

Nuclear Collective Dynamics and Density Constrained TDHF

Sait A. Umar and Volker E. Oberacker

Sait
Umar



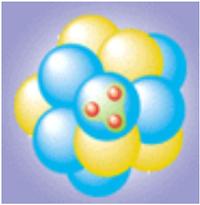
Volker
Oberacker



Research supported by:
US Department of Energy, Division of Nuclear Physics

JUSTIPEN-LACM '07, ORNL





Established Microscopic Methods (CHF-ATDHF)

• Advantages

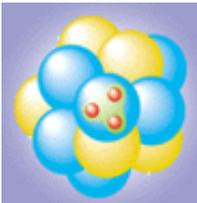
- Fully microscopic description of nuclear PES
- Use same microscopic interaction used in g.s. calculation
- Gives global information on collective potential
- Quantization via ATDHF

• Shortcomings

- Artificial introduction of constraining operators
- Collective motion not necessarily confined in constrained phase space
- Static adiabatic approximation
- Most energetically favorable state requires sudden rearrangement
- No reason why dynamical system should move along the valley of PES
- CHF calculations seldom produce the correct saddle-point

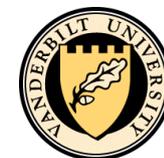
Möller, Sierk, Iwamoto, PRL 92, 072501 (2004)

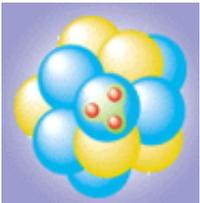




Desired Improvements

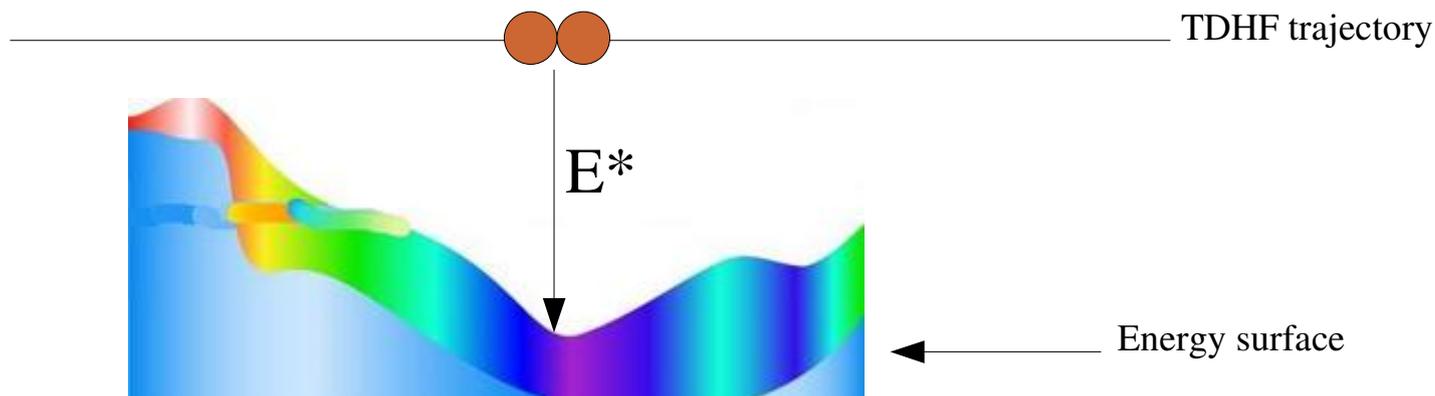
- Explore collective dynamics in terms of mean-field dynamics
 - self-organizing system selects its evolutionary path by itself following the microscopic dynamics.
- Develop dynamical methods for selecting constraining operators
 - which are not known from the outset nor from the static theory
 - should it be coordinate or constraint?
- Go beyond the static adiabatic approximation
 - Explore nonlinear dynamics between single-particle degrees of freedom and collective motion by going beyond adiabatic approximation
- Diabatic states
 - Go beyond single determinant (shape coexistence)



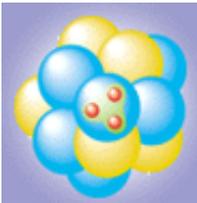


Density Constrained TDHF

- Project unhindered TDHF evolution onto the dynamical PES
 - system selects its evolutionary path by itself
 - constrains all collective degrees of freedom



- Extract internal excitation energy
 - hold the instantaneous TDHF density frozen
 - minimize the energy
 1. Cusson et al. Z. Phys. A320, 475 (1985)
 2. Umar et al. Phys. Rev. C32, 172 (1985)



Numerical Implementation

- Generalize the ordinary method of constraints

- for a single constraint $\longrightarrow \hat{H} \rightarrow \hat{H} + \lambda \hat{Q}$

- for a set of constraints $\longrightarrow \hat{H} \rightarrow \hat{H} + \sum_i \lambda_i \hat{Q}_i$

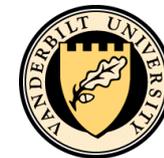
- for density constraint $\longrightarrow \hat{H} \rightarrow \hat{H} + \int d^3 r \lambda(r) \hat{\rho}(r)$

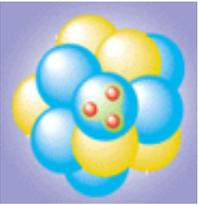
- Works as accurately as a single constraint

$$\hat{\rho}(r) = \sum_{i=1}^A \delta(\vec{r} - \vec{r}_i)$$

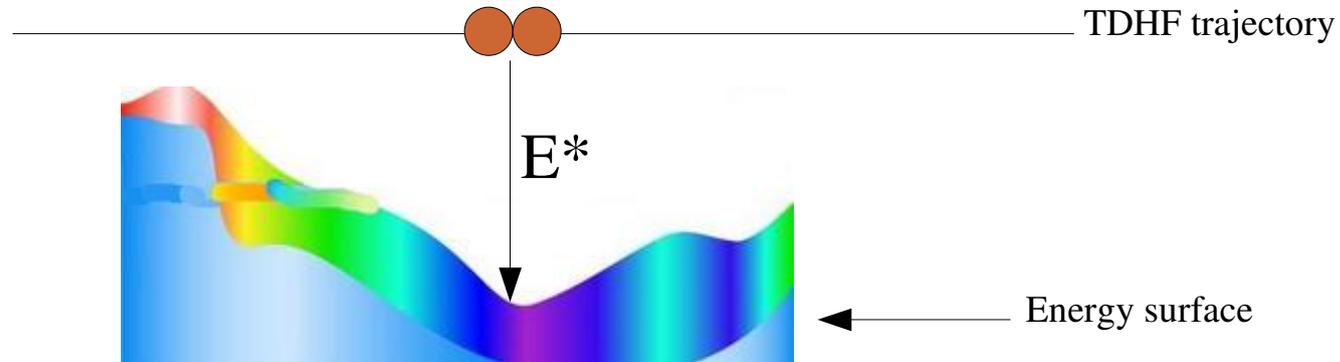
- numerical method for steering the solution to TDHF density is given in:

1. Cusson et al. Z. Phys. A320, 475 (1985)
2. Umar et al. Phys. Rev. C32, 172 (1985)





Excitation Energy

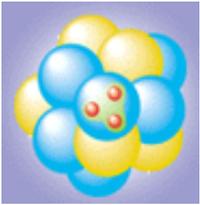


$$E^*(t) = E_{TDHF} - T_R(t) - E_{DC}(t) \longrightarrow \text{Excitation energy}$$

$$E_{TDHF}(t) = \int d^3 r \mathcal{H}(\vec{r}, t) \longrightarrow \text{Total energy is constant (includes kinetic energy)}$$

$$T_R(t) = \frac{1}{2} \mu \dot{R}^2 \longrightarrow \text{Translational kinetic energy}$$

$$E_{DC}(t) \longrightarrow \text{HF energy with constraint on } \rho_{TDHF}(\vec{r}, t) \text{ obtained from TDHF (no kinetic energy)}$$



Ion-Ion Potential

- Total energy in terms of the excitation energy is:

$$E_{TDHF} = T_R + V + E^* \quad \longrightarrow \quad V = E_{TDHF} - T_R - E^* = E_{DC}$$

- E_{DC} contains the binding energies of the two nuclei

$$V(R) \rightarrow E_{DC}(R) - E_{A_1} - E_{A_2} \quad \longrightarrow \quad \text{Subtract binding energies}$$

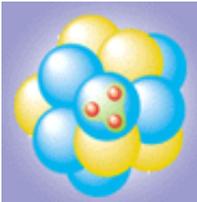
- Asymptotically correct because (no normalization needed):

$$E_{DC}(R_{max}) = E_{A_1} + E_{A_2} + \frac{Z_1 Z_2 e^2}{R_{max}} \quad \longrightarrow \quad V(R_{max}) = \frac{Z_1 Z_2 e^2}{R_{max}}$$

- Contains all of the dynamics present in TDHF; neck formation, particle exchange, deformation to all orders ...

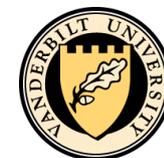
Umar, Oberacker, Phys. Rev. C 74, Rapid Communication, 021601 (2006)

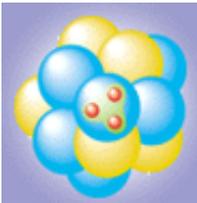




A New Generation TDHF Code

- Unrestricted 3-D Cartesian geometry
 - No fixed reaction plane
 - No rotating frame approximation (2D codes)
 - No reflection symmetry (+z/-z)
- Basis-Spline discretization for high accuracy
- Coded in Fortran-95 and OMP
- Use of modern Skyrme forces with **all** the terms (time even/odd)
- No time-reversal symmetry assumed

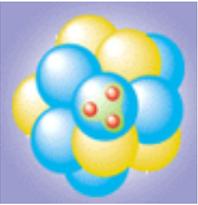




New Physics with TDHF

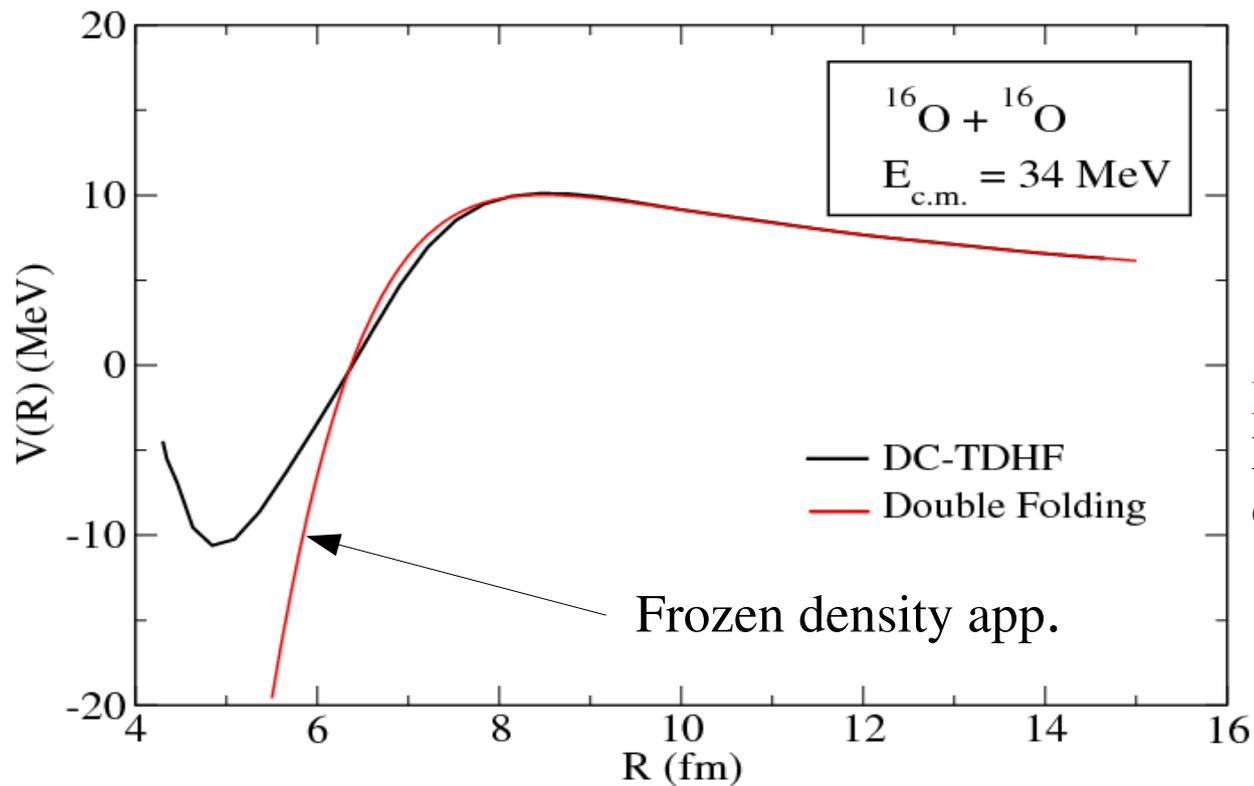
- Much improved fusion cross sections for light systems
 - New terms should be incorporated into Skyrme fits!
Umar, Oberacker, Phys. Rev. C 73, 054607 (2006)
- It is possible to calculate cross sections for deformed nuclei
 - Orientation probability determined from Coulomb excitation
Umar, Oberacker, Phys. Rev. C 74, 124606 (2006)
- New method for calculating ion-ion potentials from TDHF
 - Use the novel method of density constraint during TDHF evolution
Umar, Oberacker, Phys. Rev. C 74, Rapid Comm., 021601 (2006)
- Dynamical deformation effects in subbarrier fusion of $^{64}\text{Ni} + ^{132}\text{Sn}$
 - Study barrier distribution depending on orientation of ^{64}Ni
Umar, Oberacker, Phys. Rev. C 74, Rapid Comm., 061601 (2006)





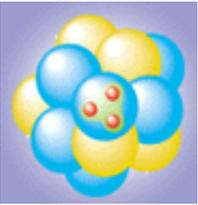
Comparison to Empirical Fusion Potentials

- DC-TDHF potential contains no parameters and normalization

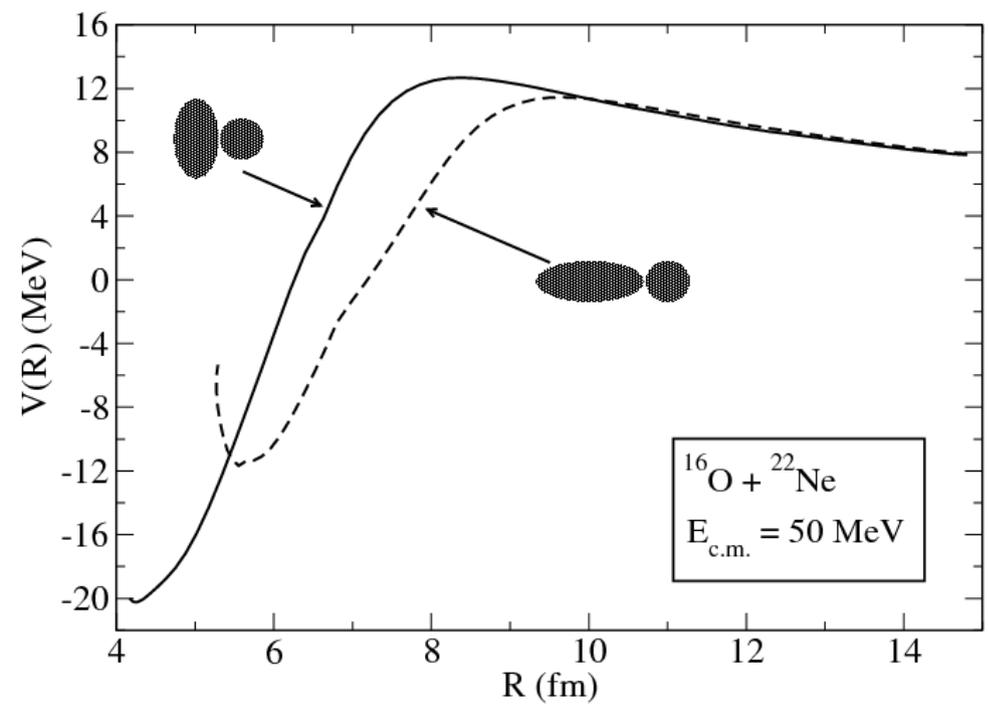
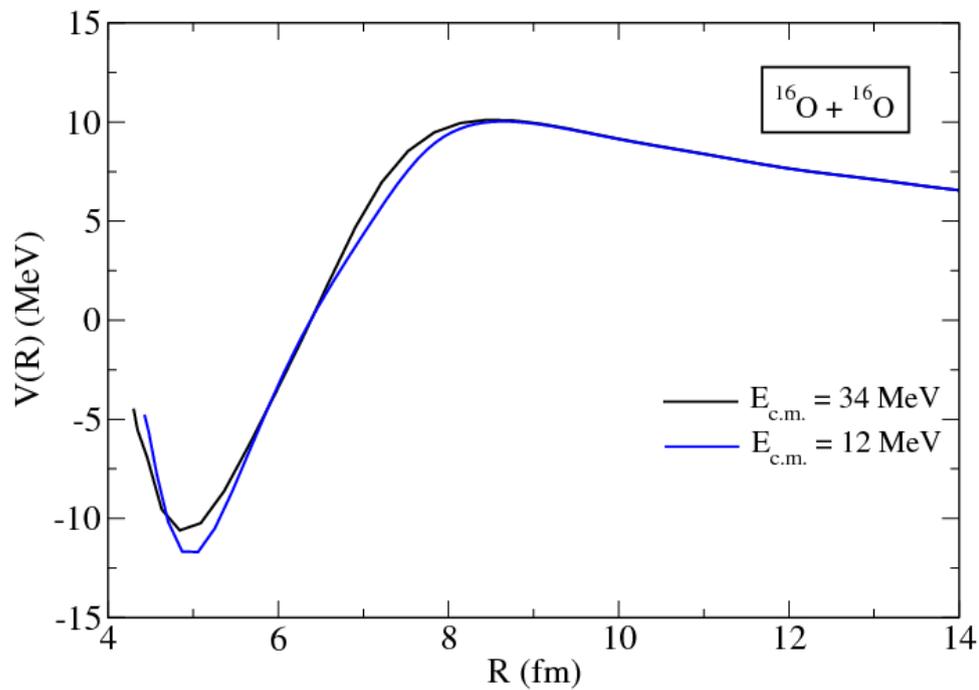


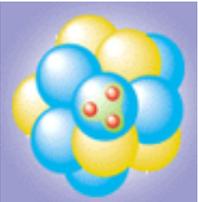
Double folding:
M3Y effective NN interaction
densities from electron scattering

- All comparisons show incredible agreement!



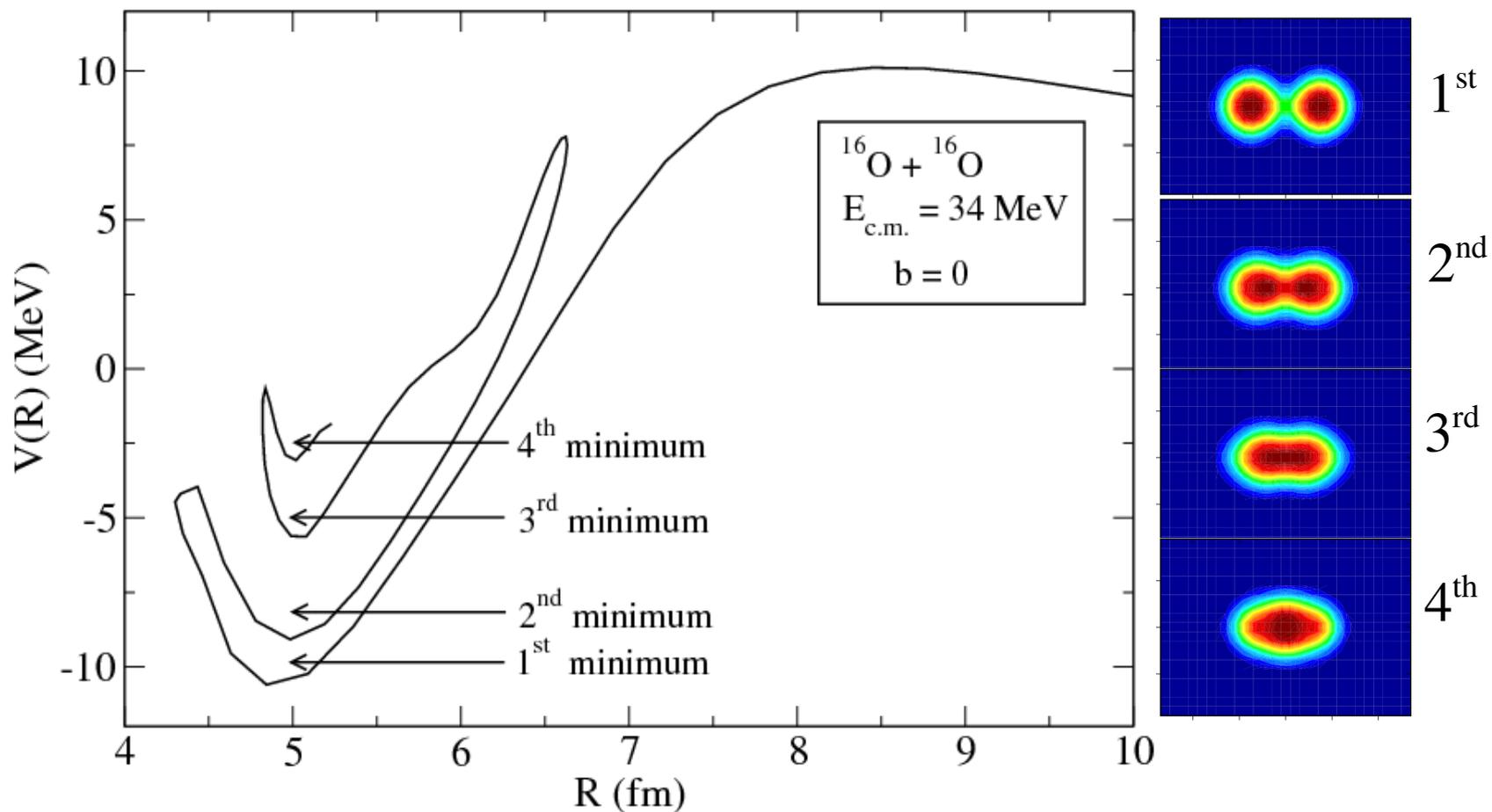
Energy and Orientation Dependence





Approach to Fusion

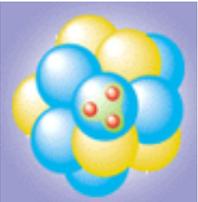
- In fusion system climbs up a potential ladder



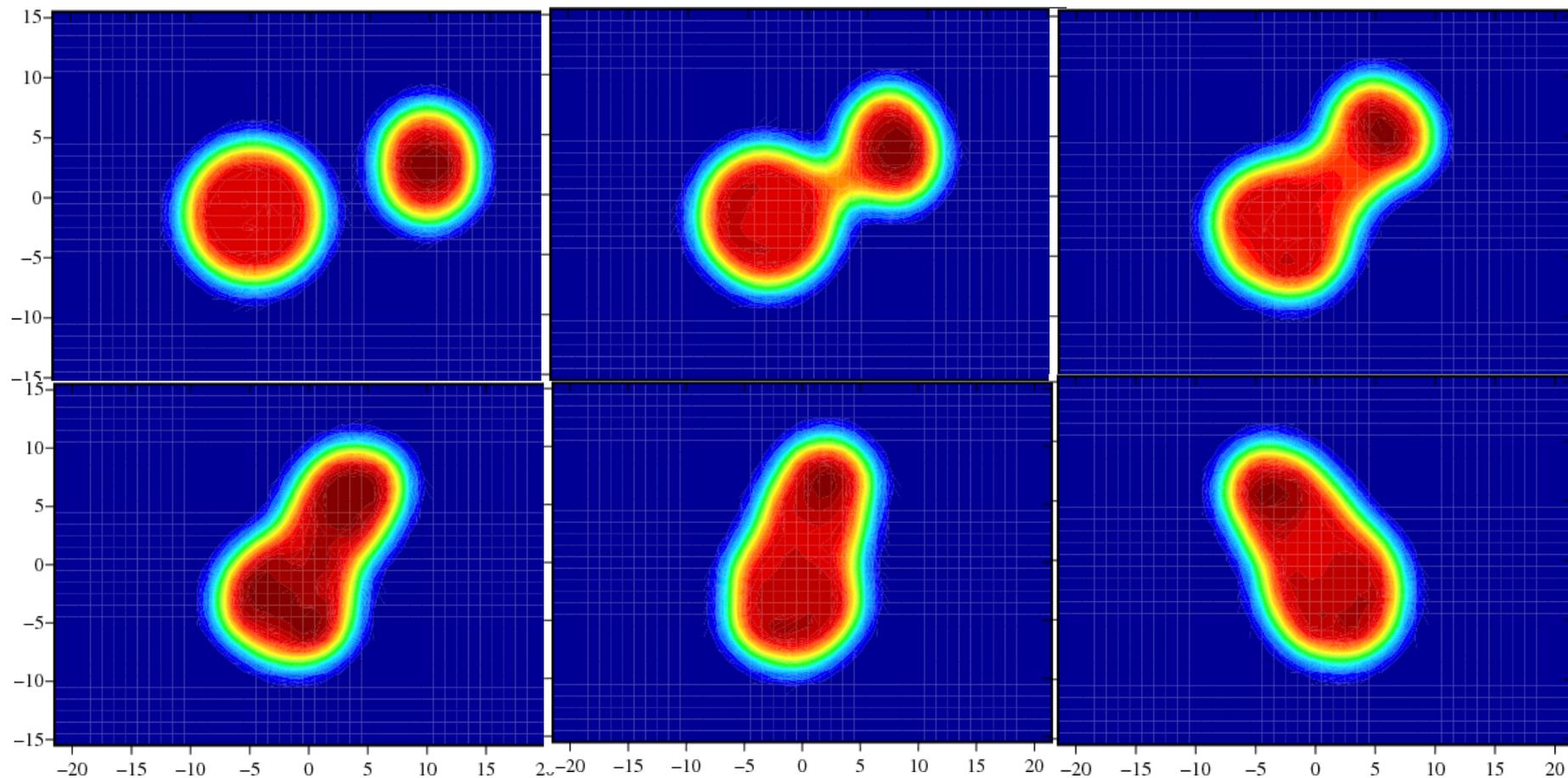
- $R(t)$ eventually becomes the compound radius

JUSTIPEN-LACM '07, ORNL

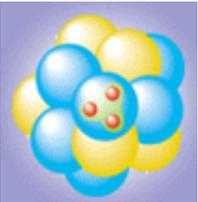




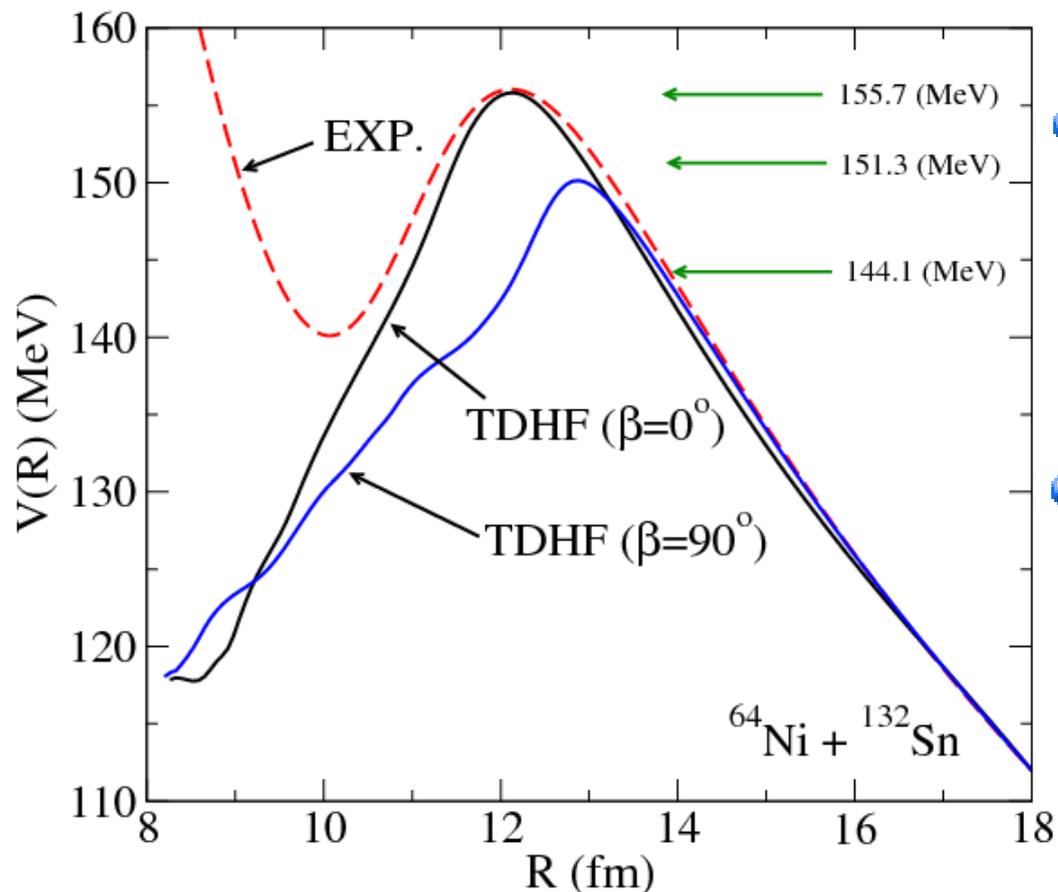
Application to Heavier Systems



● $^{64}\text{Ni} + ^{132}\text{Sn}$, $E_{\text{cm}} = 176 \text{ MeV}$, SLy5, $b = 3 \text{ fm}$



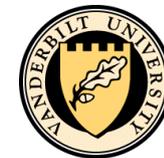
Application to Heavier Systems

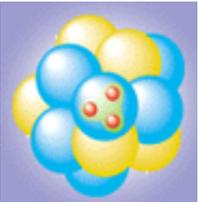


Liang et al., PRL 91, 152701-1 (2003)

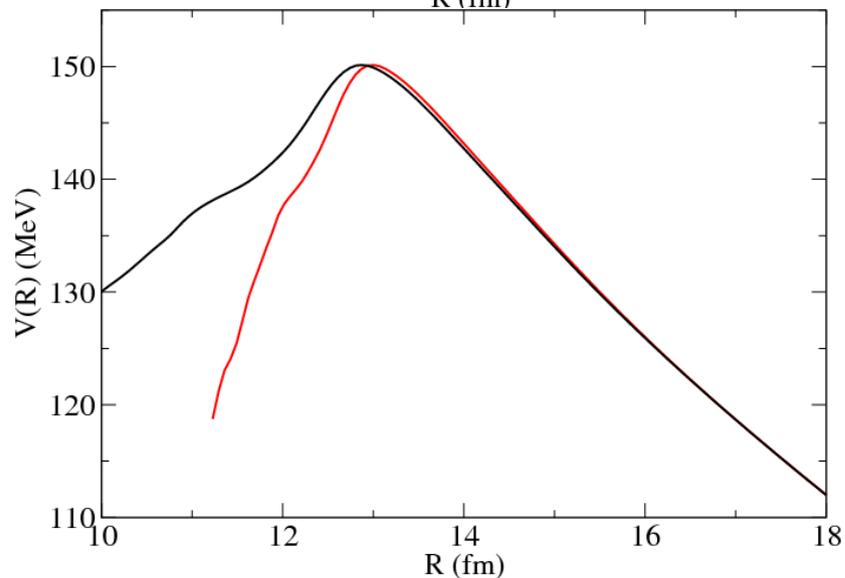
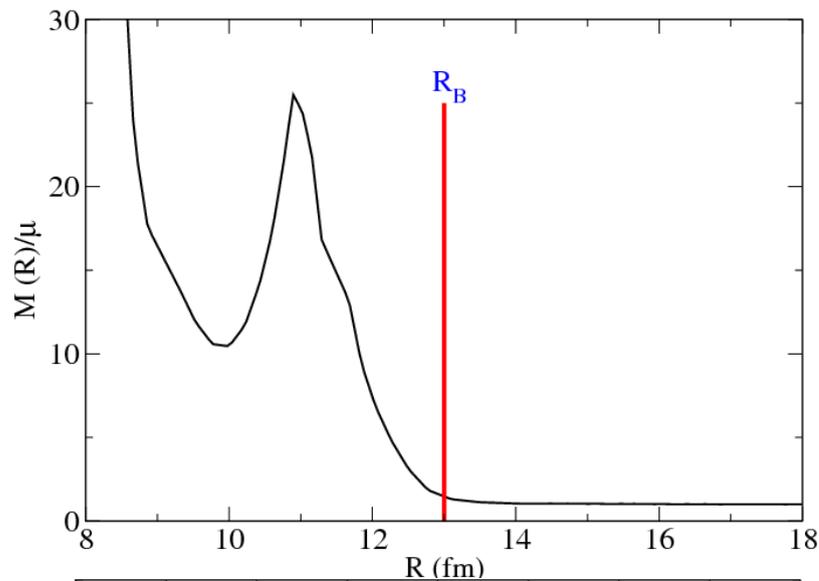
- Barrier for $\beta=0^\circ$ agrees with empirical
 - No parameter/normalization in TDHF
 - $V_B = 155.81$ MeV
 - $R_B = 12.12$ fm
- Barrier for $\beta=90^\circ$ lower
 - $V_B = 150.13$ MeV
 - $R_B = 12.87$ fm

Umar, Oberacker, Phys. Rev. C 74, Rapid Comm., 061601 (2006)





Dynamical Effective Mass



$$E_{c.m.} = \frac{1}{2} M(R) \dot{R}^2 + V(R)$$

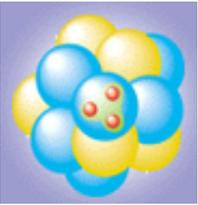
TDHF DC-TDHF

- Typical CHF type peak
- Because we are over the barrier!

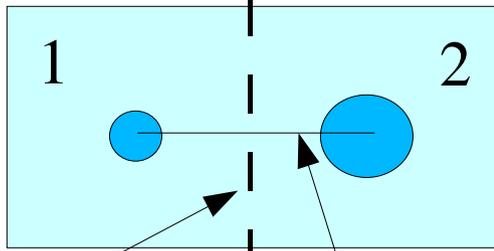
$$M(R) = \frac{2(E_{c.m.} - V(R))}{\dot{R}^2}$$

- Transform effect to $V(R)$

$$d\bar{R} = \left(\frac{M(R)}{\mu} \right)^{\frac{1}{2}} dR$$



Dynamical Reduced Mass



Dividing plane

Separation R

- Naive definition not valid for general Skyrme force

$$\mu_0(R) = m \frac{A_1(R) A_2(R)}{A_1(R) + A_2(R)}$$

- Calculate ρ_1^τ and ρ_2^τ for two halves ($\tau=n,p$)

- Calculate

$$R_i^\tau = \text{Tr}(\hat{r} \rho_i^\tau) / \text{Tr}(\rho_i^\tau)$$

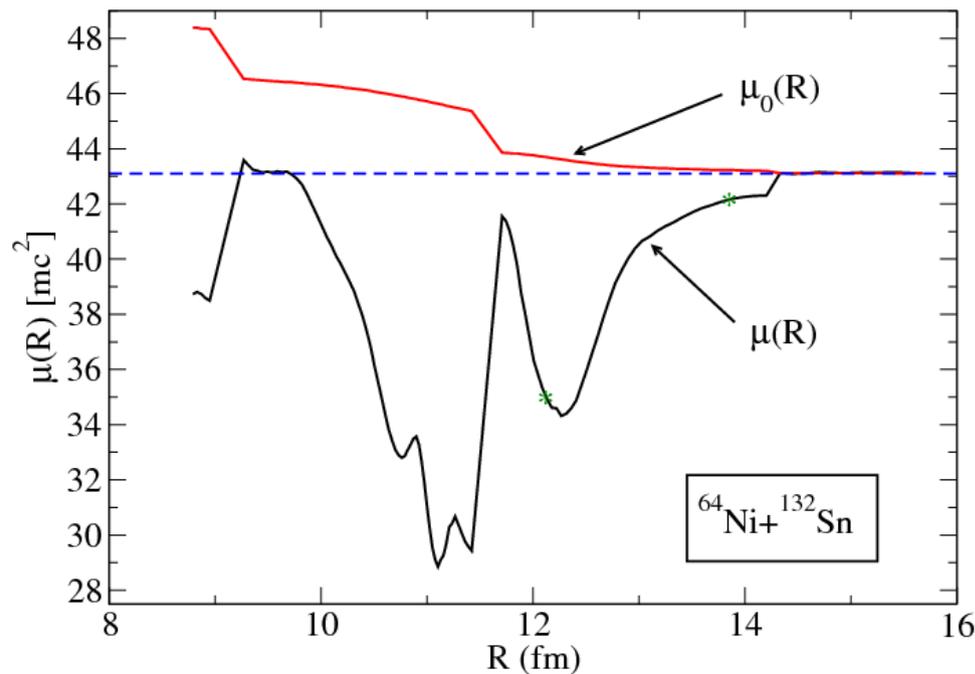
$$P_i^\tau = \text{Tr}(\hat{p} \rho_i^\tau)$$

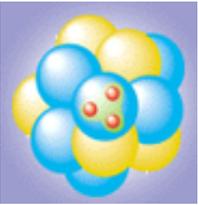
$$R_i = (N_n R_i^n + N_p R_i^p) / A_i$$

$$P_i = P_i^n + P_i^p$$

$$m_i = \frac{P_i}{dR_i/dt}$$

$$\mu(R) = \frac{m_1 m_2}{m_1 + m_2} \quad R = R_2 - R_1$$



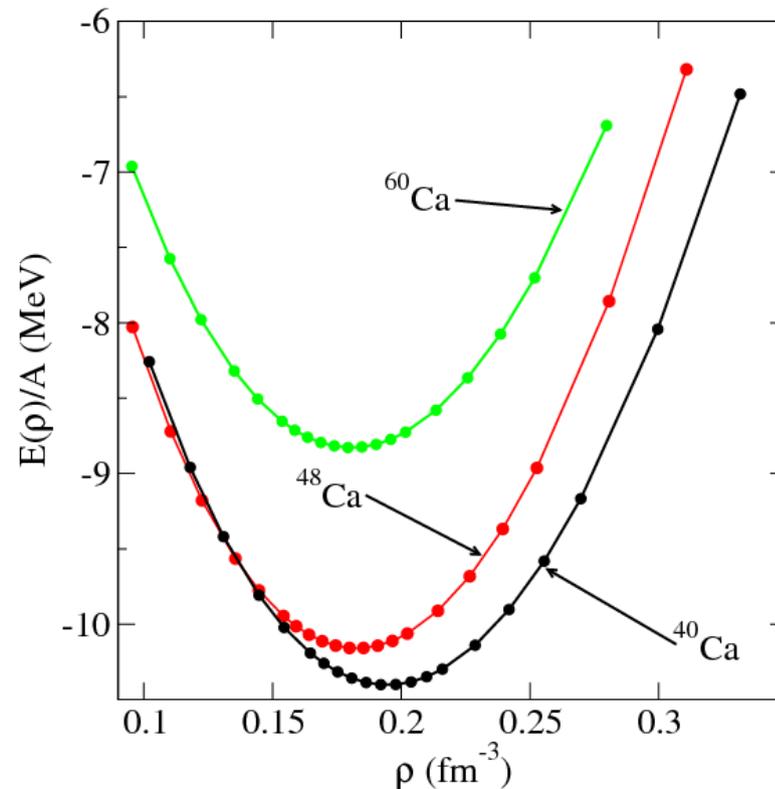
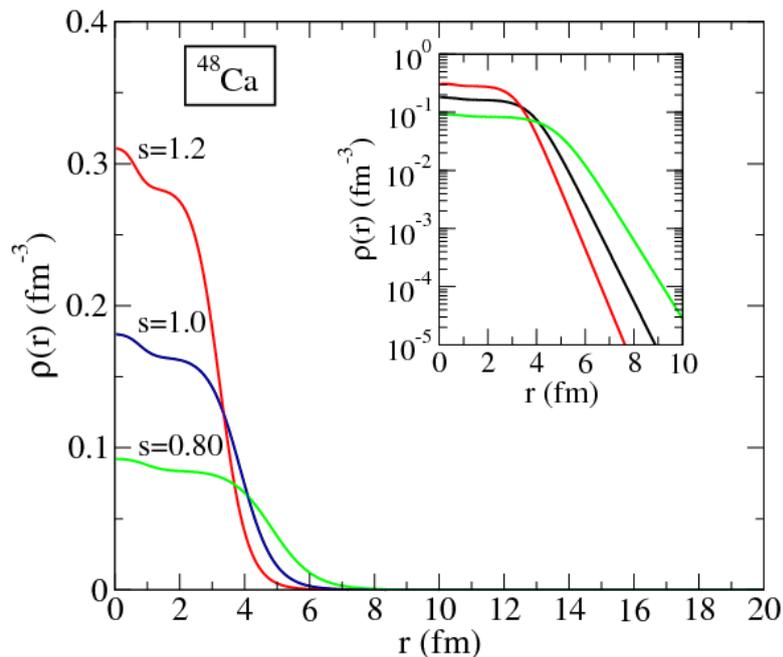


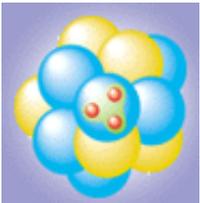
Future Directions I – EOS for Finite Nuclei

- Compress/decompress nucleus by constraining scaled density

$$\rho(r) \rightarrow N \rho(sr)$$

$$K_A = 9 \rho_0^2 \frac{\partial^2 (E/A)}{\partial \rho^2} \Big|_{\rho_0}$$





Future Directions II – Induced Fission

- Previous TDHF calculations yield fission under special conditions
 - when initialized slightly beyond the saddle point
 - starting from two-center type initial state
 - excited slabs
- Suggests that we need to go beyond single-Slater determinant
 - Pairing necessary for axial/reflection symmetric calculations to couple states with different angular momentum
 - In unrestricted 3D the coupling is there
 - Shape coexistence?

