Density-Constrained TDDFT with Application to Fission

A.S. Umar

Time-dependent DFT theory with density constraint
Fusion of light systems for astrophysics
Fission dynamics

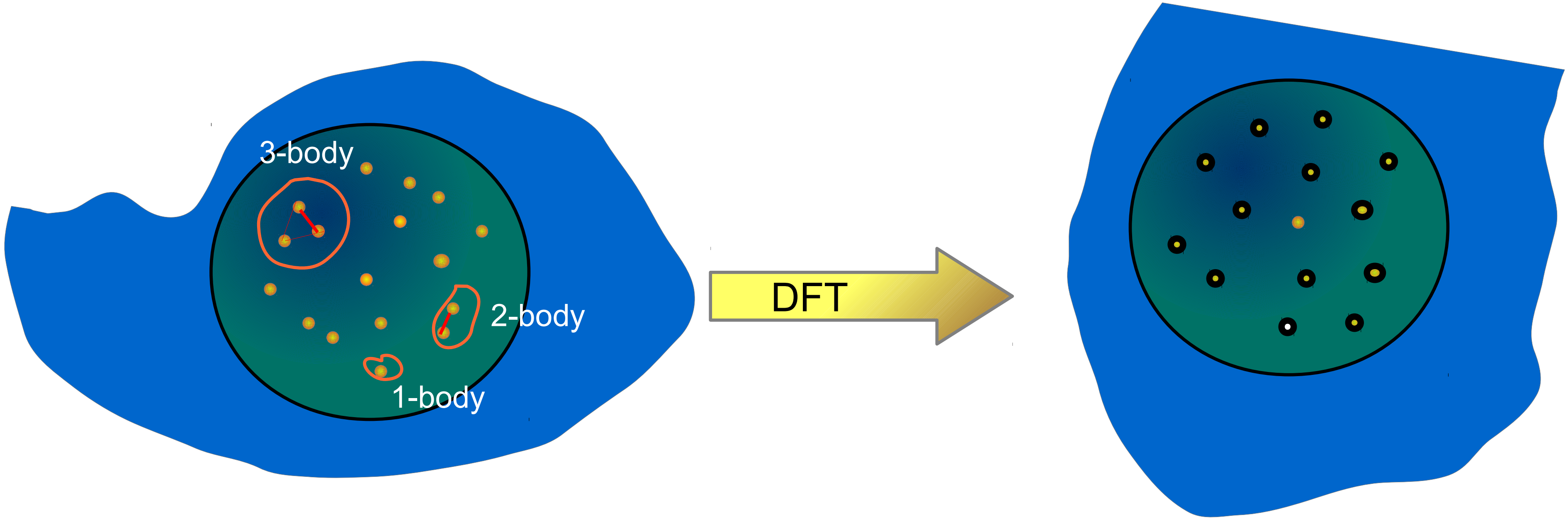
V.E. Oberacker

DC-TDHF for fusion
Fusion of neutron-rich systems
Capture for superheavy formations

Collaborators: J.A. Maruhn, P.-G. Reinhard, C. Horowitz, C. Simenel

VANDERBILT UNIVERSITY Research supported by: U.S. Department of Energy, Division of Nuclear Physics

Mean Field or Energy Density Functional (EDF)



ab-initio

$$\langle \Psi | H | \Psi \rangle = E$$

Mean-field - EDF

$$\Psi \rightarrow \Phi_{Slater}$$

$$H \rightarrow H_{eff}$$

$$E = \langle \Phi | H_{eff} | \Phi \rangle = \int d^3 r \; \{ H(\rho, \tau, \boldsymbol{j}, \boldsymbol{s}, \boldsymbol{T}, J_{\mu\nu} \; ; \boldsymbol{r}) + H_{Coulomb}(\rho_p) \}$$

Single-(one-) particle density *etc.* in terms of s.p. states

$$\rho_q(\boldsymbol{r}) = \sum_{i=1}^{A} \sum_{\sigma} \varphi_i^*(\boldsymbol{r}, \sigma, q) \varphi_i(\boldsymbol{r}, \sigma, q)$$

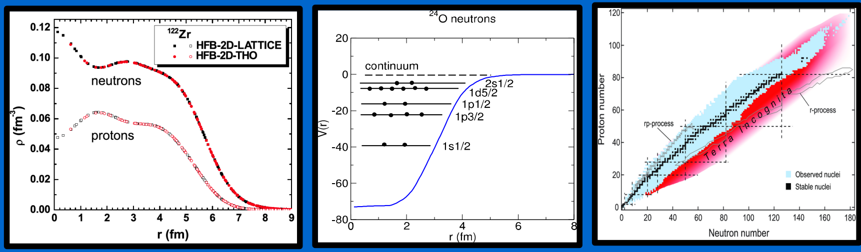
EDF in NP more complicated

$$v = v_{NN-eff} \rightarrow DFT\,(Hartee - Fock)$$

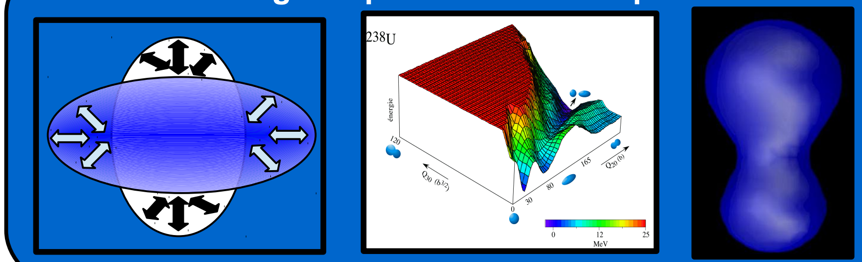
$$v \neq v_{NN-eff} \rightarrow DFT\,(Kohn - Sham)$$

Unified Theory of Structure, Low-E Reactions, and Star Matter

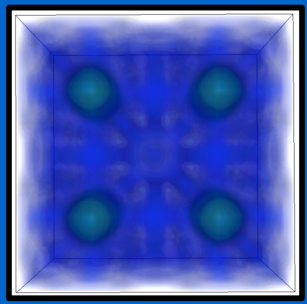
Structure



Small and large amplitude collective phenomena



Neutron Star Crust



- Time-dependent generalization TDDFT (variational or Runge-Gross)

$$\delta S = \delta \int_{t_1}^{t_2} dt \langle \Phi(t) | H_{eff} - i\hbar \partial_t | \Phi(t) \rangle = 0$$

$$i \frac{\partial}{\partial t} \varphi_\alpha = h(\rho, \tau, \boldsymbol{j}, \boldsymbol{s}, \boldsymbol{T}, J_{\mu\nu}\ ; \boldsymbol{r}) \varphi_\alpha$$

self-consistent

- Considerable effort testing TDDFT in recent years

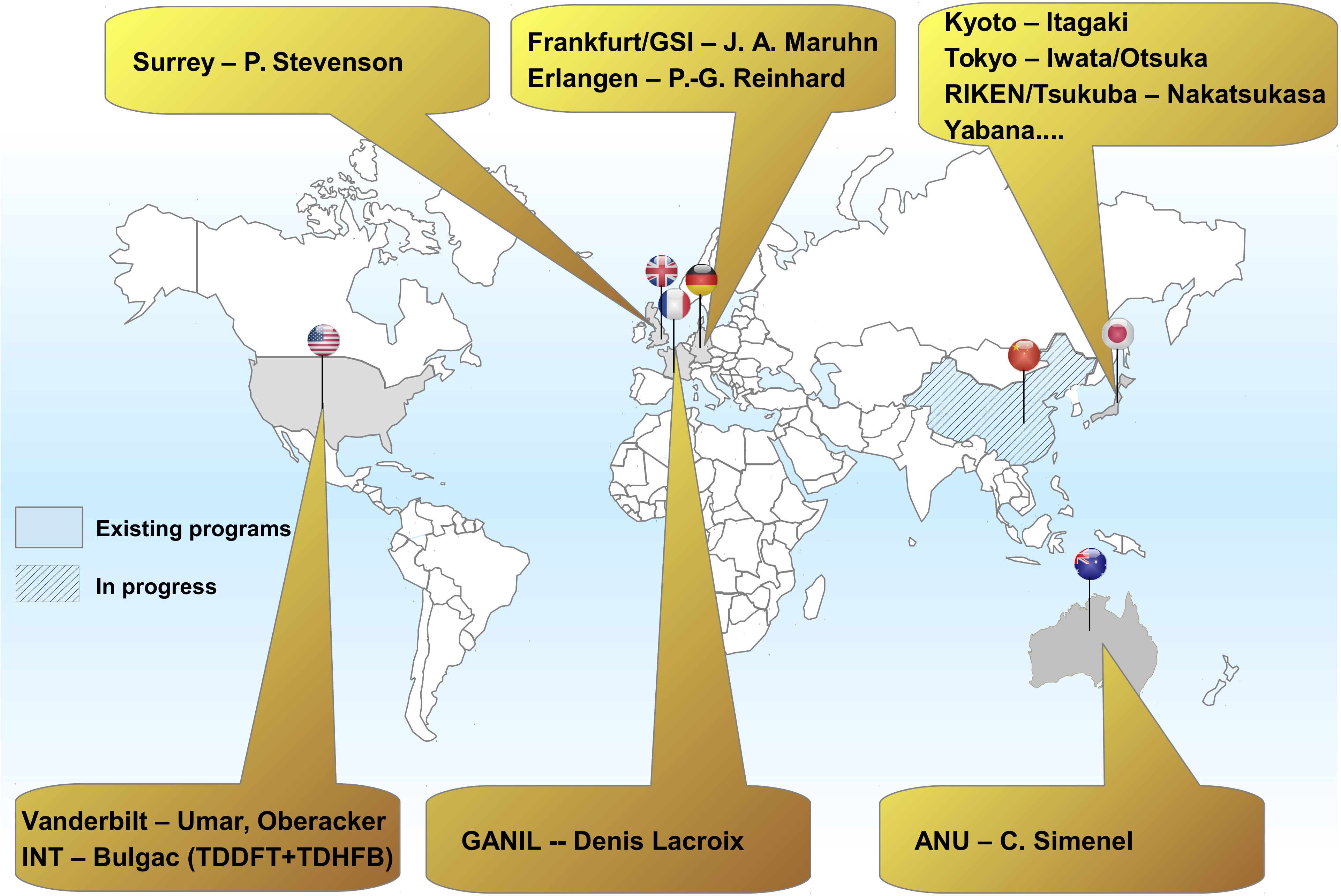
Nuclear Energy Density Functional

$$
\begin{aligned}
H_S(\boldsymbol{r}) \; = \; & \frac{\hbar^2}{2\mathrm{m}}\tau + \frac{1}{2}t_0\left(1+\frac{1}{2}x_0\right)\rho^2 - \frac{1}{2}t_0\left(\frac{1}{2}+x_0\right)\left[\rho_p^2+\rho_n^2\right] + \frac{1}{4}\left[t_1\left(1+\frac{1}{2}x_1\right)+t_2\left(1+\frac{1}{2}x_2\right)\right](\rho\tau-\boldsymbol{j}^2) \\
& -\frac{1}{4}\left[t_1\left(\frac{1}{2}+x_1\right)-t_2\left(\frac{1}{2}+x_2\right)\right]\left(\rho_p\tau_p+\rho_n\tau_n-\boldsymbol{j}_p^2-\boldsymbol{j}_n^2\right) - \frac{1}{16}\left[3t_1\left(1+\frac{1}{2}x_1\right)-t_2\left(1+\frac{1}{2}x_2\right)\right]\rho\nabla^2\rho \\
& +\frac{1}{16}\left[3t_1\left(\frac{1}{2}+x_1\right)+t_2\left(\frac{1}{2}+x_2\right)\right]\left(\rho_p\nabla^2\rho_p+\rho_n\nabla^2\rho_n\right) \\
& +\frac{1}{12}t_3\left[\rho^{\alpha+2}\left(1+\frac{1}{2}x_3\right)-\rho^\alpha\left(\rho_p^2+\rho_n^2\right)\left(x_3+\frac{1}{2}\right)\right] \\
& +\frac{1}{4}t_0x_0\boldsymbol{s}^2-\frac{1}{4}t_0(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2)+\frac{1}{24}\rho^\alpha t_3x_3\boldsymbol{s}^2-\frac{1}{24}t_3\rho^\alpha(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2) \\
& +\frac{1}{32}(t_2+3t_1)\sum_q \boldsymbol{s}_q\cdot\nabla^2\boldsymbol{s}_q-\frac{1}{32}(t_2x_2-3t_1x_1)\,\boldsymbol{s}\cdot\nabla^2\boldsymbol{s} \\
& +\frac{1}{8}(t_1x_1+t_2x_2)(\boldsymbol{s}\cdot\boldsymbol{T}-\boldsymbol{J}_{\mu\nu}^2)+\frac{1}{8}(t_2-t_1)\sum_q(\boldsymbol{s}_q\cdot\boldsymbol{T}_q-\boldsymbol{J}_{q\mu\nu}^2) \\
& -\frac{t_4}{2}\sum_{qq'}(1+\delta_{qq'})[\boldsymbol{s}_q\cdot\nabla\times\boldsymbol{j}_{q'}+\rho_q\boldsymbol{\nabla}_{\mu\nu}\cdot\boldsymbol{J}_{\mu\nu}]
\end{aligned}
$$

Time-odd terms come in pairs!
Total is TR invariant

(s,j,T) time-odd, vanish for static HF calculations of even-even nuclei
non-zero for dynamic calculations, odd mass nuclei, cranking etc.

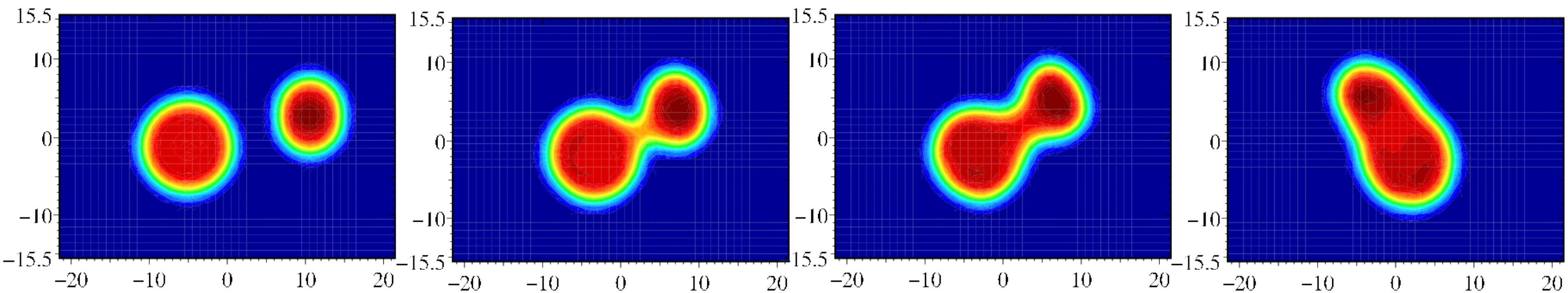
Worldwide Nuclear TDDFT Efforts (partial list)



New Vanderbilt TDDFT Code

- 3-D Cartesian lattice – no geometrical simplification
- Complete EDF including all terms (time-even, time-odd, tensor)
- Coded in Fortran-95 and OpenMP
- Basis-Spline discretization for high accuracy

***Frankfurt/Vanderbilt/Surrey code will be submitted to *Computer Physics Communications* this year**



TDDFT + Density Constraint = Microscopic Fusion Barriers

NEW

Minimize energy with density constraint during unhindered TDDFT

$$E_{DC}(t)=\min_{\rho}\{E[\rho_n,\rho_p]+\int d^3r\, v_n(\mathbf{r})[\rho_n(\mathbf{r})-\rho_n^{tddft}(\mathbf{r},t)]+\int d^3r\, v_p(\mathbf{r})[\rho_p(\mathbf{r})-\rho_p^{tddft}(\mathbf{r},t)]\}$$

Ion-Ion Potential

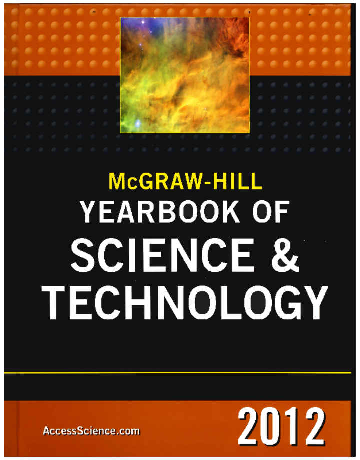
$$V(R(t))=E_{DC}(t)-E_{A_1}-E_{A_2}$$

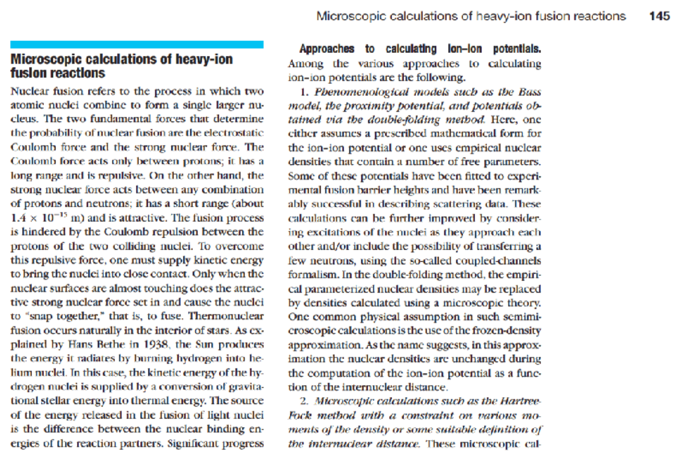
→ Subtract binding energies

Label it with ion-ion separation at time t

- DC-TDHF finds underlying microscopic potential V(R)
- Parameter-free, only depends on chosen EDF
- Dynamical, energy-dependent
- Calculate E*(t) and M(R)

★ Traditional method double-folding with frozen densities + CC





Microscopic calculations of heavy-ion fusion reactions 145

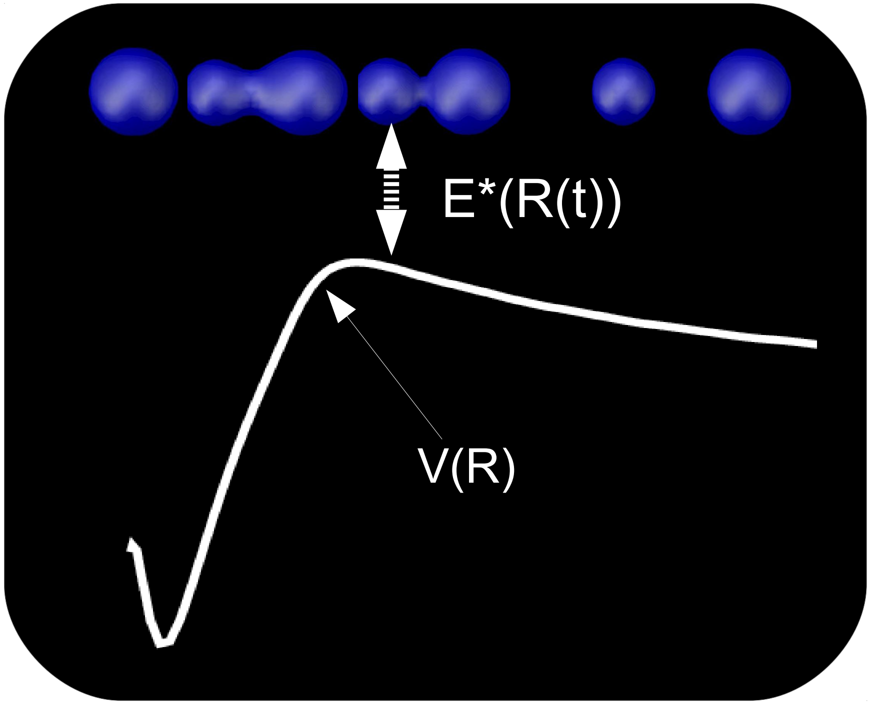
Microscopic calculations of heavy-ion fusion reactions

Nuclear fusion refers to the process in which two atomic nuclei combine to form a single larger nucleus. The two fundamental forces that determine the probability of nuclear fusion are the electrostatic Coulomb force and the strong nuclear force. The Coulomb force acts only between protons; it has a long range and is repulsive. On the other hand, the strong nuclear force acts between any combination of protons and neutrons; it has a short range (about 1.4×10^{-15} m) and is attractive. The fusion process is hindered by the Coulomb repulsion between the protons of the two colliding nuclei. To overcome this repulsive force, one must supply kinetic energy to bring the nuclei into close contact. Only when the nuclear surfaces are almost touching does the attractive strong nuclear force set in and cause the nuclei to "snap together," that is, to fuse. Thermonuclear fusion occurs naturally in the interior of stars. As explained by Hans Bethe in 1938, the Sun produces the energy it radiates by burning hydrogen into helium nuclei. In this case, the kinetic energy of the hydrogen nuclei is supplied by a conversion of gravitational stellar energy into thermal energy. The source of the energy released in the fusion of light nuclei is the difference between the nuclear binding energies of the reaction partners. Significant progress

Approaches to calculating ion–ion potentials. Among the various approaches to calculating ion–ion potentials are the following.

1. *Phenomenological models such as the Bass model, the proximity potential, and potentials obtained via the double-folding method.* Here, one either assumes a prescribed mathematical form for the ion–ion potential or one uses empirical nuclear densities that contain a number of free parameters. Some of these potentials have been fitted to experimental fusion barrier heights and have been remarkably successful in describing scattering data. These calculations can be further improved by considering excitations of the nuclei as they approach each other and/or include the possibility of transferring a few neutrons, using the so-called coupled-channels formalism. In the double-folding method, the empirical parameterized nuclear densities may be replaced by densities calculated using a microscopic theory. One common physical assumption in such semimicroscopic calculations is the use of the frozen-density approximation. As the name suggests, in this approximation the nuclear densities are unchanged during the computation of the ion–ion potential as a function of the internuclear distance.

2. *Microscopic calculations such as the Hartree-Fock method with a constraint on various moments of the density or some suitable definition of the internuclear distance.* These microscopic cal-



Numerical Implementation

- Standard 1-body constraint Q becomes

$$\lambda\hat{Q} \longrightarrow \int d^3r\, \lambda(\mathbf{r})\hat{\rho}(\mathbf{r}) = \lambda(\mathbf{r})$$

1-body

- Iterative scheme for lambda is

$$\lambda^{n+1}(\mathbf{r}) = \lambda^{n}(\mathbf{r}) + c_0 \frac{\delta\rho^{n+1/2}}{2x_0\rho^{n}(\mathbf{r}) + d_0}$$

$$\delta\rho^{n+1/2}(\mathbf{r}) \equiv \rho^{n+1/2}(\mathbf{r}) - \rho_0(\mathbf{r})$$

- Full iteration becomes (c_0, d_0 parameters)

$$\chi_\lambda^{n+1} = \mathcal{O}[\chi_\lambda^{n+1/2} - x_0(\lambda^{n+1}(\mathbf{r}) - \lambda^{n}(\mathbf{r}) + \delta\lambda^{n}(\mathbf{r}))\chi_\lambda^{n+1/2}]$$

$$\delta\lambda^{n}(\mathbf{r}) = c_0 \frac{\rho^{n}(\mathbf{r}) - \rho_0(\mathbf{r})}{2x_0\rho^{n}(\mathbf{r}) + d_0}$$

VANDERBILT UNIVERSITY

A.S. Umar *et al.*, *Phys. Rev. C* **32**, 172 (1985)

Recent Applications of the Method (last three years)

Neutron-rich systems – Superheavy formations

Microscopic study of the 132,124Sn+96Zr reactions
V.E. Oberacker, A.S. Umar, J.A. Maruhn, and P.-G. Reinhard, **PRC** 82, 034603 (2010)
Dynamic microscopic study of pre-equilibrium giant resonance excitation and fusion in 132Sn+48Ca and 124Sn+40Ca
V.E. Oberacker, A.S. Umar, J.A. Maruhn, and P.-G. Reinhard, **PRC** 85, 034609 (2012)
Microscopic study of Ca+Ca fusion
R. Keser, A.S. Umar and V.E. Oberacker, **PRC** 85, 044606 (2012)
Microscopic analysis of sub-barrier fusion enhancement in 132Sn+40Ca versus 132Sn+48Ca
V.E. Oberacker and A.S. Umar, **PRC** 87, 034611 (2013)
Entrance channel dynamics of hot and cold fusion reactions leading to superheavy elements
A.S. Umar, V.E. Oberacker, J.A. Maruhn, and P.-G. Reinhard, **PRC** 81, 064607 (2010).

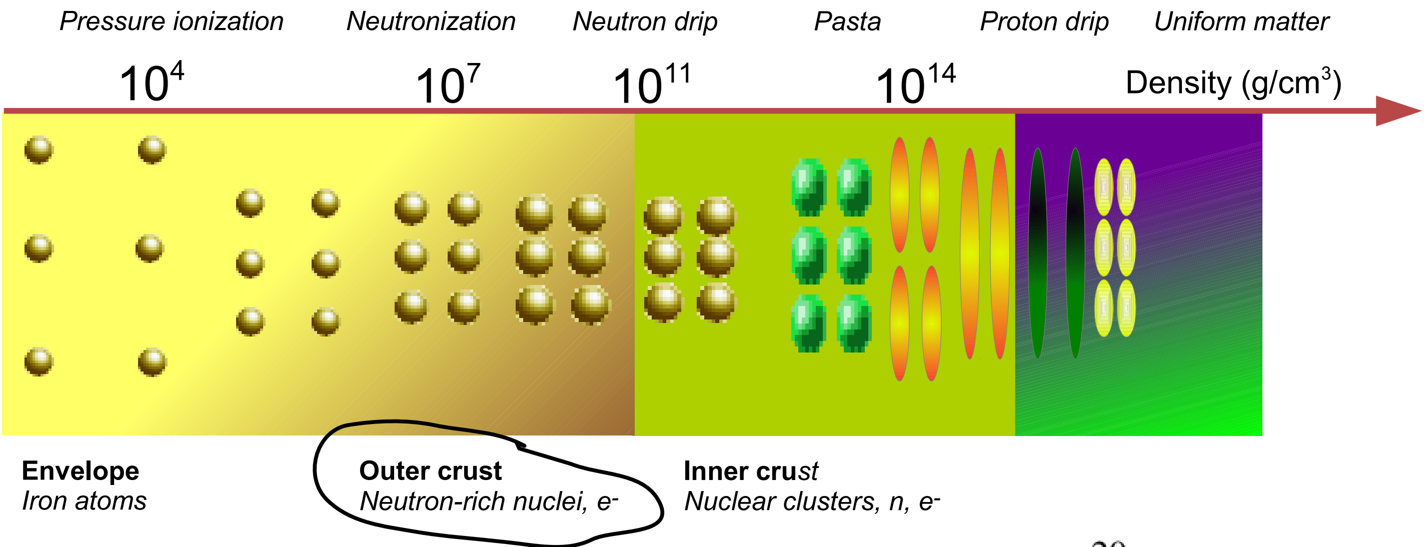
Light systems - astrophysics

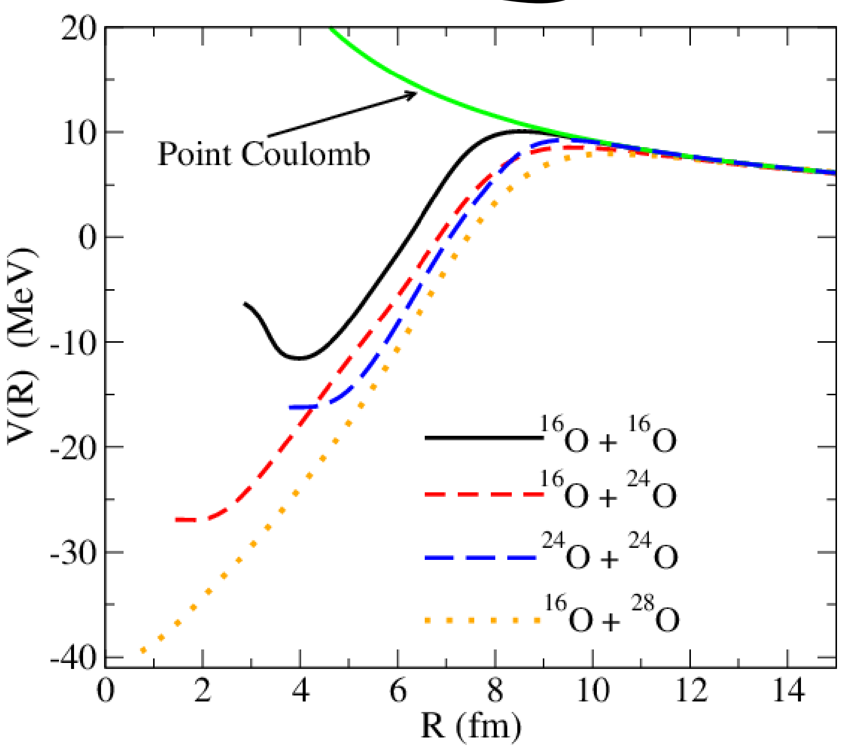
Microscopic Study of the Triple-α Reaction
A.S. Umar, J.A. Maruhn, N. Itagaki, and V.E. Oberacker, **PRL** 104, 212503 (2010)
Linear-Chain Structure of Three-Alpha Clusters in ^{12}C, ^{16}C, and ^{20}C
J.A. Maruhn, N. Loebl, A.S. Umar, N. Itagaki, M. Kimura, H. Horiuchi, and A. Tohsaki, **MPL** A, 25, 1866 (2010)
Localization in light nuclei
P.-G. Reinhard, J. A. Maruhn, A. S. Umar, and V. E. Oberacker, **PRC** 83, 034312 (2011)
Microscopic composition of ion-ion interaction potentials
A.S. Umar, V.E. Oberacker, J.A. Maruhn, and P.-G. Reinhard, **PRC** 85, 017602 (2012)
Microscopic sub-barrier fusion calculations for the neutron star crust
A.S. Umar, V.E. Oberacker, and C. J. Horowitz, **PRC** 85, 055801 (2012)

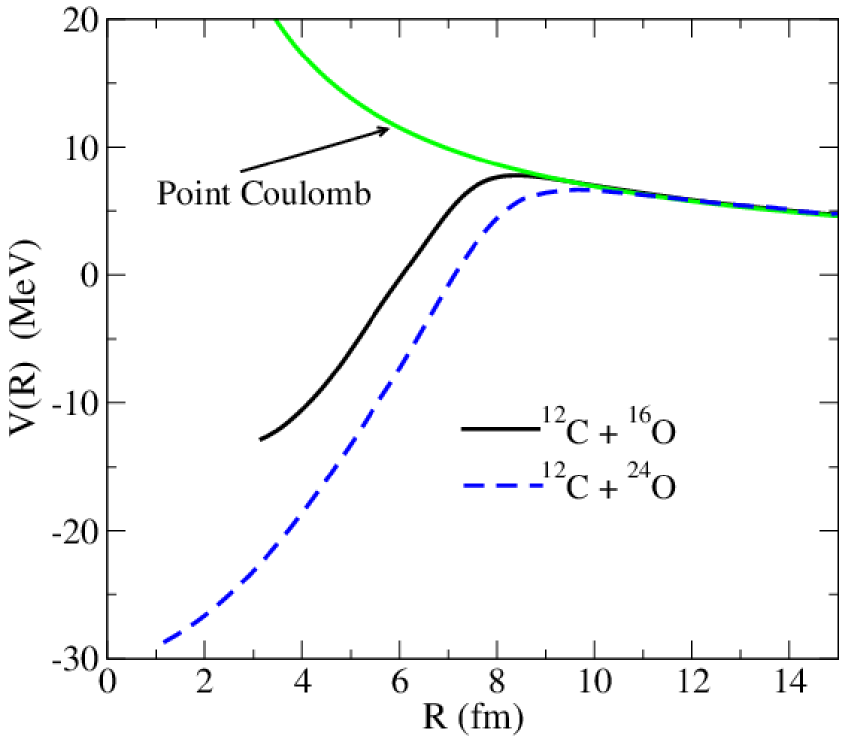
Fission and miscellaneous

Microscopic description of nuclear fission dynamics
A.S. Umar, V.E. Oberacker, J.A. Maruhn, and P.-G. Reinhard, **JPG** 37, (2010) 064037
Single-particle dissipation in a time-dependent Hartree-Fock approach studied from a phase-space perspective
N. Loebl, A. S. Umar, J.A. Maruhn, P.-G. Reinhard, P.D. Stevenson, and V. E. Oberacker, **PRC** 86, 024608 (2012)
Time-dependent coupled-cluster method for atomic nuclei
D. A. Pigg, G. Hagen, H. Nam, and T. Papenbrock, **PRC** 86, 014308 (2012)

Reactions Relevant for Neutron Star Crust



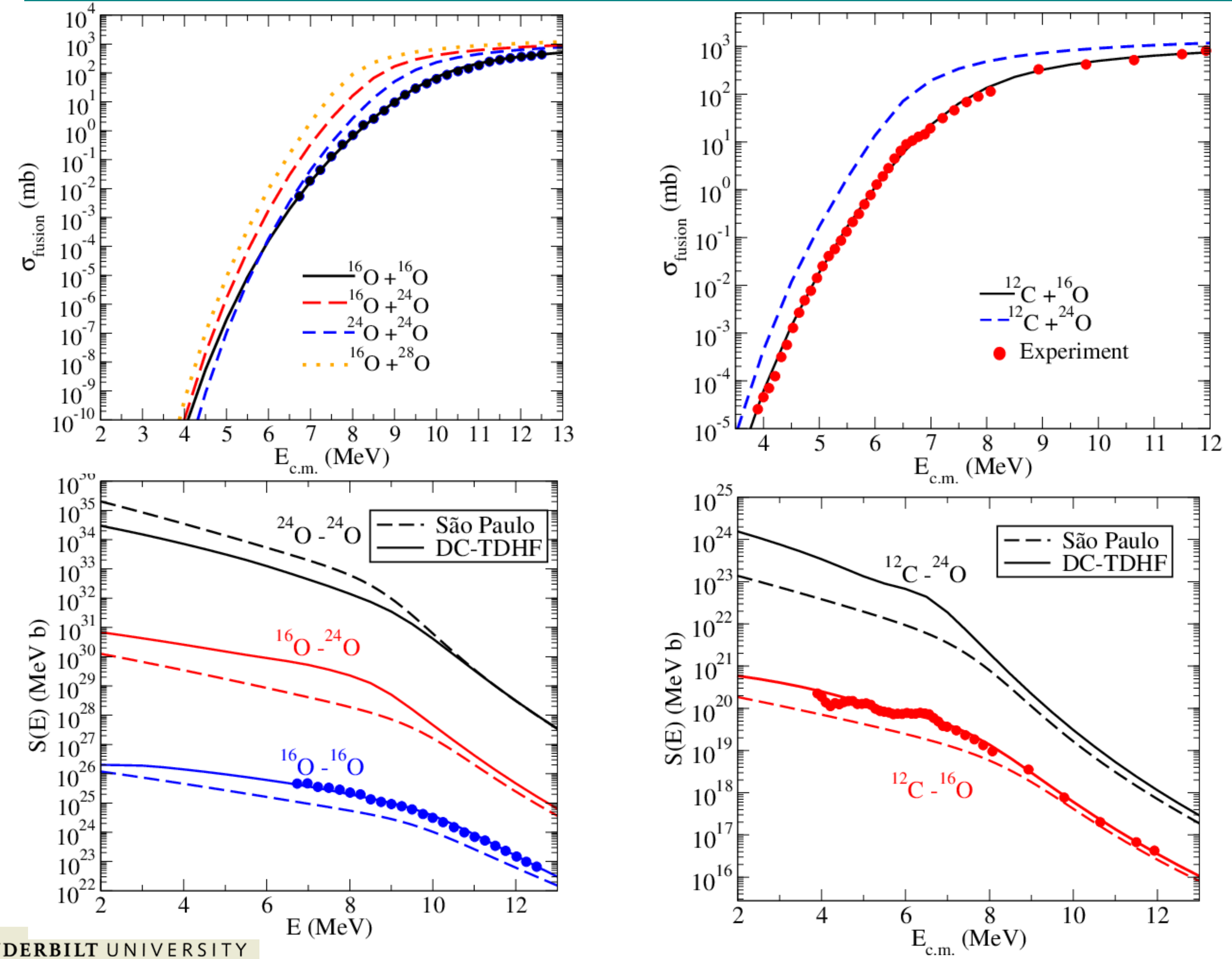




VANDERBILT UNIVERSITY

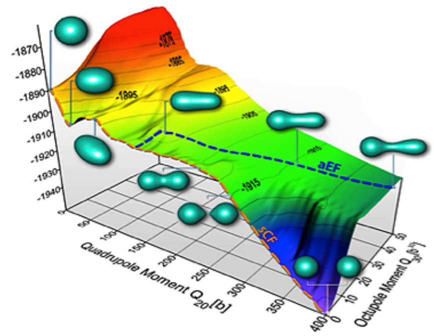
A.S. Umar, V.E. Oberacker, and C. J. Horowitz, **PRC** 85, 055801 (2012)

S-Factors for Reactions Relevant for Neutron Star Crust



Nuclear Fission

- Almost all of the theoretical work focuses on static fission barrier properties
- Static-Adiabatic self-consistent calculation of barriers in terms of collective degrees of freedom
- Improved by configuration mixing, projections, etc.



Baran, Staszczak, Dobaczewski, Nazarewicz, J. Mod. Phys. E16, 443 (2007)
(HF+BCS, GCM+GOA+Cranking)

Pei, Nazarewicz, Sheikh, Kerman, Phys. Rev. Lett. 102, 192501 (2009)
(Finite-temperature DFT or HFB)

Burvenich, Bender, Maruhn, Reinhard, PRC 69, 014307 (2004)
(RMF + Skyrme HF systematics)

Bender, Heenen, Bonche, PRC 70, 054304 (2004)
(HF+BCS, angular momentum projection)

Dobrowolski, Goutte, Berger, J. Mod. Phys. E17, 81 (2008)
(HFB with Gogny + GCM)

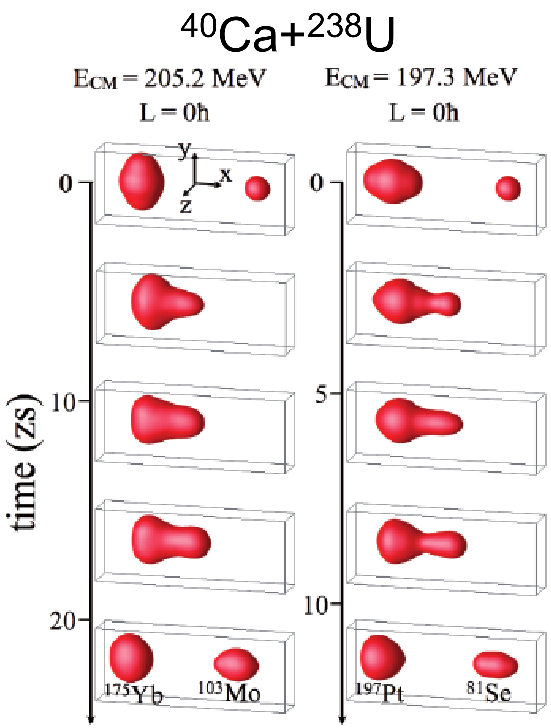
Types of Fission Dynamics

- Spontaneous or Prompt FIssion
- Induced Fission (neutrons etc.)

Start from ground or excited state

- Quasi-Fission
- Fusion-Fission

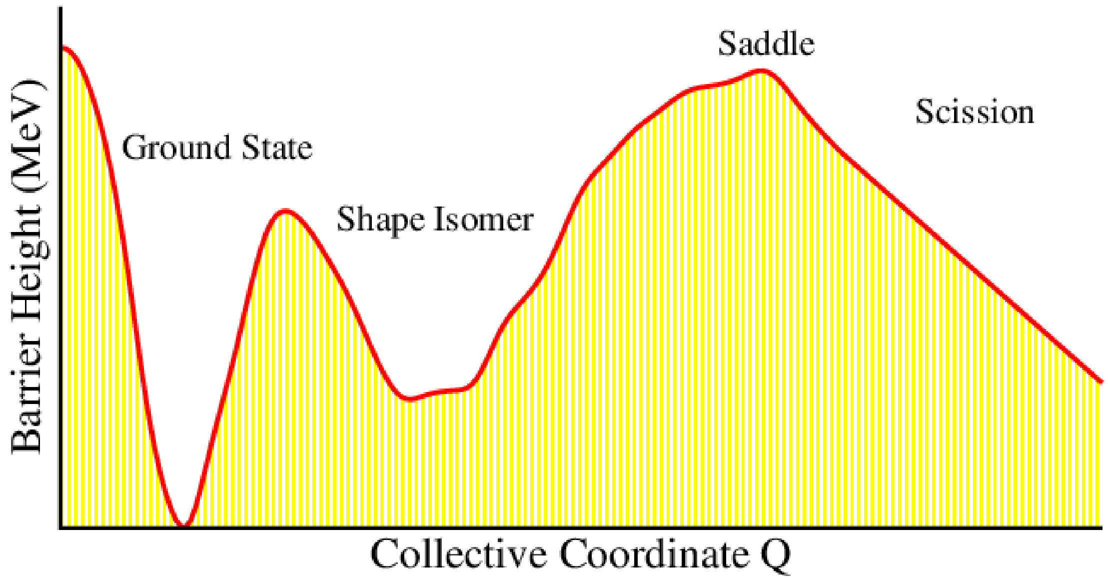
Product of heavy-ion reactions
Important for superheavy formations



QF and FF may be amenable to study directly with TDDFT
(see C. Simenel, EPJA **48**, 152 (2012))

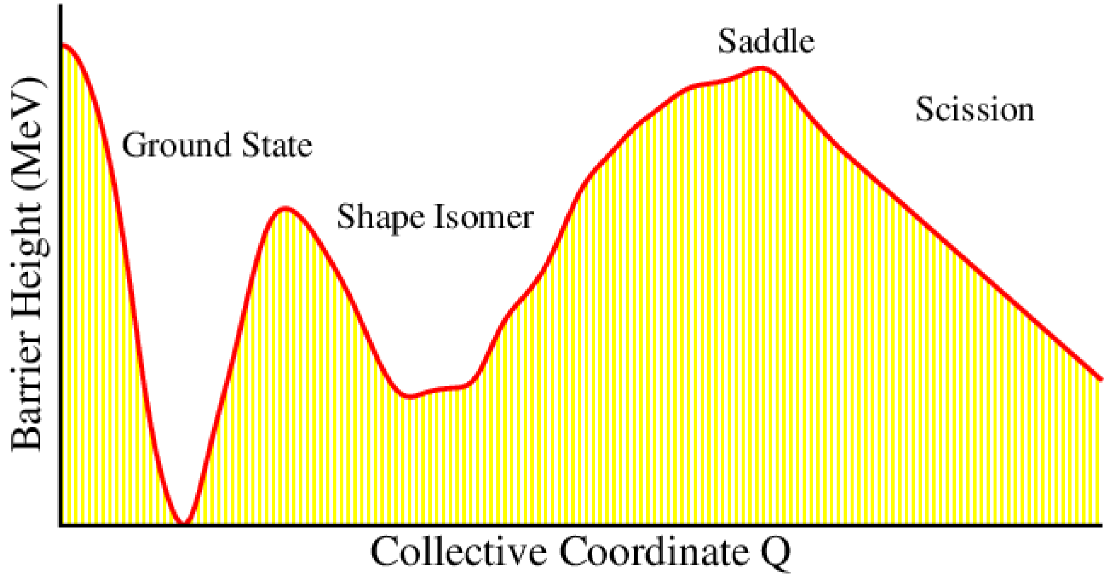
We are currently studying QF in $^{48}Ca+^{248}Cm$

Dynamics of Nuclear Fission - I



- Effective potential barrier description may be an oversimplification
- In a many-body system different states see different barriers
- Dynamical system may not follow the static PES path
- Certain symmetry breakings are not included in adiabatic-static approach
- How do we restore broken symmetries?

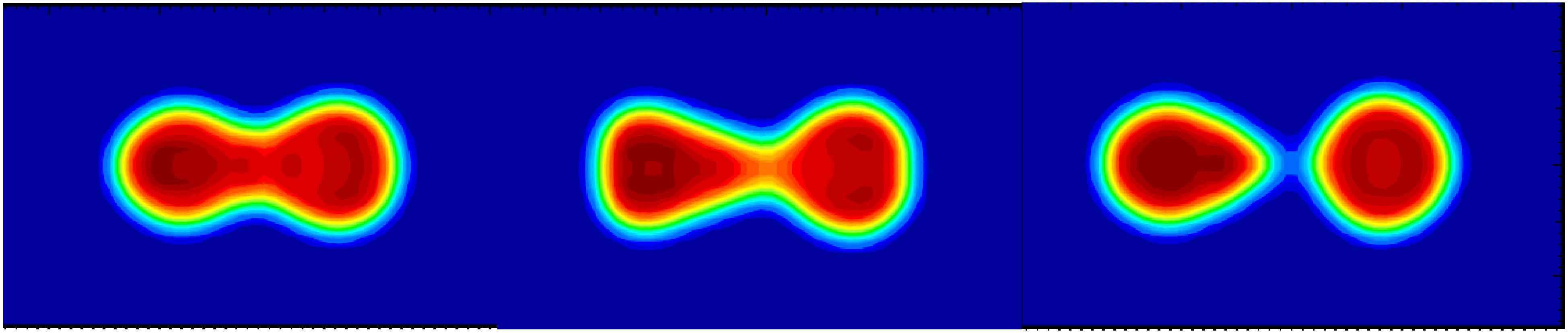
Dynamics of Nuclear Fission - II



- Understanding the *dynamics* of prompt and induced fission is a challenge
- By dynamics we mean real-time microscopic dynamics – not in collective subspace
- Is TDHF-TDDFT suitable to study some aspects of fission dynamics?
- Periodic TDHF equations are too hard to solve for spontaneous fission
- Multi-configuration or stochastic dynamics may be necessary

Fission Efforts

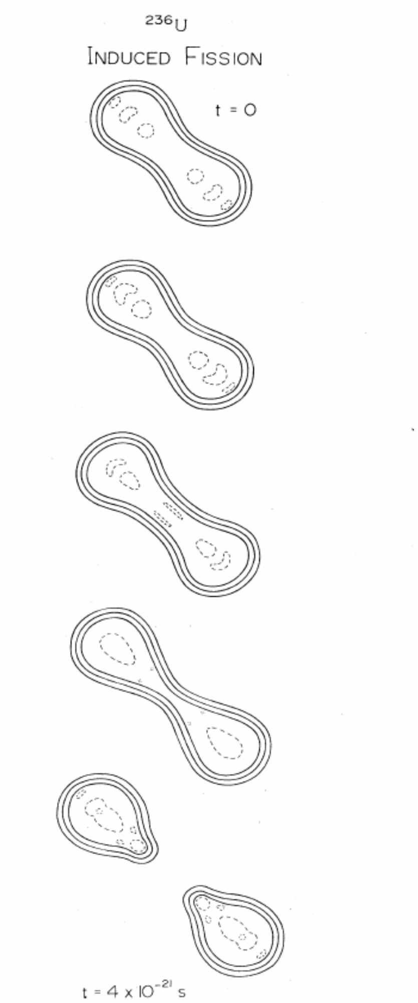
- Historical attempts to use TDHF for fission dynamics
- Our attempts to use TDHF for fission dynamics
- Fusion-fission, quasi-fission studies using TDHF and DC-TDHF
- One success – not yet explained!



Fission – TDHF - History

- Most well known attempt to study fission via TDHF:

Dynamics of Induced Fission, ***Negele, Koonin, Möller, Nix, Sierk, PRC 17, 1098 (1978)***



- Nucleus is initialized via quadrupole constraint with energy 1 MeV below and beyond the saddle point.

- Crude numerical methods; axial symmetry, reflection symmetry, no spin-orbit, BKN force.

- To break symmetries and couple angular momenta time-dependent BCS was introduced in conjunction TDHF calculations. Only reason?

- Results depend strongly on gap parameter.

ergies or ternary α events. Furthermore, there exists a conceptually clear program in which, in principle, the initial adiabatic TDHF wave function provides an ensemble of initial conditions from which all fission observables may be unambiguously calculated microscopically without any free parameters.

Fission – TDHF - History

- Other fission studies using TDHF:

Dietrich, Nemeth, Z. Phys. A300, 183 (1981)

- Fission studied with TDHF for slabs by giving a collective boost to the initial HF state
  1. Fission was not seen when using small velocity field for boost but higher fields resulted in fission.
  2. Instead, the initial states were constructed by exciting single particle states into higher unoccupied states. Easier to induce fission from these configurations.

Okolowicz, Irvine, Nemeth, J. Phys. G 9, 1385 (1983)

- Nucleus is initialized inside and just outside of the barrier and given a **quadrupole boost**
- Two different method used to create the initial HF states:
  1. A single center regular HF state – no fission achieved for different initializations.
  2. A spherical two-center initial HF state leads to fission almost always.

Jung, Cassing, Mosel, Cusson. NP A477, 256(1988)

- Studied multi-fragmentation and fission using TDHF (very adhoc).
  1. Initialize by multiplying density with some r-dependent function c(**r**).
  2. Boost by exp(i**k**·**r**) but with **k** having different sign for different parts of the nucleus. Limiting $k > 0.5\ \mathrm{fm}^{-1}$

Fission – TDHF – Suggestion!

- In studying fusion with TDHF we sometimes see states that are coalesced and show kind of a resonance behavior.
- For light nuclei these have been associated with shape-isomers and nuclear molecular resonances.
- In heavy systems these intermediary states may:

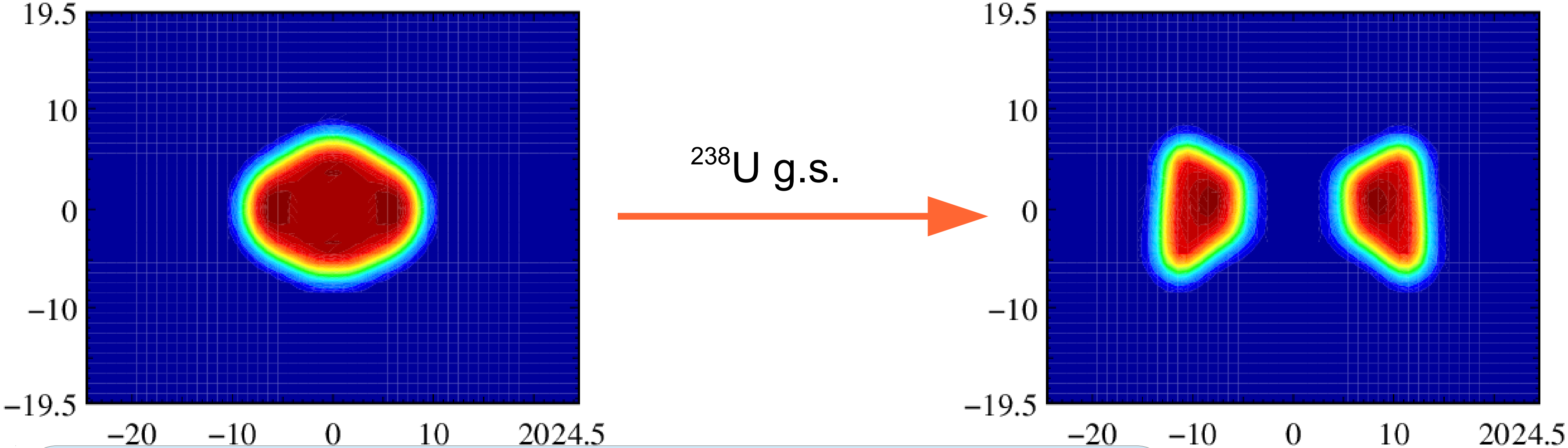
K.T.R. Davies et al.
PRC 24, 2576 (1981)

bits a kind of resonance behavior. Therefore, it is tempting to speculate[52] that these characteristics might be associated with single-particle wave functions which are approximate eigenstates[53] of the instantaneous Hartree-Fock (HF) Hamiltonian $h(t_f)$ as $t_f \to \infty$. The many-body wave function constructed from these single-particle wave functions could then be considered a "transition state" to processes that are not taken into account in TDHF theory.[52]

[52]Private comm. A.K. Kerman

Initiating Fission with Boosts

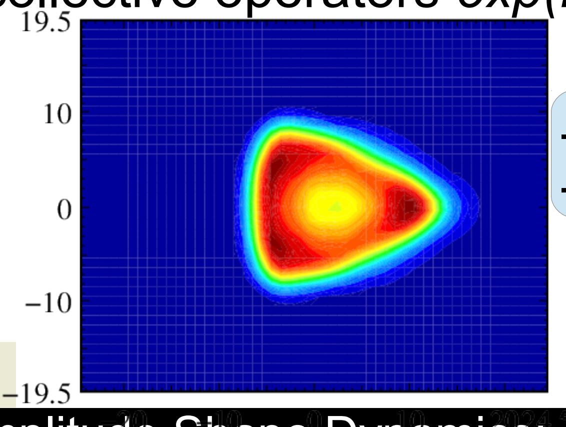
- Simple *exp(i**k**·**r**)* boost with ***k*** having opposite sign for each half



- k_x ~ 0.4 fm^{-1} limit for breakup
- about 700 MeV excitation!
- symmetric fission
- asymmetric boost makes the c.m. move, box problems

Bertsch et al.
PRC 17, 1646 (1978)
find E/A > 2 MeV

- Boost using collective operators $exp(i\alpha q_{20} + i\beta q_{30})$ etc.



- Similar to above case, need very large boosts
- Is there a magic boost operator?

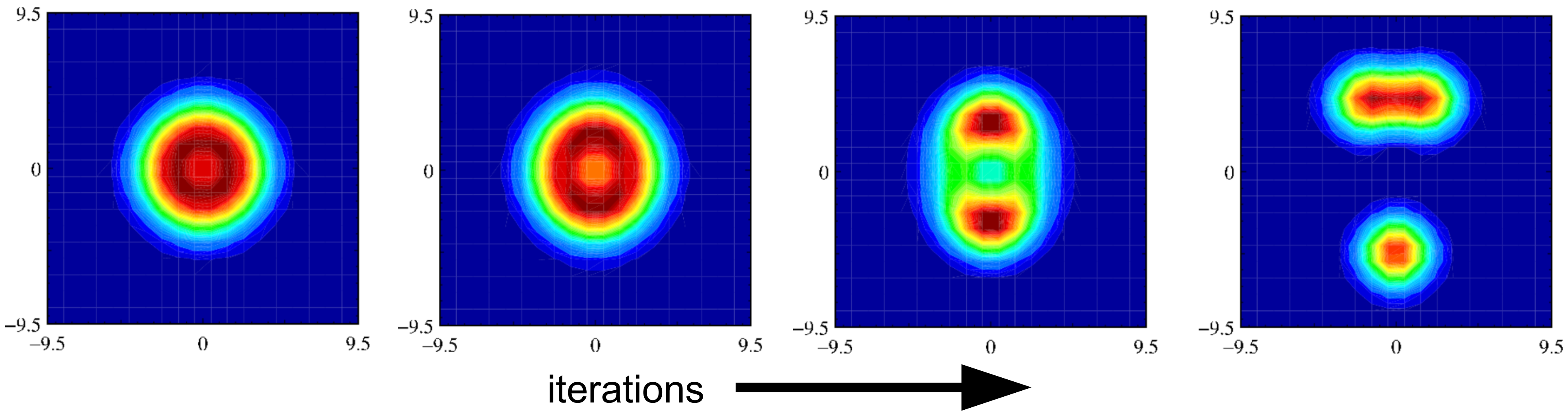
Initializing with excited states

- Construct excited states by promoting s.p. levels

- generate g.s. wavefunctions and store
- read them into the Gram-Schmidt routine when running HF again
- orthogonalize selected state(s) to all of the g.s. wavefunctions

$$\langle \Phi | \Phi' \rangle = det\left(\langle \varphi_i | \varphi'_j \rangle \right) = 0$$

- For light nuclei very interesting breakups occur during the static iteration!

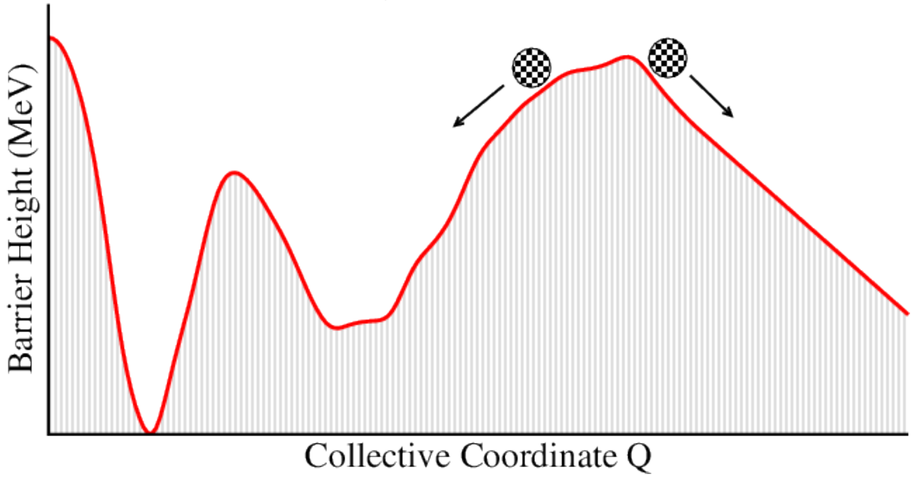


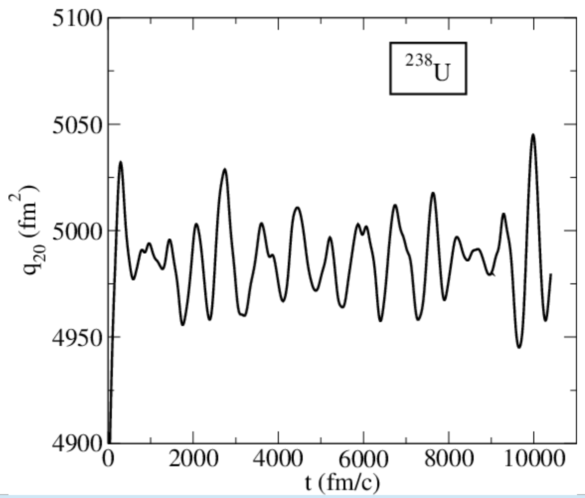
12C* promote 1*p* to 2*s*

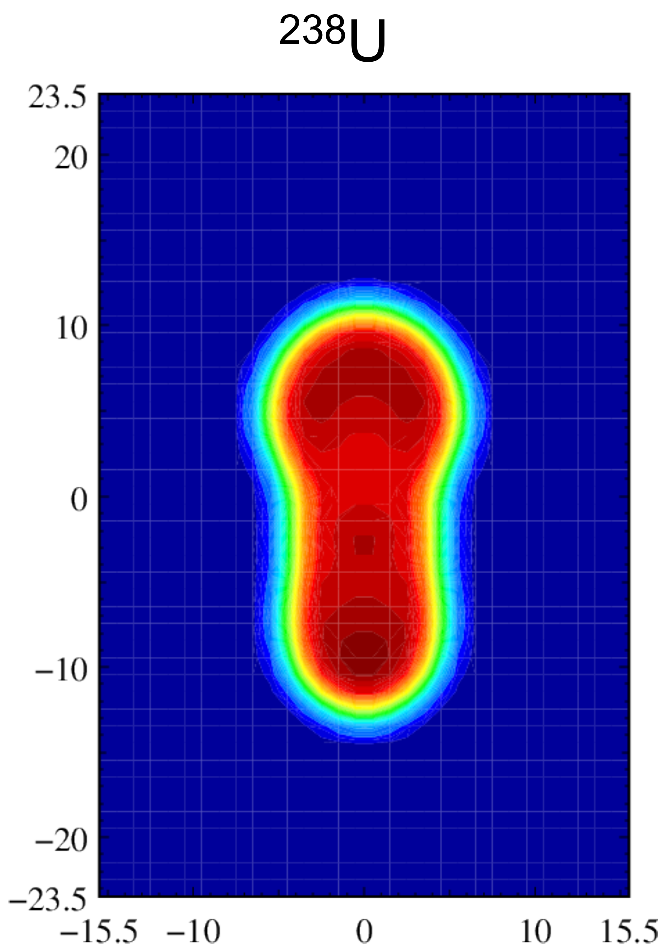
- Harder for heavier systems – the effect not as pronounced
- Is there a way to select particular states to excite in induced fission?

Roll Down Approach

- Initialize the system close to the saddle point and let it evolve via TDHF



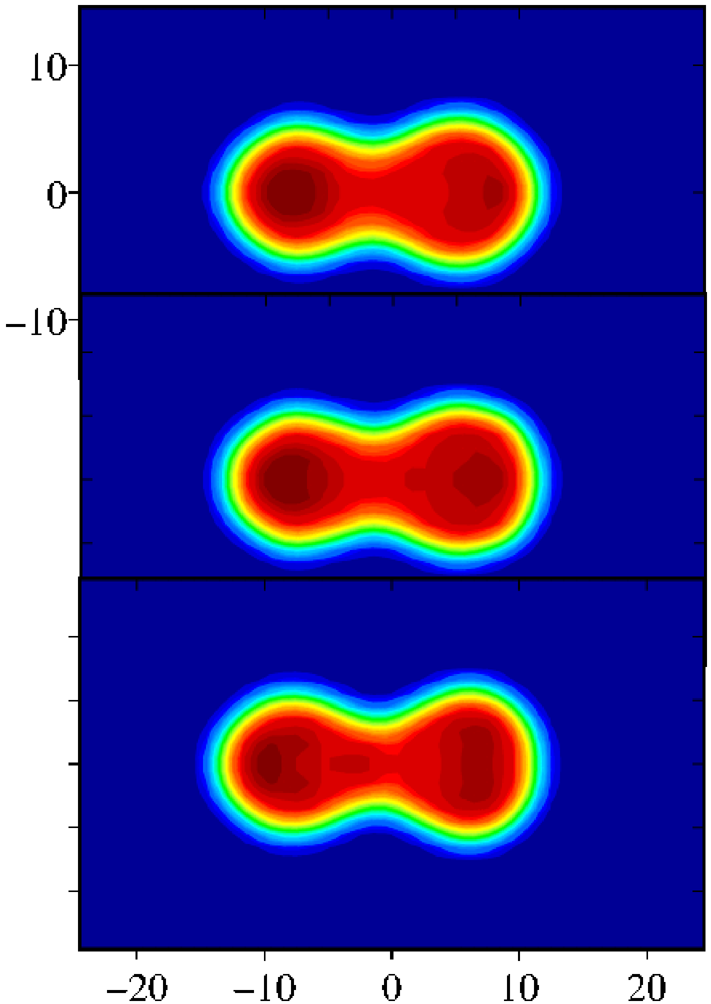




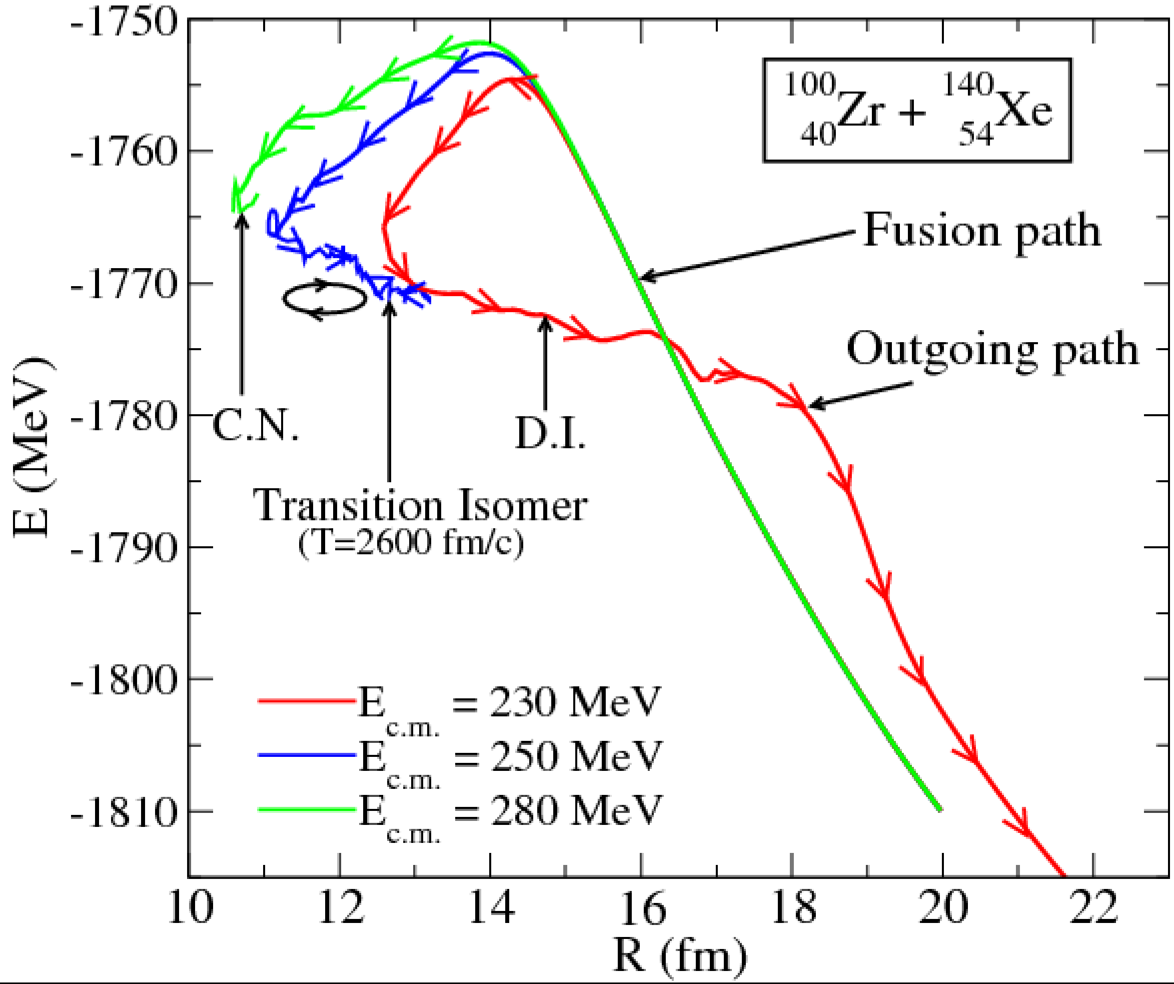
- with no boost or reasonable collective boosts system does not fission
- in all of these the system has difficulty reorganizing to have two center configuration
- tried with and without pairing (frozen in TDHF)

Different approach – fission after a collision

- Recently, we have investigated fission after a low-energy collision
- We have studied collision of $^{100}Zr + ^{140}Xe \rightarrow ^{240}Pu^*$
- Long-time oscillatory behavior, followed up to 2600 fm/c (Ecm=250 MeV)

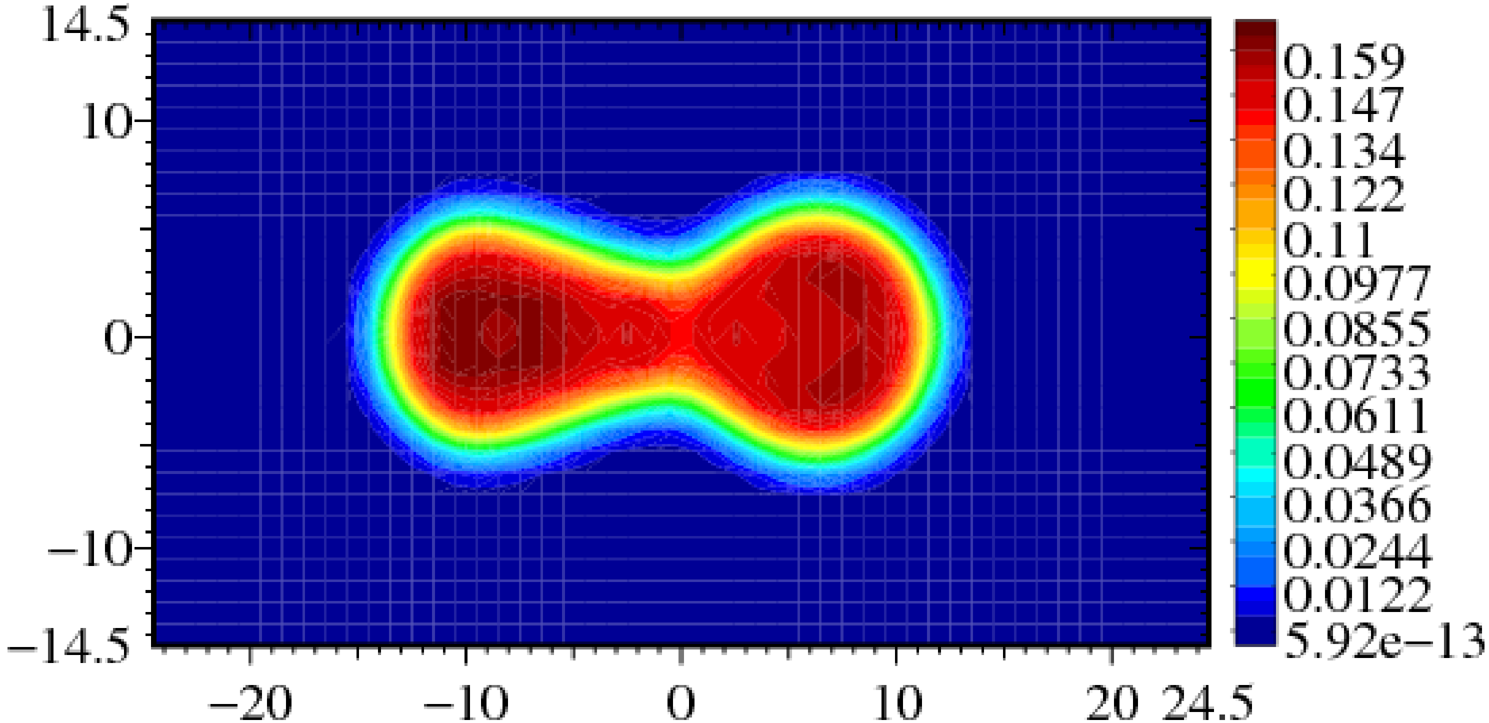


DC-TDHF



Unconstrained Fusion/Fission Isomer

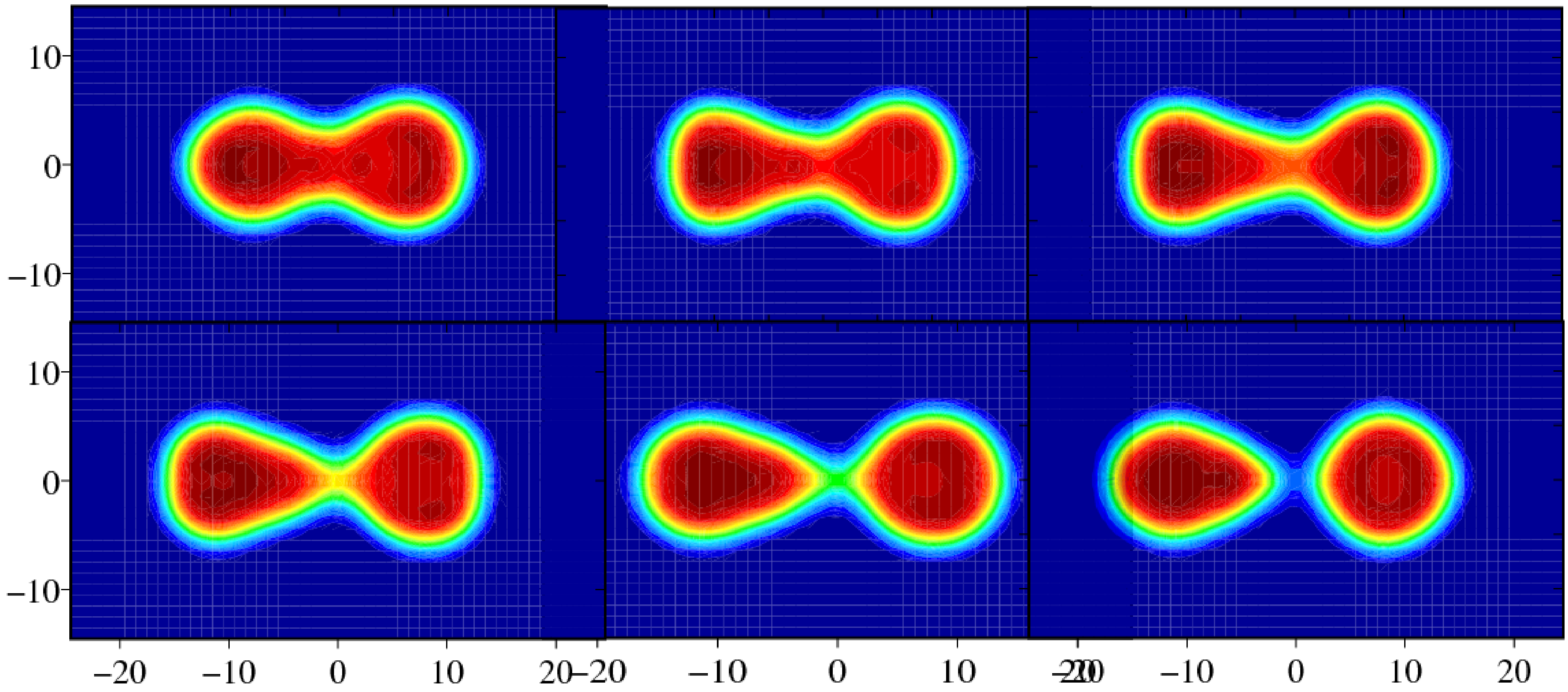
- Start from TDHF fusion state and minimize energy by DC
- Starting from DC-TDHF result minimize energy with no constraint



β_2=2.27 Q_{20}=230 b Q_{30}=-28 $b^{3/2}$

Initiation of Fission

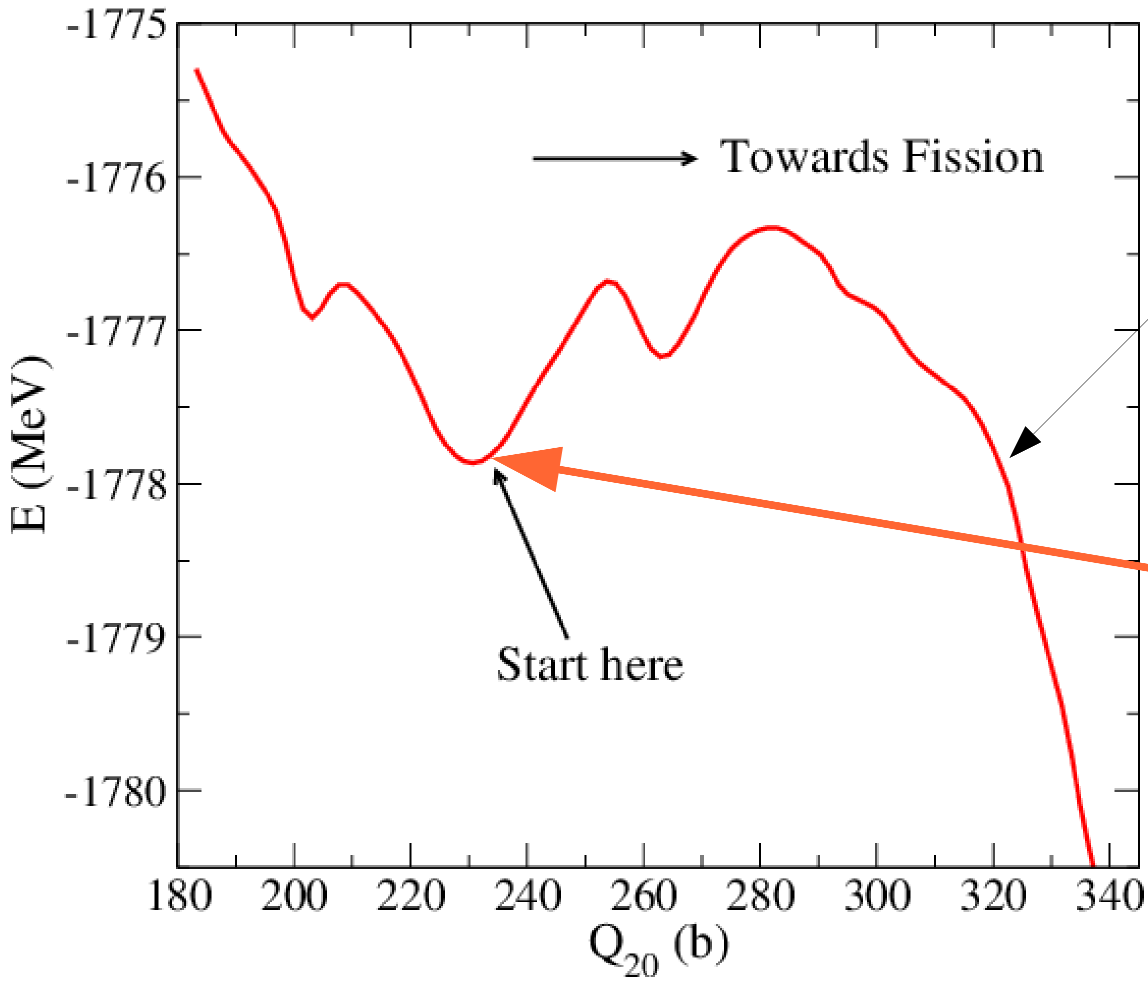
- Boost this state by a unitary collective boost operator $e^{ip\,q_{20}(\boldsymbol{r})}$ where for p = 0.0025 we get 7.5 MeV excitation



SHOW MOVIE!

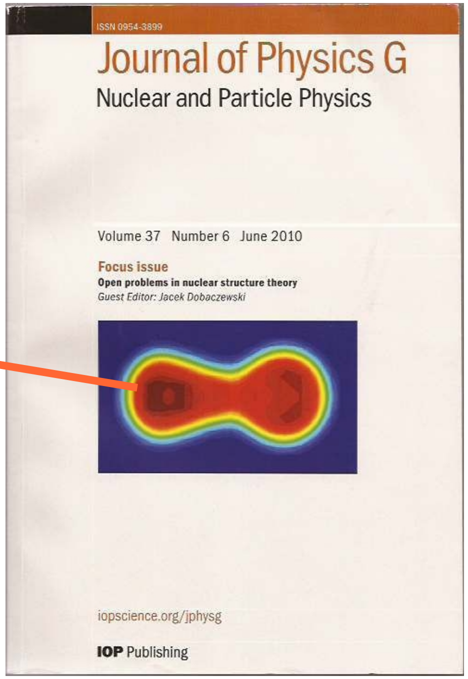
Fission Path

- Follow fission path with DC-TDHF



A_1, Z_1=106, 42

A_2, Z_2=134, 52



Further Experimentation and a Special Case

- Obtained the 238U initial state from Skyax with BCS-LN (SLy4)

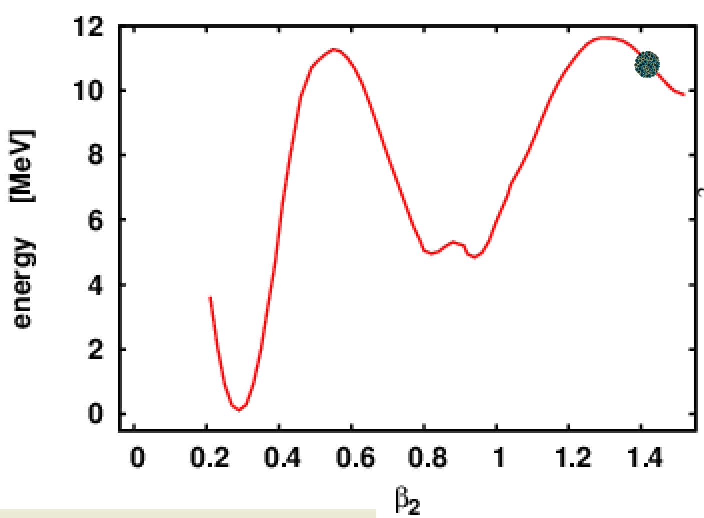
  a) Do a density-constraint to reproduce the same density in 3D with no L-N

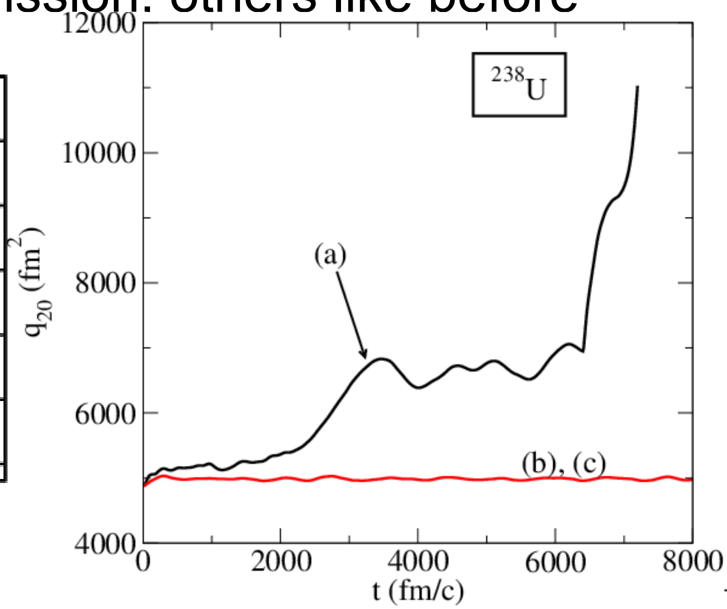
  b) Do a density-constraint to reproduce the same density in 3D with L-N

  c) Do a q2 constraint to reproduce the same density in 3D with L-N

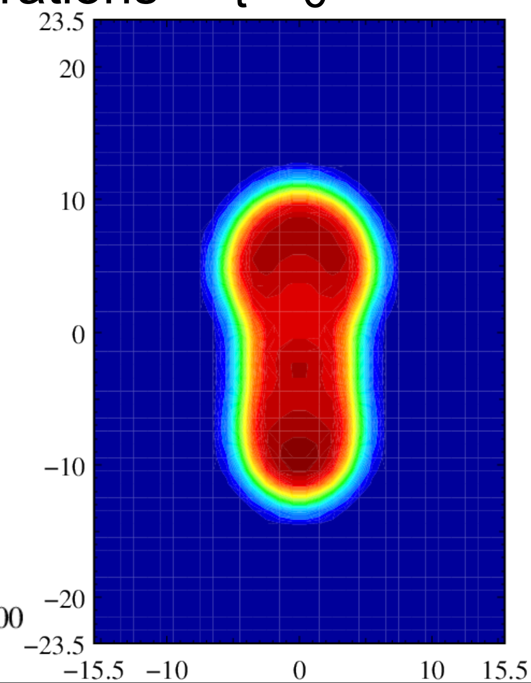
Energies (no c.m. correction): $E_{(a)}$ = -1761.2 MeV
$E_{(b)}$ = -1762.9 MeV ($E_{g.s.}$=-1772 MeV)
$E_{(c)}$ = -1763.4 MeV

- Initialize TDHF with **<u>no boost</u>** using the above configurations
- Only case (a) can go to fission, others like before

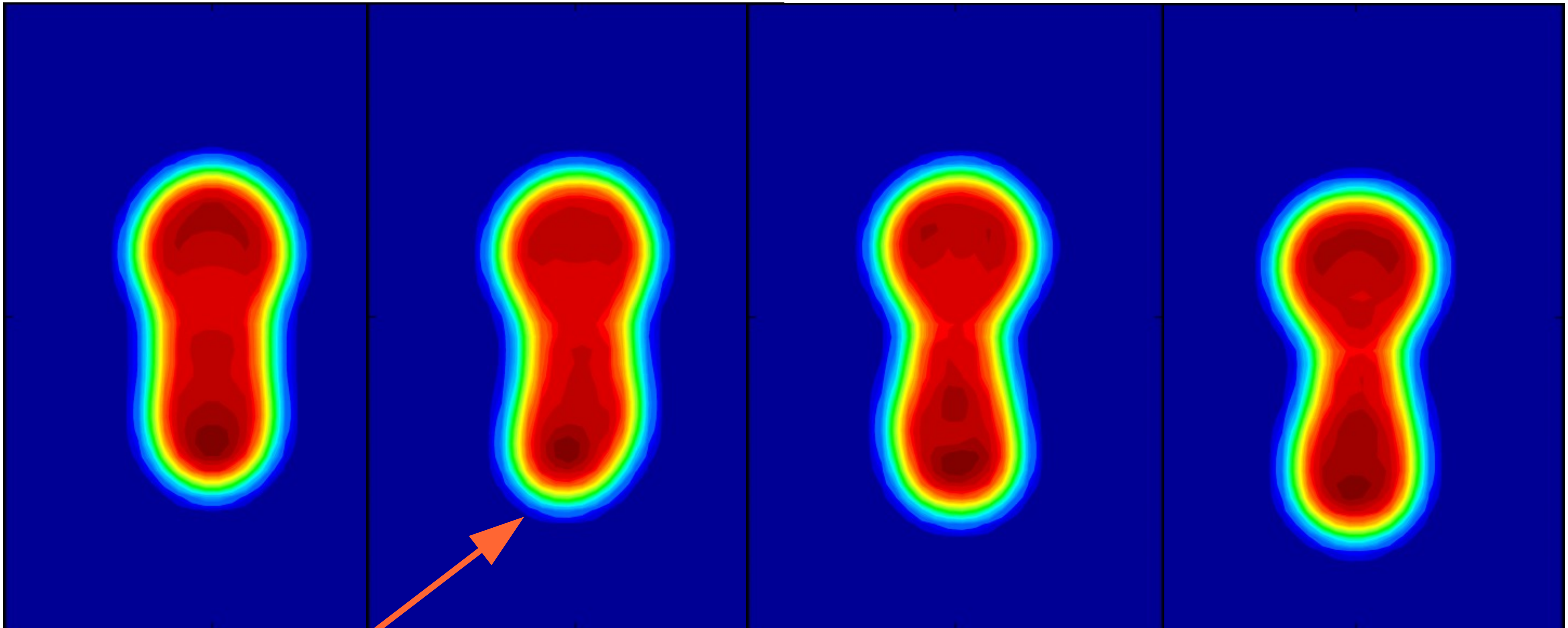




t = 0



Details of the Dynamics with No Boost



t=0

t=6400 fm/c

Boost t=6400fm/c state with |**k**|=0.02-0.03 fm^{-1} → SHOW MOVIE!

E*=5-10 MeV

Note the q_{31} symmetry breaking (also q_{11})!

A_1, Z_1 = 134.5, 51.8

A_2, Z_2 = 103.5, 40.2

How Do We Make Progress?

We can say that we have a reasonable handle on fusion

We may have a handle on quasi-fission

Understanding of fission dynamics is an outstanding challenge in NP

Can we describe many-body quantal fission with TDDFT? Does the KS theory apply here? If yes, what are the ingredients?

Issues with initialization must be better understood for prompt and induced fission. When a neutron transfers its energy to the nucleus what mode or state does this energy go into? What is this state in TDDFT?

Too many variables in the problem, collective boost operator, boost strength, different initial and final states, ...

Brute numerical force may not be sufficient – need more insight