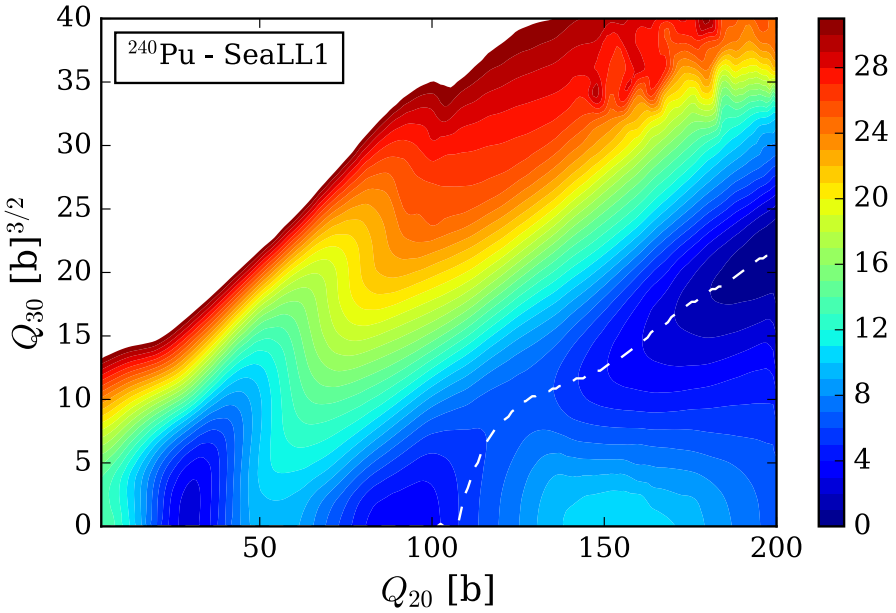
The single particle energy levels of ^{208}Pb calculated with SeaLL1 match well with Exp.

Deformation properties

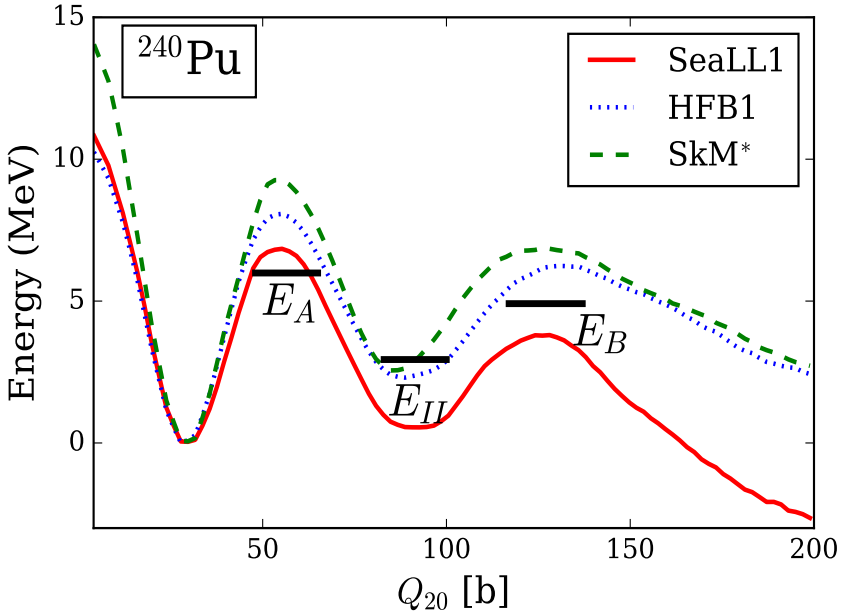
Q_{20} 

Q_{30} 

Potential energy surface of ^{240}Pu



Fission pathway of ^{240}Pu



- Reasonable potential energy surface of ^{240}Pu
- Fission barriers comparable to experiments.
- Lower fission isomer.

Experimental values (horizontal lines) from P. Möller *et al*. Phys. Rev. C 79, 064304

- Nuclear density functional theory (DFT) is the only microscopic, global approach to the structure of nuclei throughout the nuclear chart.

- We developed a qualitatively new NEDF with minimum number of parameters.

- This NEDF yields global masses and radii as good as any other competing NEDFs which contain much more parameters.

- This NEDF also gives a reasonable potential energy surface and fission pathway for ^{240}Pu.

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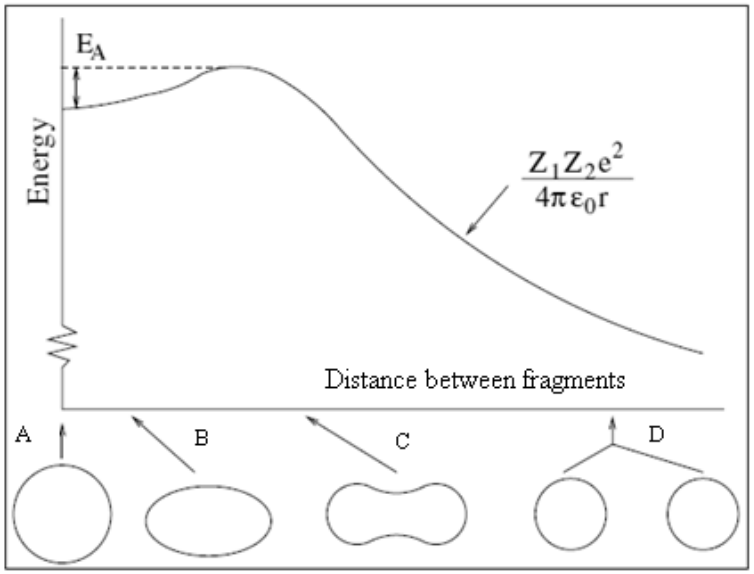
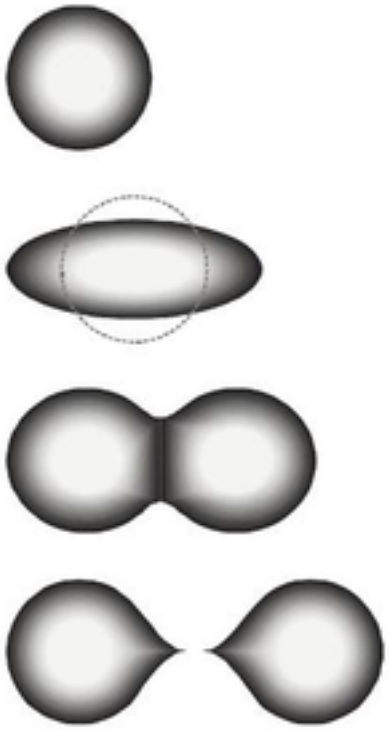
Nuclear fission: overview

- Observed by Hahn and Strassmann (1939).
- Interpreted by Meitner and Frisch, Bohr and Wheeler (1939) as the Coulomb-driven division of a classically charged liquid drop in competition with the surface tension of the liquid drop.

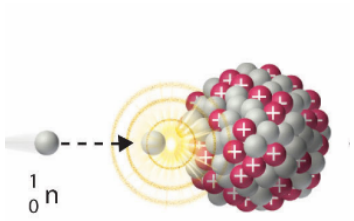




Nuclear fission: overview

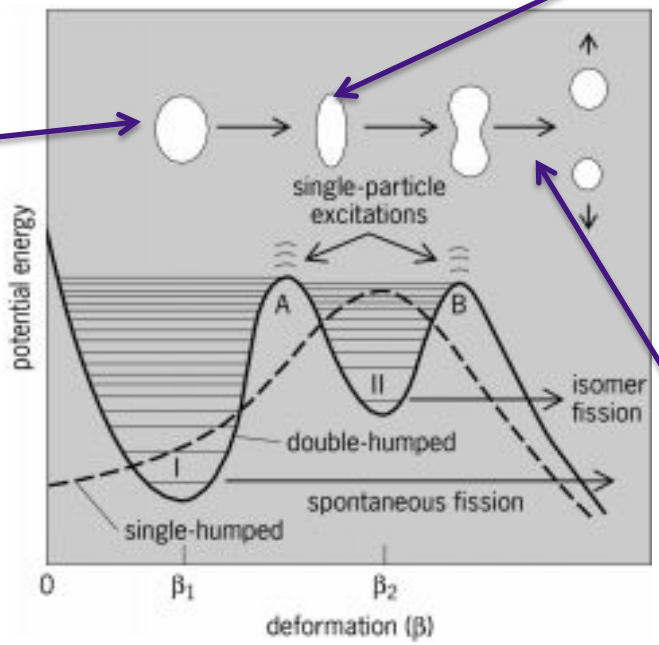
Quantum shell effects lead to a double-humped fission barrier.

The impinging neutron on ^{239}Pu, leads to the formation of an excited state, the compound nucleus (^{240}Pu) .



The nucleus evolves for a very long time from its ground state shape towards the top of the fission.

$$t_1 \approx 10^9 \text{ fm/c}$$



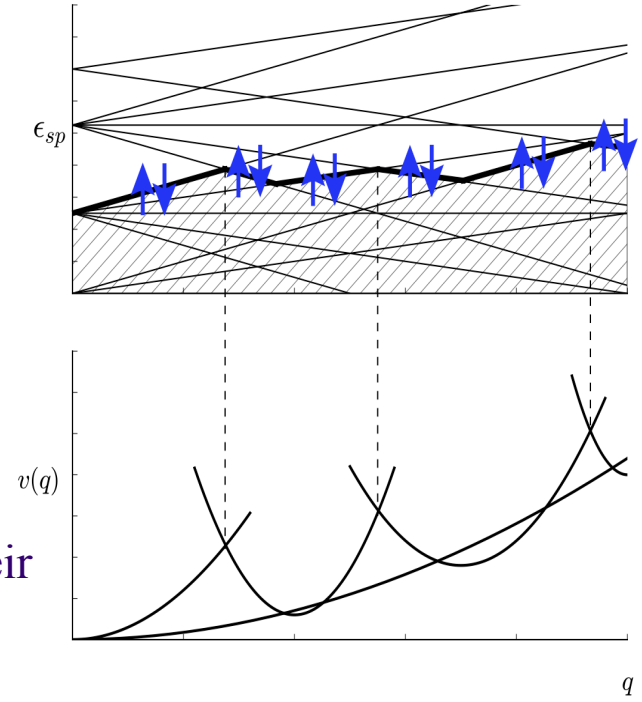
The Coulomb repulsion overcomes surface tension and the nucleus starts its descent to scission, where the two fission fragments are formed.

$$t_2 \approx 10^3 \sim 10^4 \text{ fm/c}$$

Importance of pairing interaction

Pairing plays an important role in the nuclear shape dynamics.

- While a nucleus elongates, the Fermi surface becomes oblate. Its sphericity can be restored only by redistributing the nucleons on different energy levels.
- Each single-particle level doublet is occupied with time-reversed quantum numbers (in the shaded area)
- At each crossing two nucleons change their angular momenta (m,-m) => (m',-m') "Cooper pair" => "Cooper pair"



Pairing interaction is the most effective mechanism at performing such transitions

- Fission dynamics is a very complex process. From saddle to scission, fission dynamics is a non-adiabatic, large amplitude collective motion.

- It still did not reach a microscopic description for 80 years after the discovery.

- Two recent developments make the microscopic framework of fission possible:

  - The time-dependent extension of DFT, TDDFT, for superfluid systems in the local density approximation (LDA), dubbed “time dependent superfluid local density approximation (TDSLDA)”

  - The emergence of powerful supercomputers: a large number of CPUs, and GPU acceleration.

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Time-dependent density functional theory (TDDFT)

TDDFT is an extension of DFT,

- The conceptual and computational foundations are analogous.
- TD Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(1,\cdots,A,t)=\left\{\sum_{i=1}^{A}-\frac{\hbar^2}{2m}\Delta_i+V(1,\cdots,A,t)\right\}\Psi(1,\cdots,A,t)$$

- The (TD) wavefunction still has a one-to-one correspondence to the one-body local density:

$$\Psi(1,...,A,t)\Leftrightarrow\Psi[n]\Leftrightarrow n(\mathbf{r},t)=\sum_k|\phi_k(\mathbf{r},t)|^2$$

Time-dependent density functional theory (TDDFT)

- TDDFT equation for superfluid system:

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} h_{\uparrow,\uparrow}(\mathbf{r},t) & h_{\uparrow,\downarrow}(\mathbf{r},t) & 0 & \Delta(\mathbf{r},t) \\ h_{\downarrow,\uparrow}(\mathbf{r},t) & h_{\downarrow,\downarrow}(\mathbf{r},t) & -\Delta(\mathbf{r},t) & 0 \\ 0 & -\Delta^*(\mathbf{r},t) & -h^*_{\uparrow,\uparrow}(\mathbf{r},t) & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & 0 & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) & -h^*_{\downarrow,\downarrow}(\mathbf{r},t) \end{pmatrix} \begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix}$$

Put in a lattice system, the number of PDEs is $4N_xN_yN_z$

- The Hamiltonian contains the local densities introduced earlier, and current density $\boldsymbol{j}(\boldsymbol{r},\boldsymbol{t})$, required by Galilean invariance:

$$h(\boldsymbol{r},t) = h[n(\boldsymbol{r},t),\tau(\boldsymbol{r},t),\boldsymbol{J}(\boldsymbol{r},t),\boldsymbol{\nabla}n(\boldsymbol{r},t),\boldsymbol{j}(\boldsymbol{r},t)], \quad \Delta(\boldsymbol{r},t) = \Delta[\nu(\boldsymbol{r},t)]$$

$$\boldsymbol{j}(r,t) = \sum_k 2\ \mathrm{Im}\ \left(v_{k\uparrow}(\boldsymbol{r},t)\boldsymbol{\nabla}v^*_{k\uparrow}(\boldsymbol{r},t) + v_{k\downarrow}(\boldsymbol{r},t)\boldsymbol{\nabla}v^*_{k\downarrow}(\boldsymbol{r},t)\right)$$

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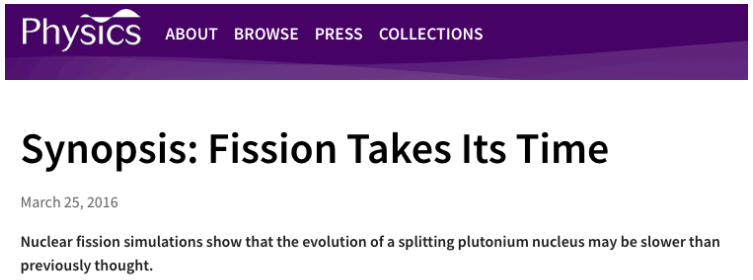
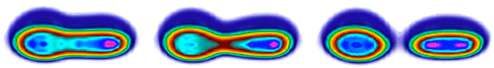
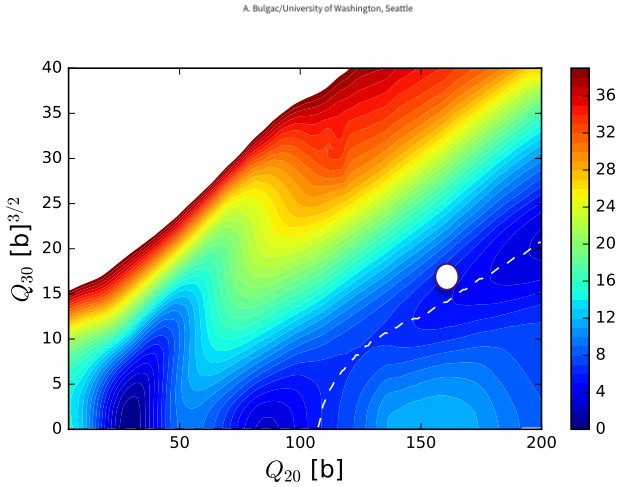
Numerical Implementation

A. Bulgac, P. Magierski, K.J. Roche, I. Stetcu, *Induced Fission of ^{240}Pu within a Real-Time Microscopic Framework*, Phys. Rev. Lett. 116, 122504 (2016)



- EDF: SLy4
- Pairing coupling: $g_0 = -233$ MeV
- Simulation box: $22.5 \times 22.5 \times 40$ fm^3, $dx = 1.25$ fm
- Time step: $\Delta t \approx 0.119$ fm/c
- Number of PDEs: $4N_xN_yN_z \approx 5 \times 10^4$
- Initial configuration: beyond the outer fission barrier (see figure)





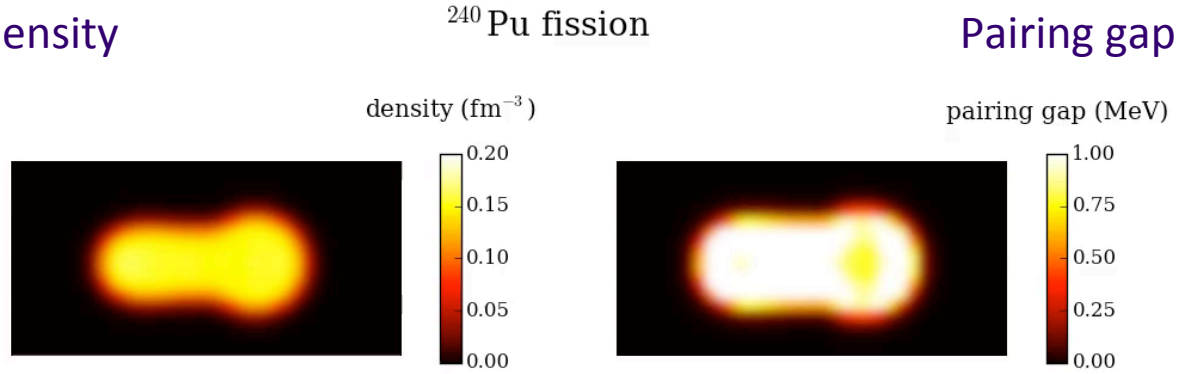
We have the following improvement:

- Larger box: $30 \times 30 \times 60\ \mathrm{fm}^3, \quad dx = 1.25\ \mathrm{fm}$
- larger number of PDEs: $\approx 5 \times 10^5$
- smaller time step: $\Delta t \approx 0.03\ \mathrm{fm/c}$
- number of GPUs: 1730
- wall time: $3.7\ \mathrm{h}/(1000\ \mathrm{fm/c})$

Titan Cray XK7

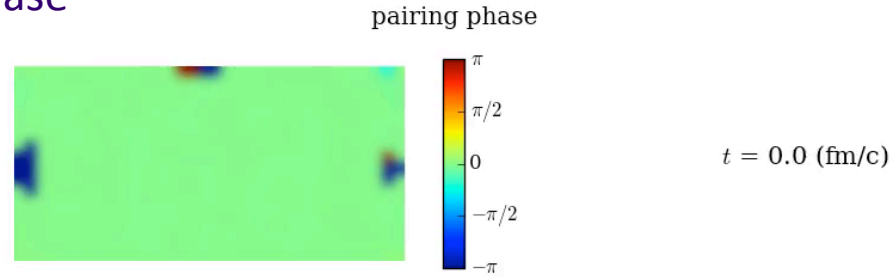
Movie: ^{240}Pu fission

Nucleon density



Pairing gap

Pairing phase



Fission fragments properties

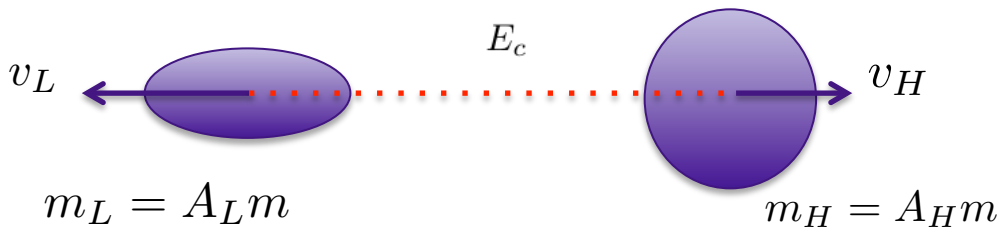
The quality of the agreement with experimental observations is surprisingly good.

t_{sc}	TKE ^{syst}	TKE	A_L^{syst}	A_L	N_L^{syst}	N_L	Z_L^{syst}	Z_L
12259	177.26	173.42	100.55	101.7	60.69	61.3	39.81	40.4

t_{sc} : (fm/c), TKE: (MeV)

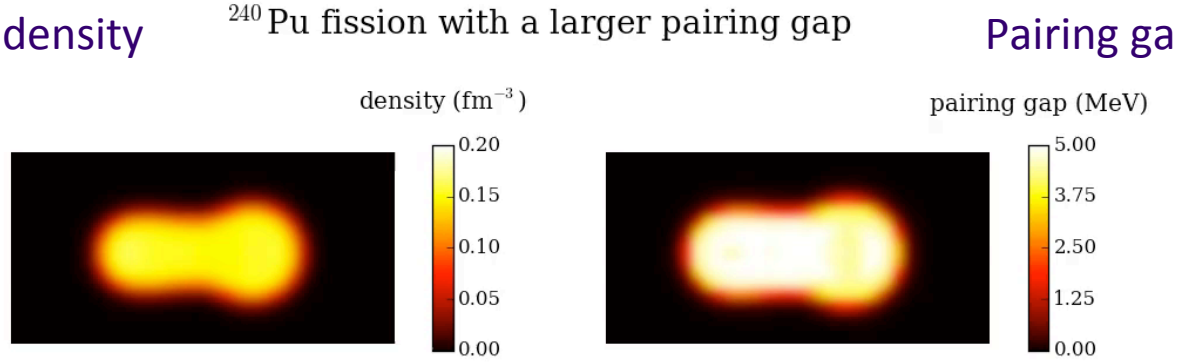
Total kinetic energy (TKE) :

$$\mathrm{TKE} = \frac{1}{2} m_L v_L^2 + \frac{1}{2} m_H v_H^2 + E_c$$



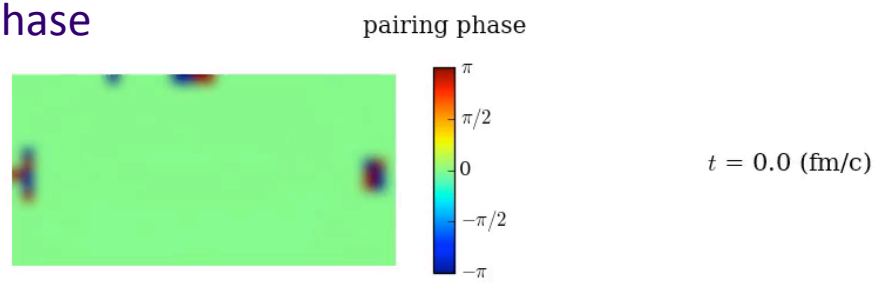
Movie: ^{240}Pu fission with $g_0 = -333$ MeV

Nucleon density

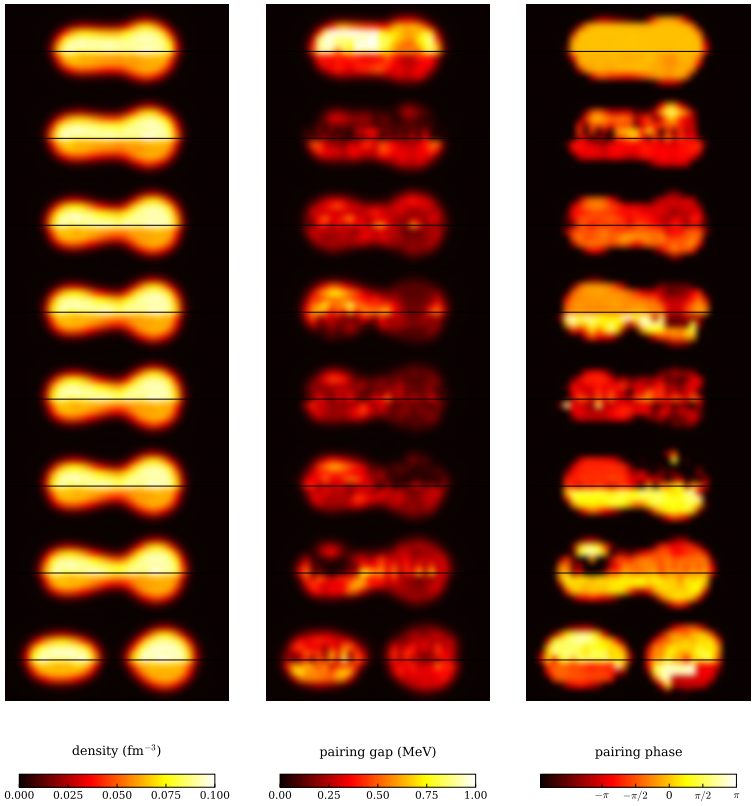


Pairing gap

Pairing phase

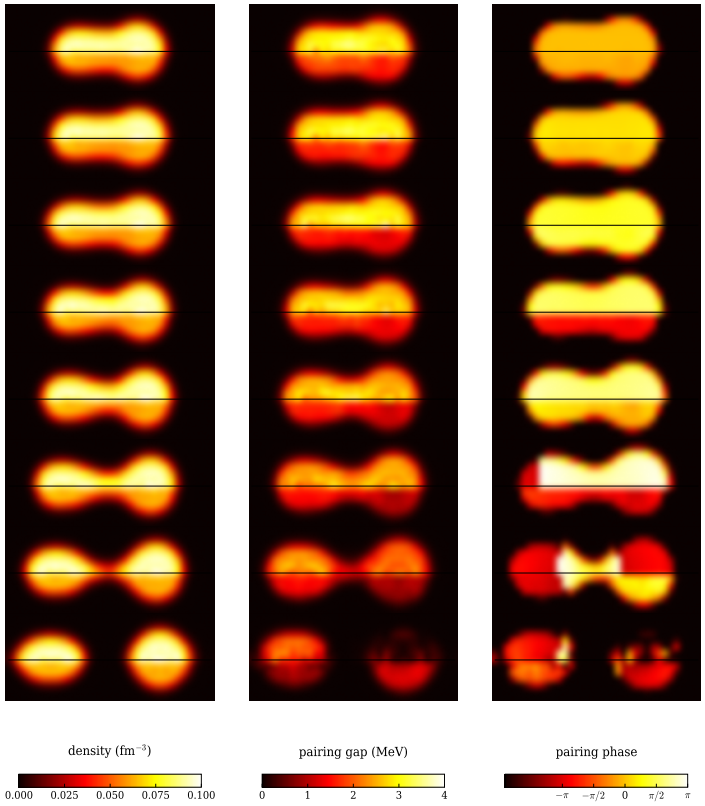


^{240}Pu fission with the normal pairing gap



Normal pairing strength, saddle to scission 14000 fm/c

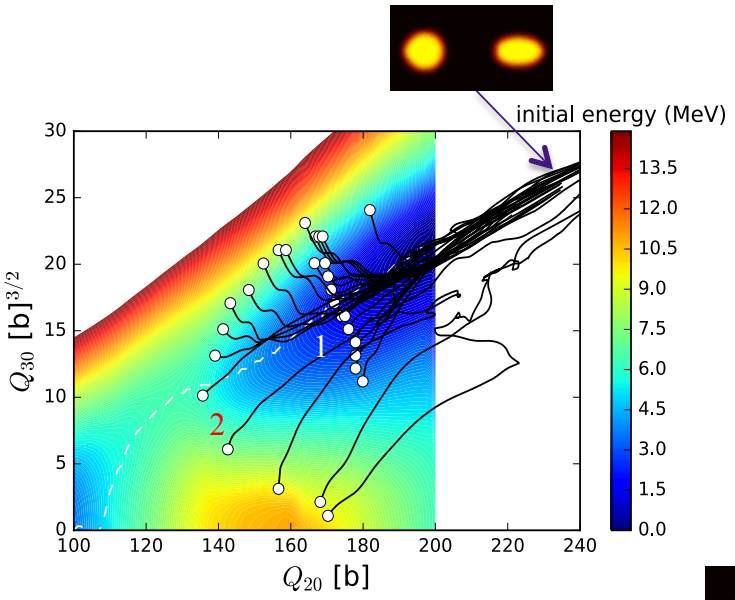
^{240}Pu fission with a larger pairing gap

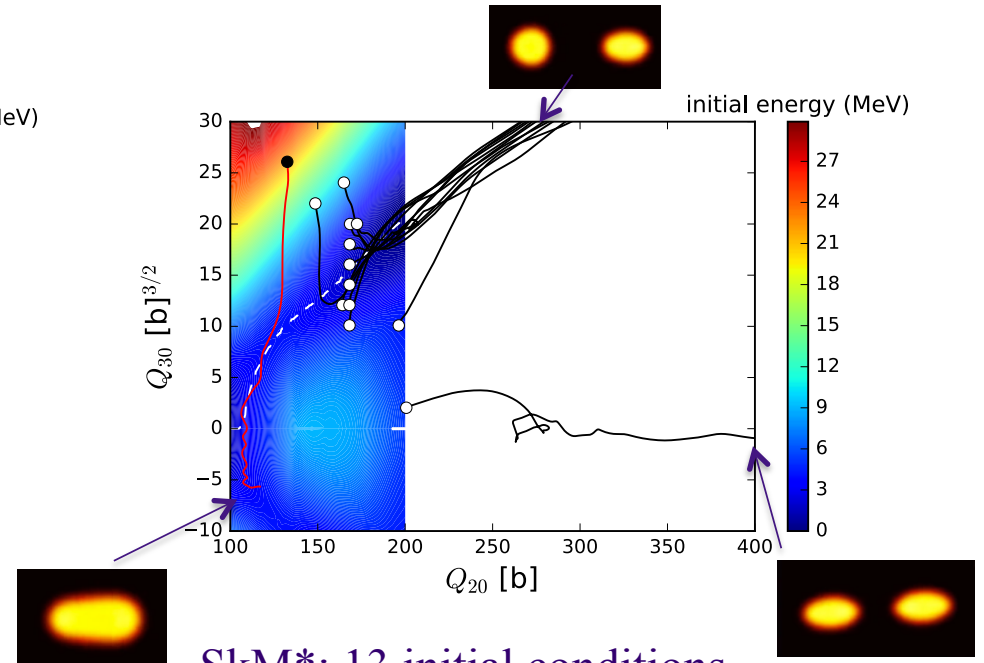


Enhanced pairing strength, saddle to scission 1400 fm/c !!!

A. Bulgac, S. Jin, P. Magierski, K. Roche, I. Stetcu:
Microscopic theory of nuclear fission, arXiv:1704.00689

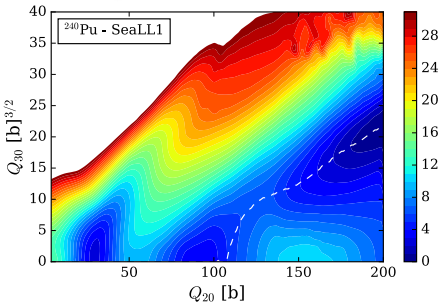
Different initial conditions and EDFs

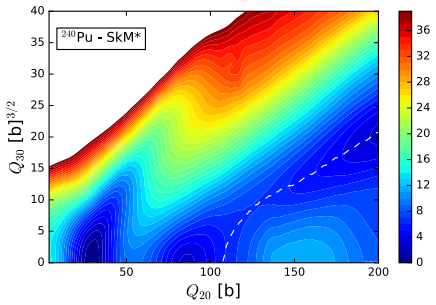




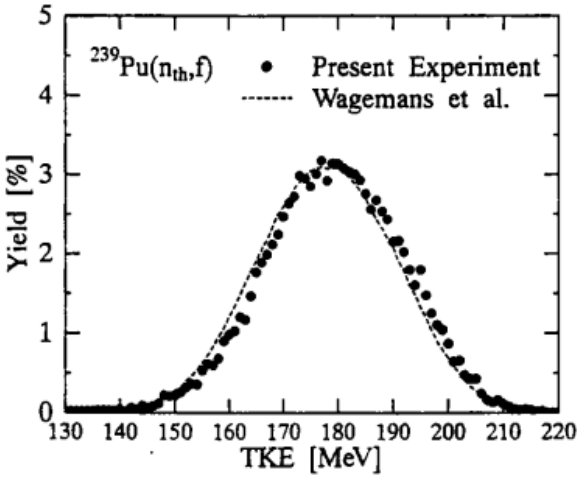
SeaLL1: 2 sets, 32 initial conditions

SkM*: 13 initial conditions.

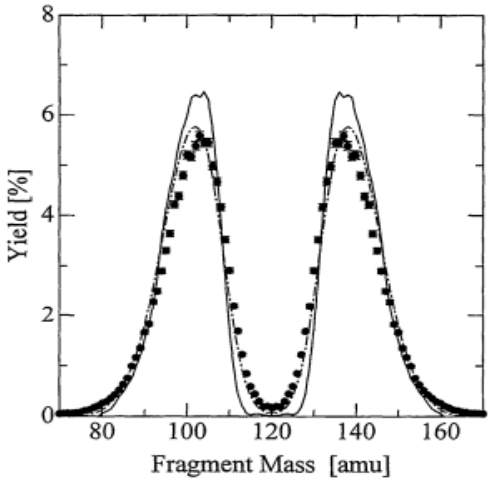




Label	$\overline{\text{TKE}}$	σ_{TKE}	$\overline{A_L}$	σ_{A_L}	$\overline{N_L}$	σ_{N_L}	$\overline{Z_L}$	σ_{Z_L}
SeaLL1-1	178.05	2.27	104.9	0.74	63.33	0.47	41.53	0.27
SeaLL1-2	177.81	2.76	103.85	0.87	62.75	0.5	41.10	0.4
SkM*	172.38	7.72	104.2	5.31	62.75	3.44	41.44	1.88
Syst.	177.26	~ 15	100.55	~ 10	60.69		39.81	



Nishio *et al.* JNST, 32.5.404



Nishio *et al.* JNST, 37.11.941

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Summary

- Nuclear energy density functional theory (DFT) and its extension, TDDFT are powerful theoretical tools to study static properties and dynamics of nuclei throughout the nuclear chart.

- We developed a new NEDF, “SeaLL1”, with the minimal number of independent parameters and achieved very good agreement with experiment for various nuclear static properties: masses, radii, shell structure, deformation properties

- We studied the induced fission of ^{240}Pu with TDDFT and obtained a good agreement of the average fission fragments (FF) properties with experiments.

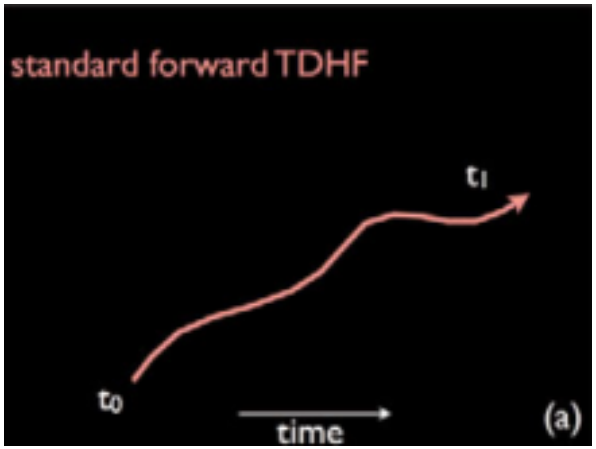
- We also explored the factors that will impact on the fission dynamics and FF properties: pairing interaction, initial conditions and EDFs.

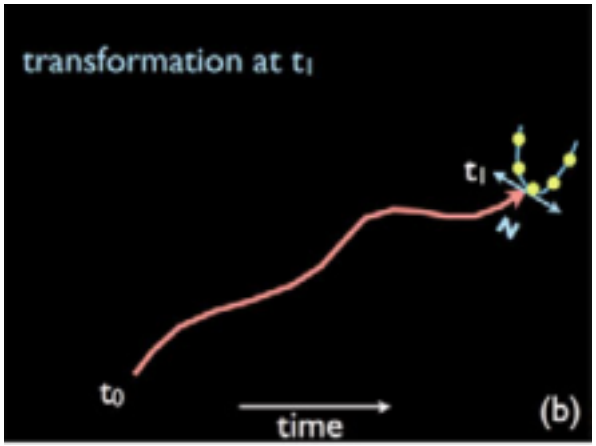
Future work

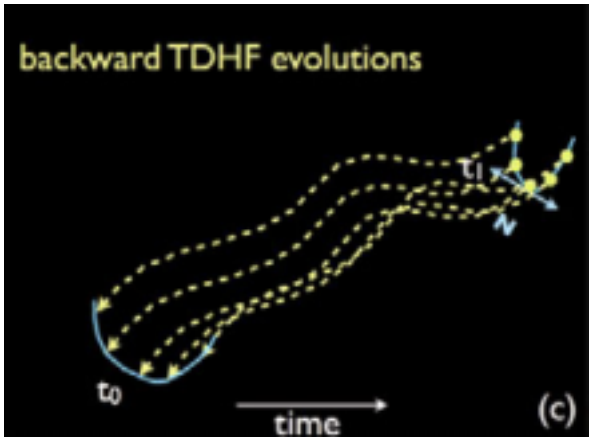
- Calculate the fluctuations of fission fragment observables using Ballian-Véneroni (BV) 's principle

The Balian-Véneroni prescription:

$$\sigma_X^2(t_1) = \lim_{\varepsilon \to 0} \frac{\mathrm{Tr}\{[\rho(t_0) - \rho_X(t_0, \varepsilon)]^2\}}{2\varepsilon^2} \qquad \rho_X(t_1, \varepsilon) = e^{i\varepsilon \hat{X}} \rho(t_1) e^{-i\varepsilon \hat{X}}$$







- Study the fusion of superheavy nucleus Z>>100 using TDDFT

Papers written so far

- A. Bulgac, S. Jin, P. Magierski, K.J. Roche, N. Schunck, and I. Stetcu, *Nuclear Fission: from more phenomenology and adjusted parameters to more fundamental theory and increased predictive power* , arXiv:1705.00052
- A. Bulgac, S. Jin, P. Magierski, K.J. Roche, and I. Stetcu, *Microscopic theory of nuclear fission* , arXiv:1704.00689
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