

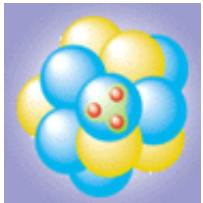
Heavy-Ion Fusion Using Density-Constrained TDHF

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JUSTIPEN-LACM '08, ORNL





Microscopic Methods for PES (CHF-ATDHF)

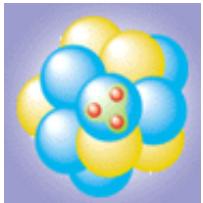
● Advantages

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

● Shortcomings

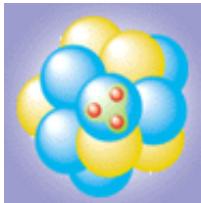
- Artificial introduction of constraining operators
- Collective motion not necessarily confined in constrained phase space
- Static adiabatic approximation
- Most energetically favorable state requires sudden rearrangement
- No reason why dynamical system should move along the valley of PES
- CHF calculations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

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



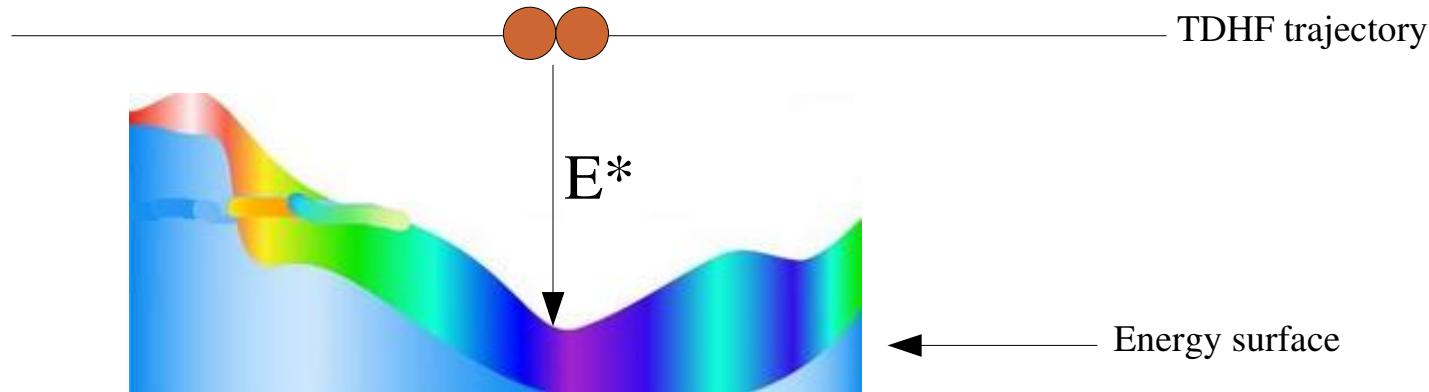
Phenomenological Fusion Barriers

- All information taken from static properties of nuclei
 - These may be correct prior to nuclear overlap but different after
- Use frozen densities when nuclei overlap
 - Typically Fermi densities fitted to experimental data
- Phenomenological heavy-ion interaction potentials
 - Wood-Saxon, Proximity, double-folding, W-A
 - Several free parameters
- Use few excited states (2-3)
 - Coupling potentials for excitations derived in simple models (rigid rotor, harmonic vibrator)
 - $B(E\lambda)$ values taken from experimental data
- Rotating frame approximation
 - To reduce the number of channels
- Allow for neutron transfer
 - Based on Q-values

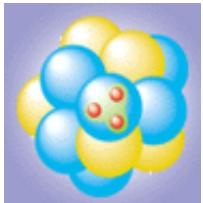


Density-Constrained TDHF

- 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



Implementation

- Generalize the ordinary method of constraints

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

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

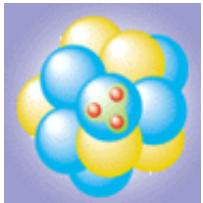
- for density constraint $\rightarrow \hat{H} \rightarrow \hat{H} + \int d^3 r \lambda_q(r) \hat{\rho}_q(r)$

- Works as accurately as a single constraint

- 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)





Ion-Ion Potential

*Umar, Oberacker, Phys. Rev. C **74**, 021601(R) (2006)*

- Total energy in terms of the excitation energy is:

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

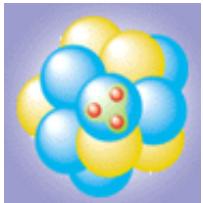
- E_{DC} contains the binding energies of the two nuclei

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

- Asymptotically correct (no normalization needed):

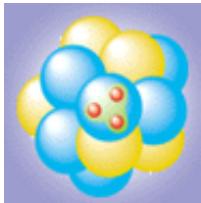
$$E_{DC}(R_{max}) = E_{A_1} + E_{A_2} + \frac{Z_1 Z_2 e^2}{R_{max}} \quad \longrightarrow \quad V(R_{max}) = \frac{Z_1 Z_2 e^2}{R_{max}}$$

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



A New Generation TDHF Code

- Unrestricted 3-D Cartesian geometry
 - No fixed reaction plane
 - 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
- Much improved fusion cross sections for light systems
Umar, Oberacker, Phys. Rev. C 73, 054607 (2006)
- It is possible to calculate cross sections for deformed nuclei
Umar, Oberacker, Phys. Rev. C 74, 124606 (2006)
- Calculate EOS for finite nuclei
Umar, Oberacker, Phys. Rev. C 76, 024316 (2007)



Additional Terms in Energy Density

New Terms

$$t_0, t_3 \rightarrow \frac{1}{4} t_0 x_0 \vec{s}^2 - \frac{1}{4} t_0 (\vec{s}_n^2 + \vec{s}_p^2) + \frac{1}{24} \rho^\alpha t_3 x_3 \vec{s}^2 - \frac{1}{24} t_3 \rho^\alpha (\vec{s}_n^2 + \vec{s}_p^2)$$

$$t_1, t_2 \rightarrow \frac{1}{32} (t_2 + 3t_1) \sum_q \vec{s}_q \cdot \nabla^2 \vec{s}_q - \frac{1}{32} (t_2 x_2 - 3t_1 x_1) \vec{s} \cdot \nabla^2 \vec{s} + \frac{1}{8} (t_1 x_1 + t_2 x_2) (\vec{s} \cdot \vec{T} - \overleftrightarrow{J}^2) + \frac{1}{8} (t_2 - t_1) \sum_q (\vec{s}_q \cdot \vec{T}_q - \overleftrightarrow{J}_q^2)$$

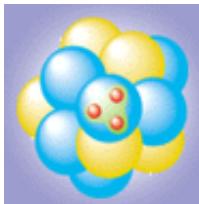
$$t_4 \rightarrow -\frac{t_4}{2} \sum_{qq'} (1 + \delta_{qq'}) [\vec{s}_q \cdot \nabla \times \vec{j}_{q'} + \rho_q \overleftrightarrow{\nabla} \cdot \overleftrightarrow{J}]$$

Old Term

$$\rho \tau - \vec{j}^2$$

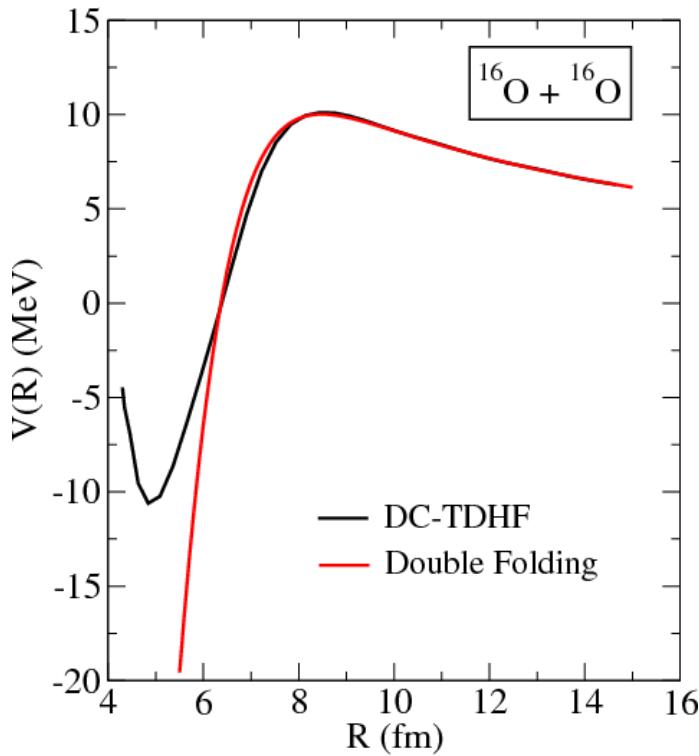
JUSTIPEN-LACM '08, ORNL





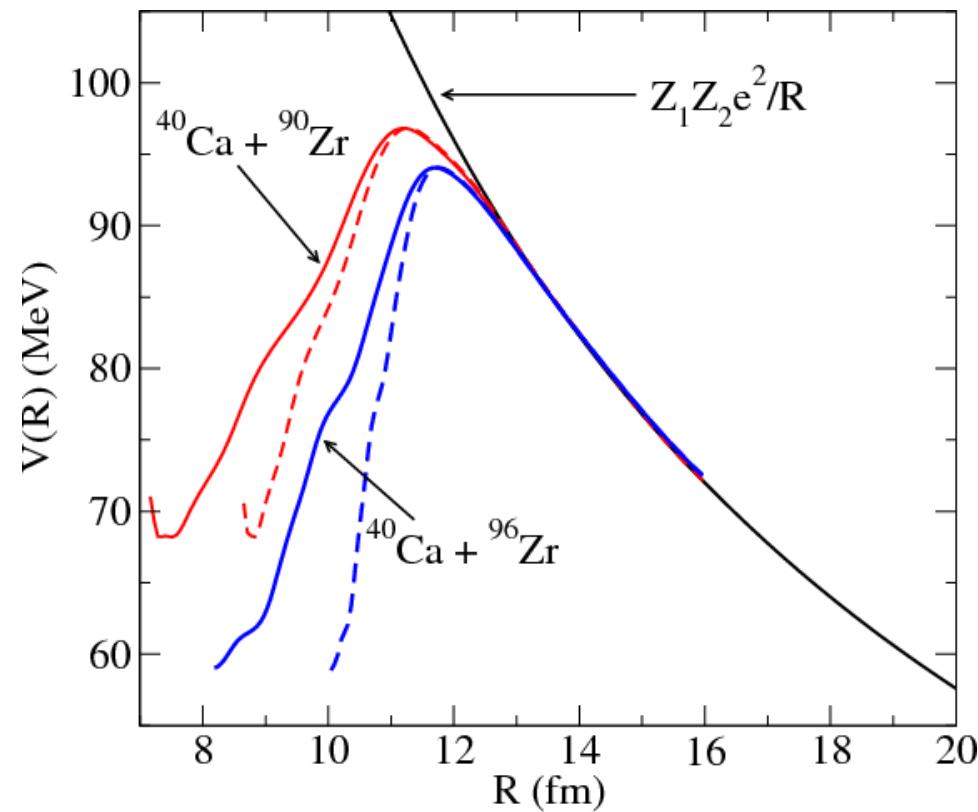
Comparison to Empirical Fusion Potentials

- DC-TDHF potential contains no parameters and normalization

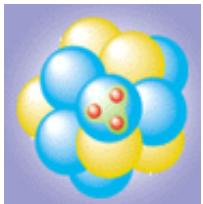


Double folding:

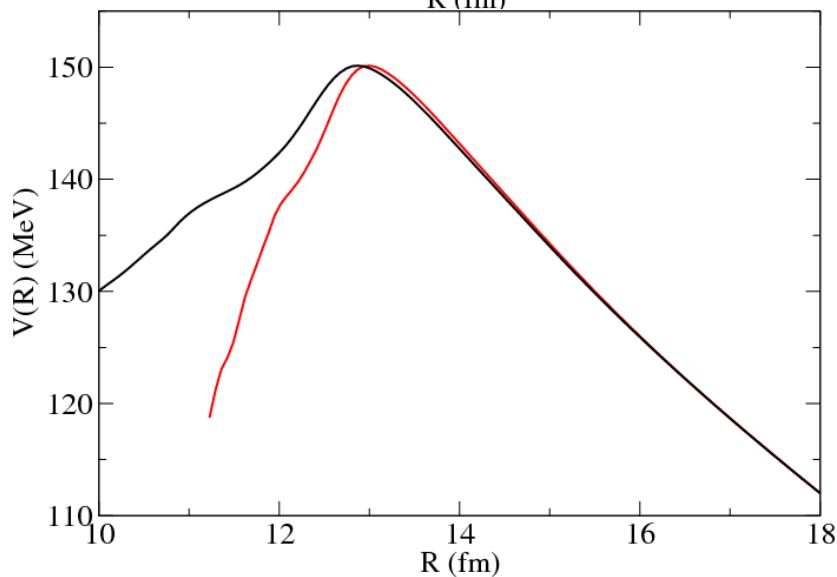
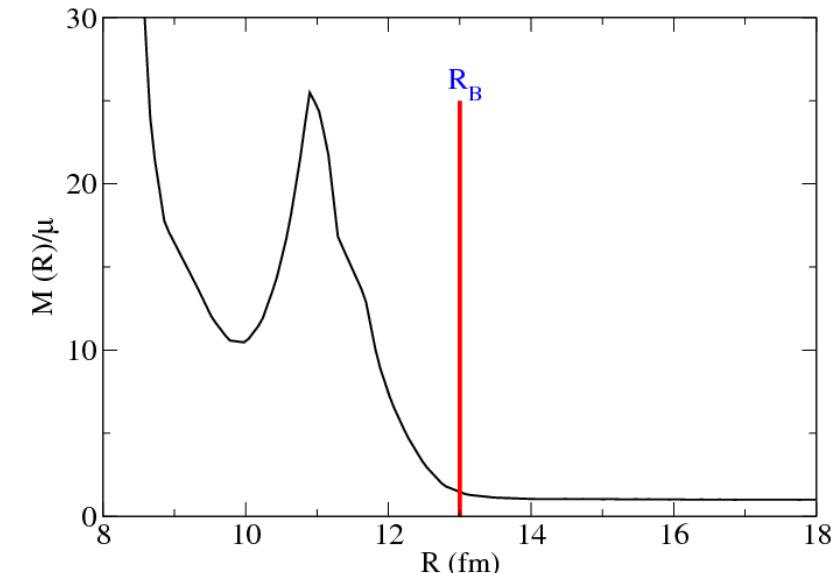
M3Y effective NN interaction
densities from electron scattering



- All comparisons show incredible agreement!



Dynamical Effective Mass



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

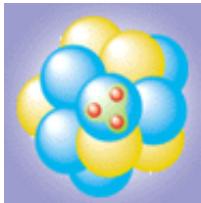
TDHF DC-TDHF

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

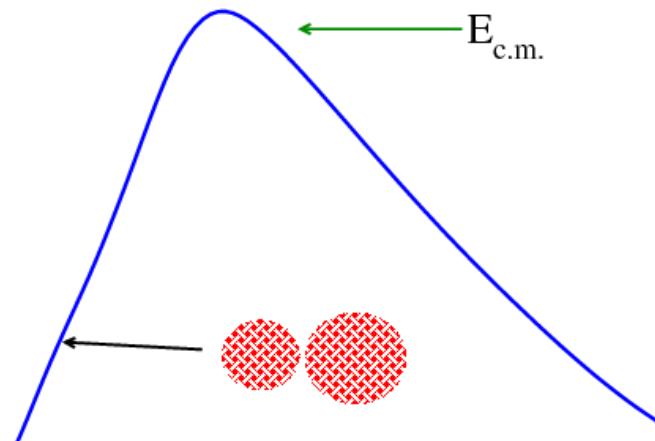
$$M(R) = \frac{2(E_{c.m.} - V(R))}{\dot{R}^2}$$

- ➋ Transform effect to $V(R)$

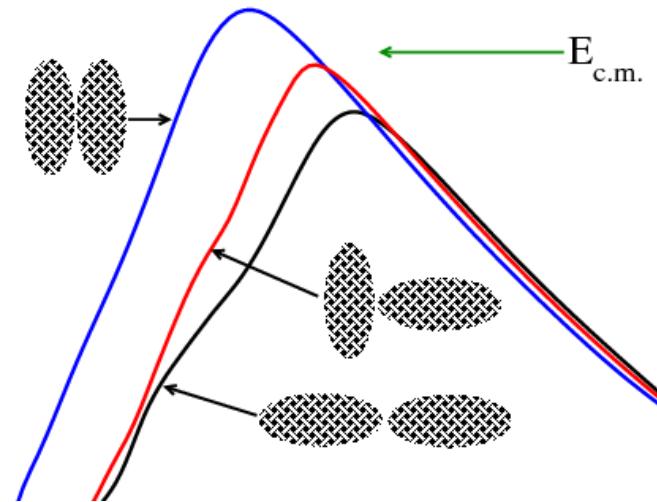
$$d\bar{R} = \left(\frac{M(R)}{\mu} \right)^{\frac{1}{2}} dR$$



Initial Alignment for Deformed Nuclei

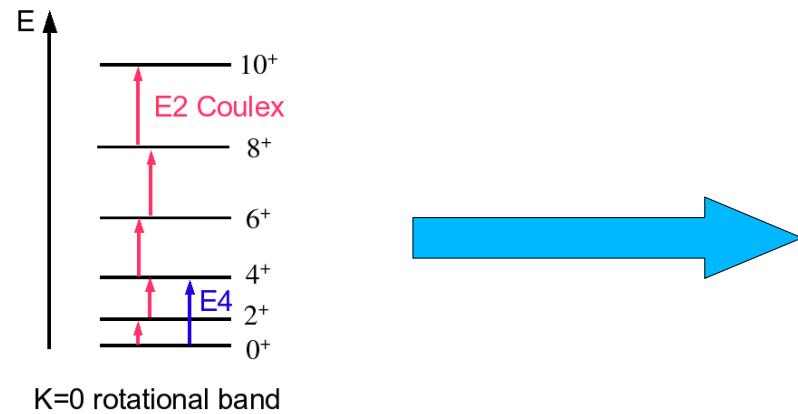


Spherical nuclei → single barrier

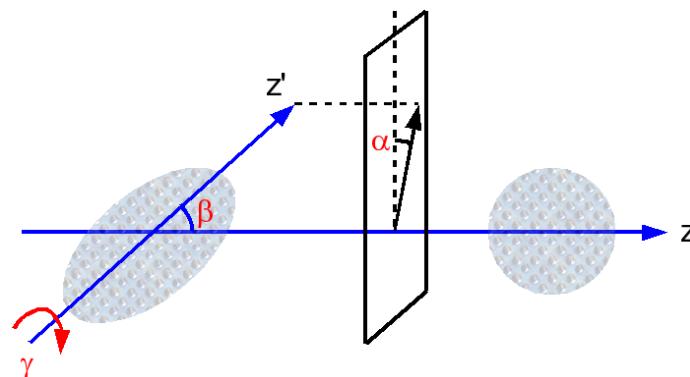


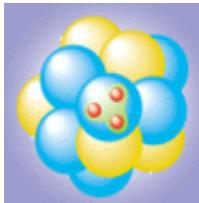
Deformed nuclei → barrier distribution

- Dynamical alignment due to Coulomb excitation



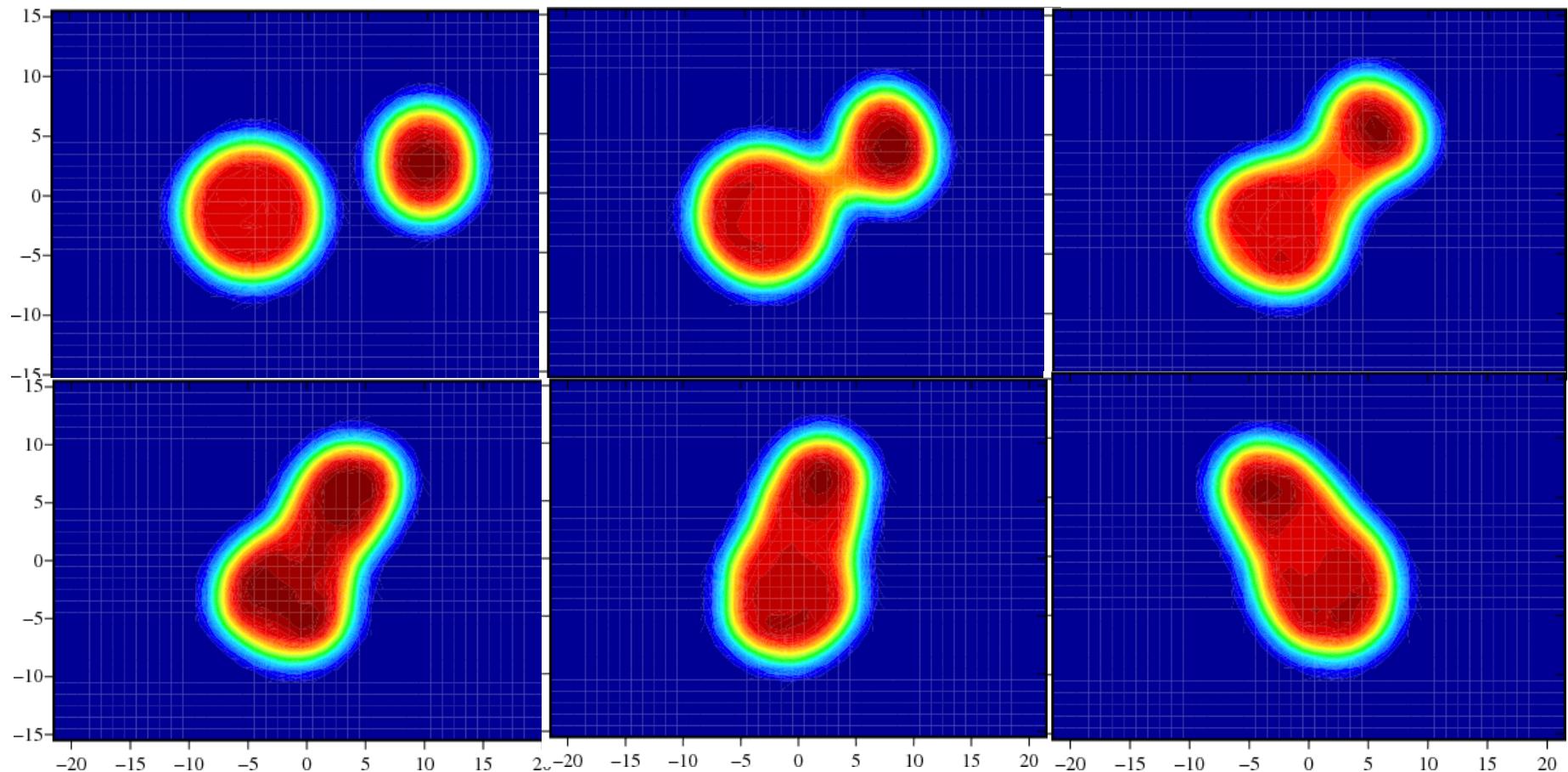
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$^{64}\text{Ni} + ^{132}\text{Sn}$ Fusion

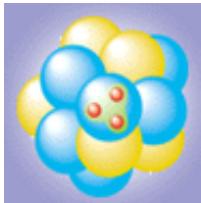
- 3D HF (SLy4) gives oblate deformation for ^{64}Ni : $Q_{zz}(n) = -0.85$ b, $Q_{zz}(p) = -0.59$ b



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

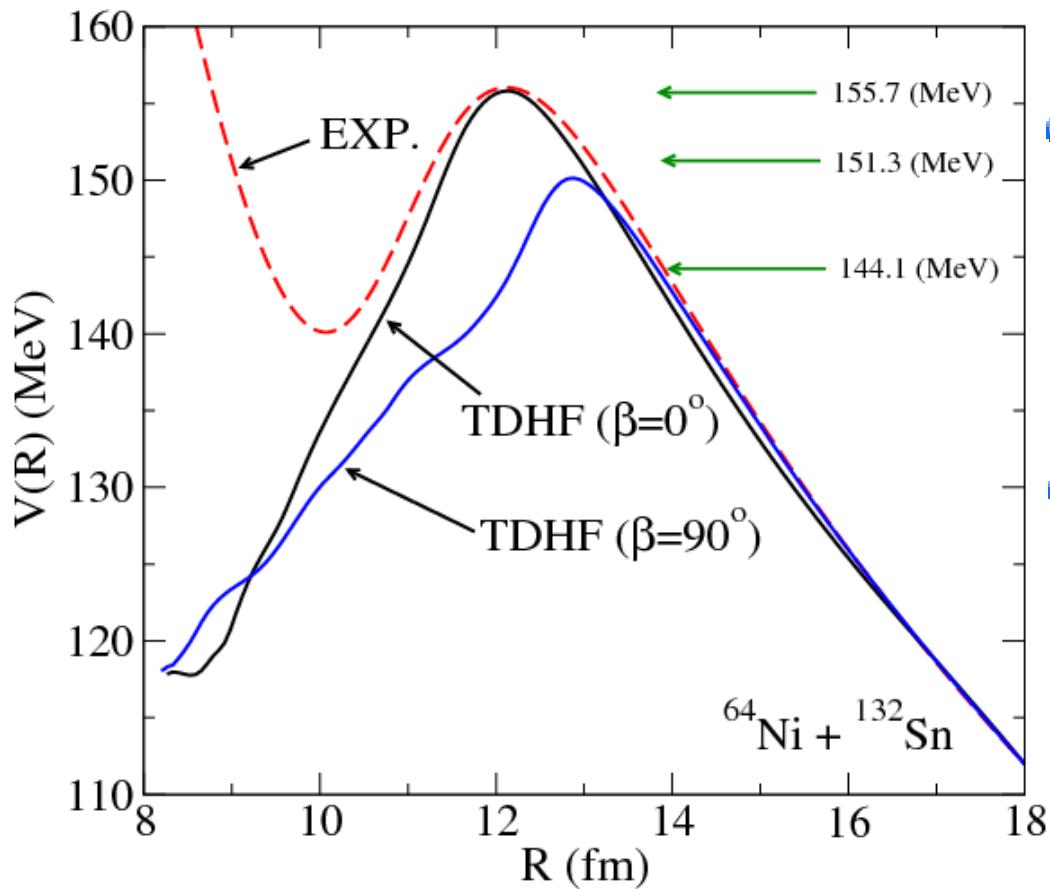
JUSTIPEN-LACM '08, ORNL





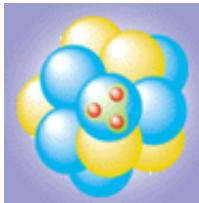
$^{64}\text{Ni} + ^{132}\text{Sn}$ Limiting Barriers

Umar, Oberacker, *Phys. Rev. C* **74**, 061601(R) (2006)
Umar, Oberacker, *Phys. Rev. C* **76**, 014614 (2007)



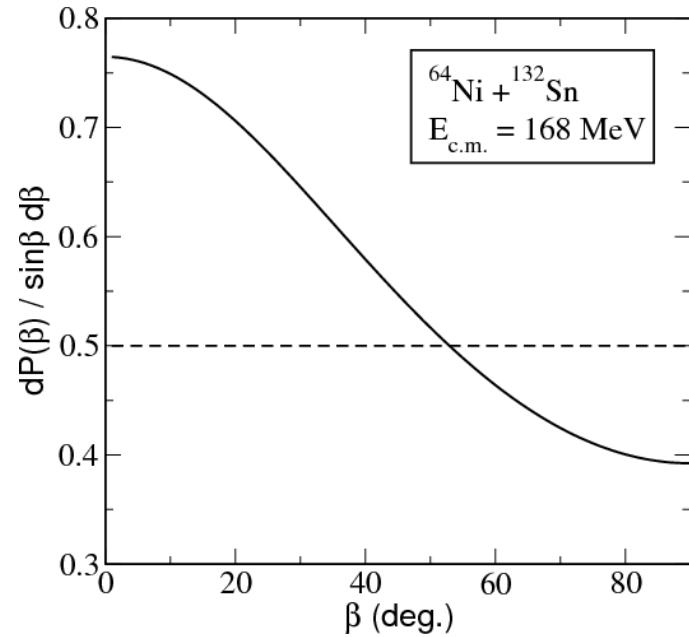
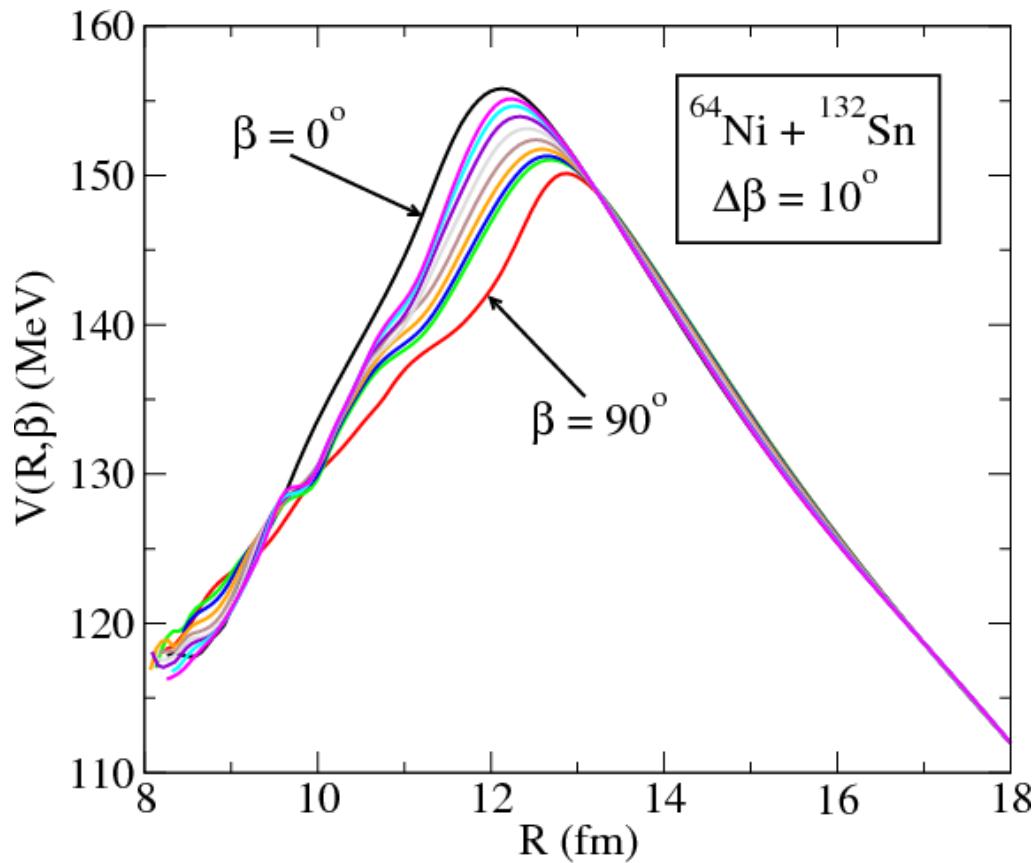
Liang et al., PRL 91, 152701-1 (2003)

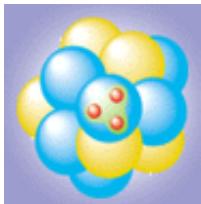
- Barrier for $\beta=0^\circ$ agrees with empirical
 - No parameter/normalization in TDHF
 - $V_B = 155.81$ MeV
 - $R_B = 12.12$ fm
- Barrier for $\beta=90^\circ$ lower
 - $V_B = 150.13$ MeV
 - $R_B = 12.87$ fm



$^{64}\text{Ni} + ^{132}\text{Sn}$ Complete Set of Barriers

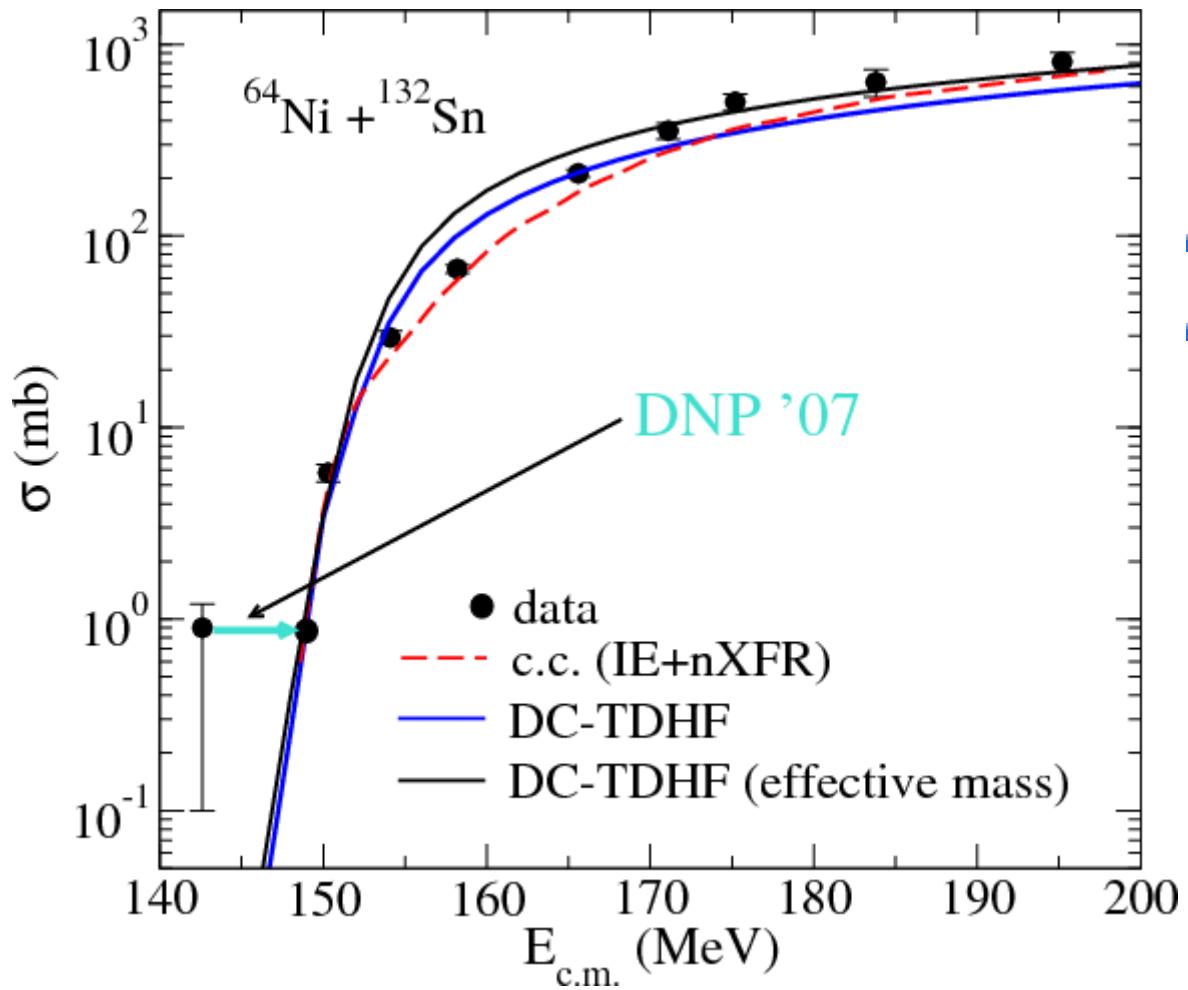
Umar and Oberacker, Phys. Rev. C76, 014614 (2007)





$^{64}\text{Ni} + ^{132}\text{Sn}$ Fusion Cross-Section

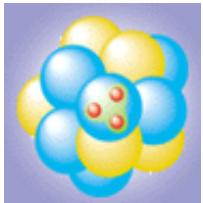
Umar and Oberacker, Phys. Rev. C76, 014614 (2007)



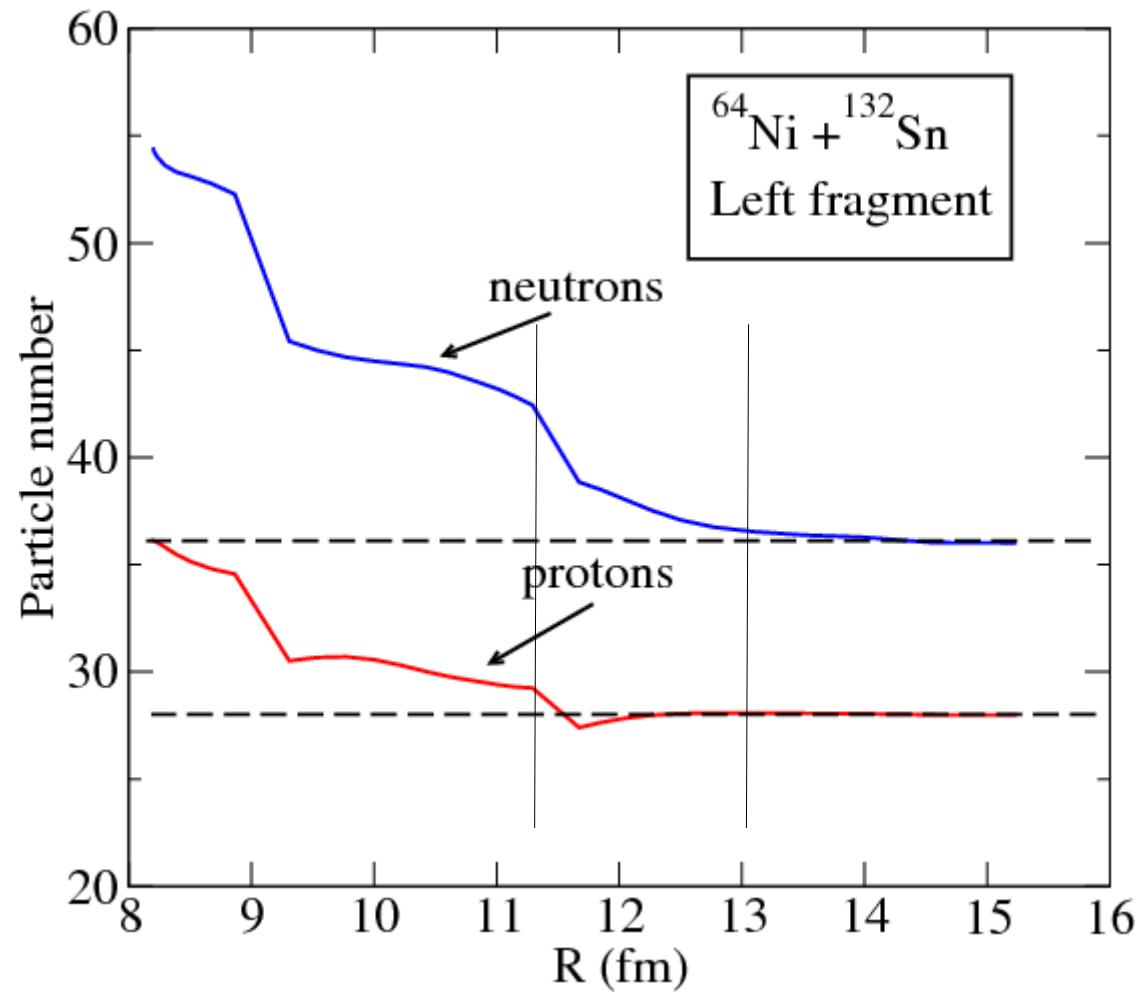
- Use IWBC
- Average over orientations

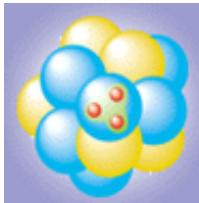
$$\sigma_f(E_{\text{c.m.}}) = \int_0^1 d\cos(\beta) P(\beta) \sigma(E_{\text{c.m.}}, \beta)$$

Exp. Data
J.F. Liang *et al.*,
PRL 91, 152701 (2003)
PRC 75, 054607 (2007)



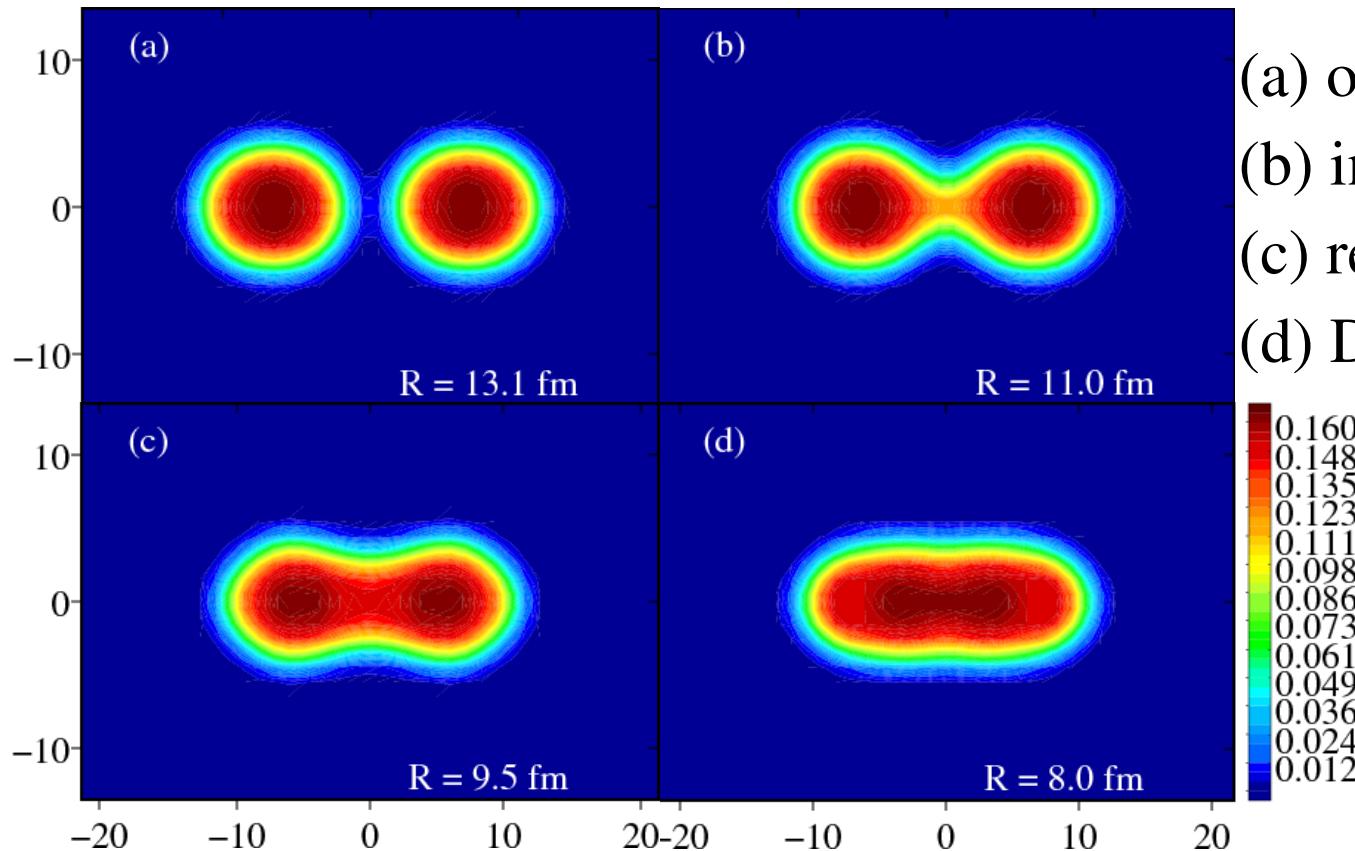
$^{64}\text{Ni} + ^{132}\text{Sn}$ Particle Transfer



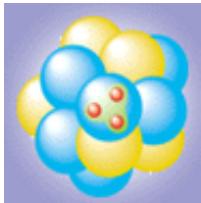


$^{64}\text{Ni} + ^{64}\text{Ni}$ Fusion ($\beta_1=90^\circ$, $\beta_2=90^\circ$)

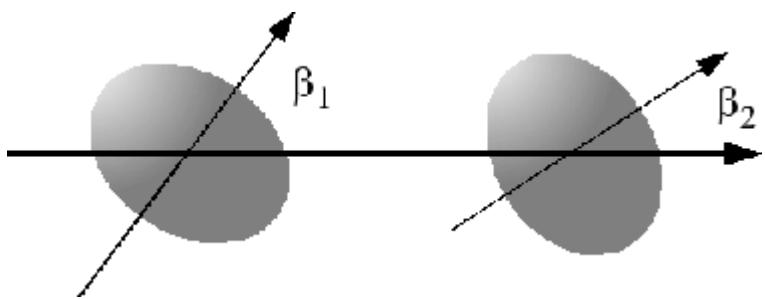
- Interesting neutron rich identical system



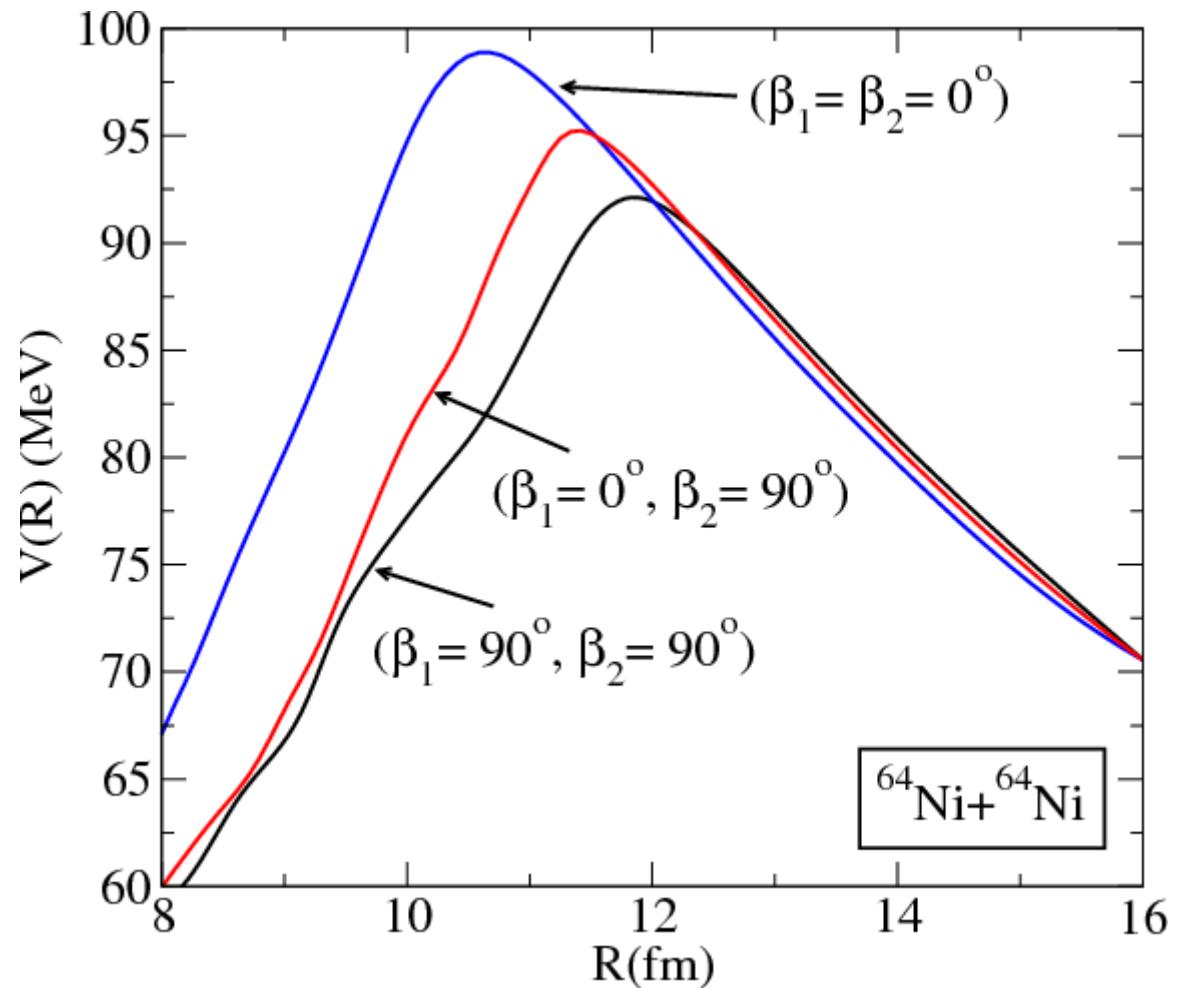
Turning points for $E_{\text{cm}} = 86 \text{ MeV}$



$^{64}\text{Ni} + ^{64}\text{Ni}$ Limiting Barriers



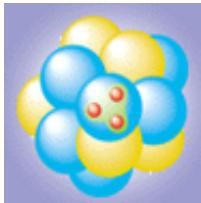
- Variation with Euler angle α_i is negligible!



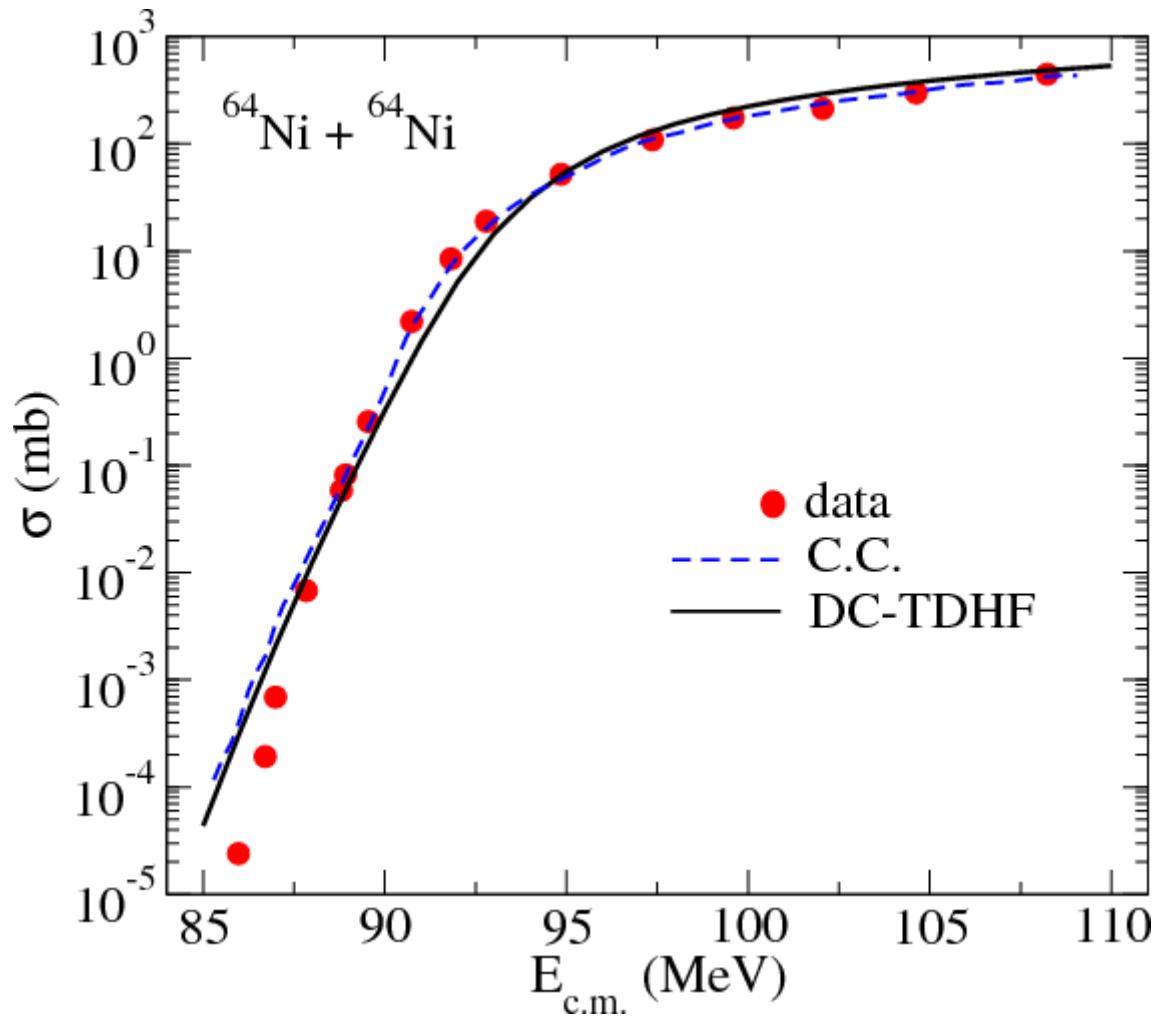
arXiv:0709.3972v1 [nucl-th]

JUSTIPEN-LACM '08, ORNL



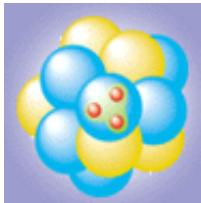


$^{64}\text{Ni} + ^{64}\text{Ni}$ Fusion Cross-Section



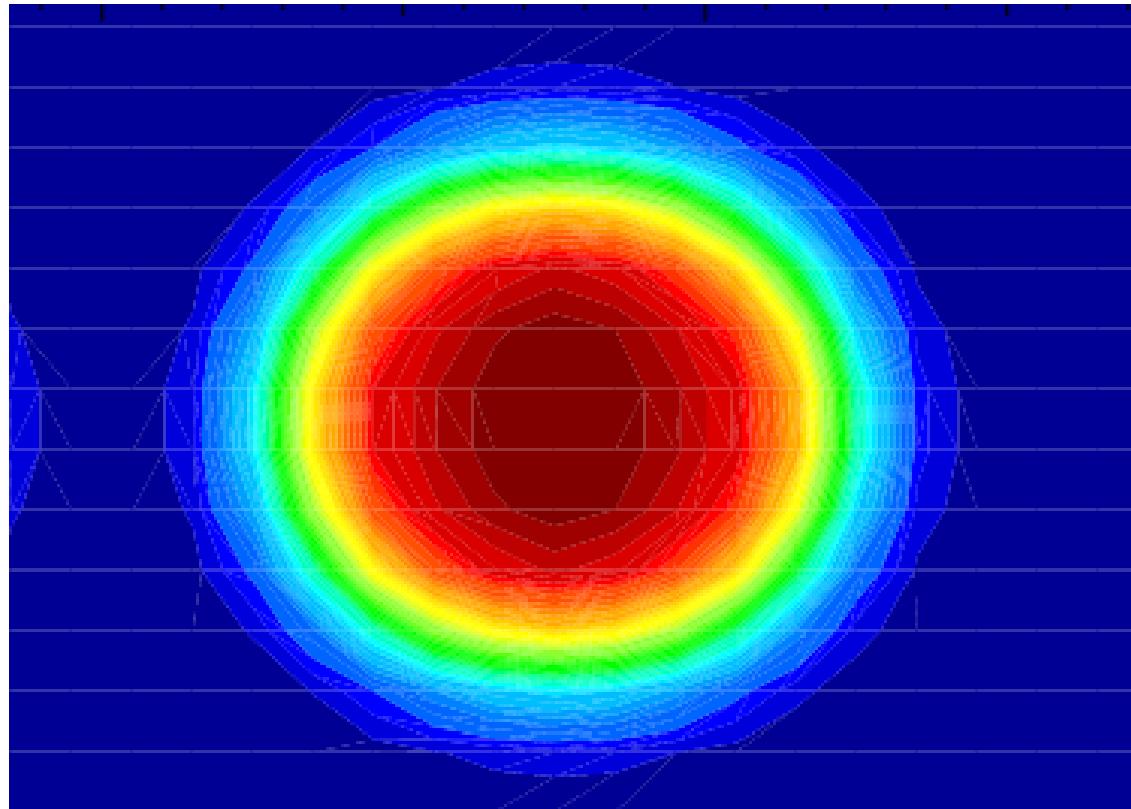
- Problem at low energies
 - Compression potential
Mişicu, Esbensen, PRL 96, 112701 (2006)
 - Modify inner turning point
Ichikawa, Hagino, Iwamoto,
PRC 75, 064612 (2007)

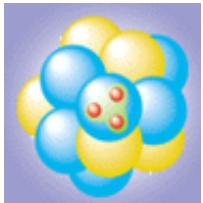
Exp. Data
C.L. Jiang *et al.*,
PRL 93, 012701 (2004)



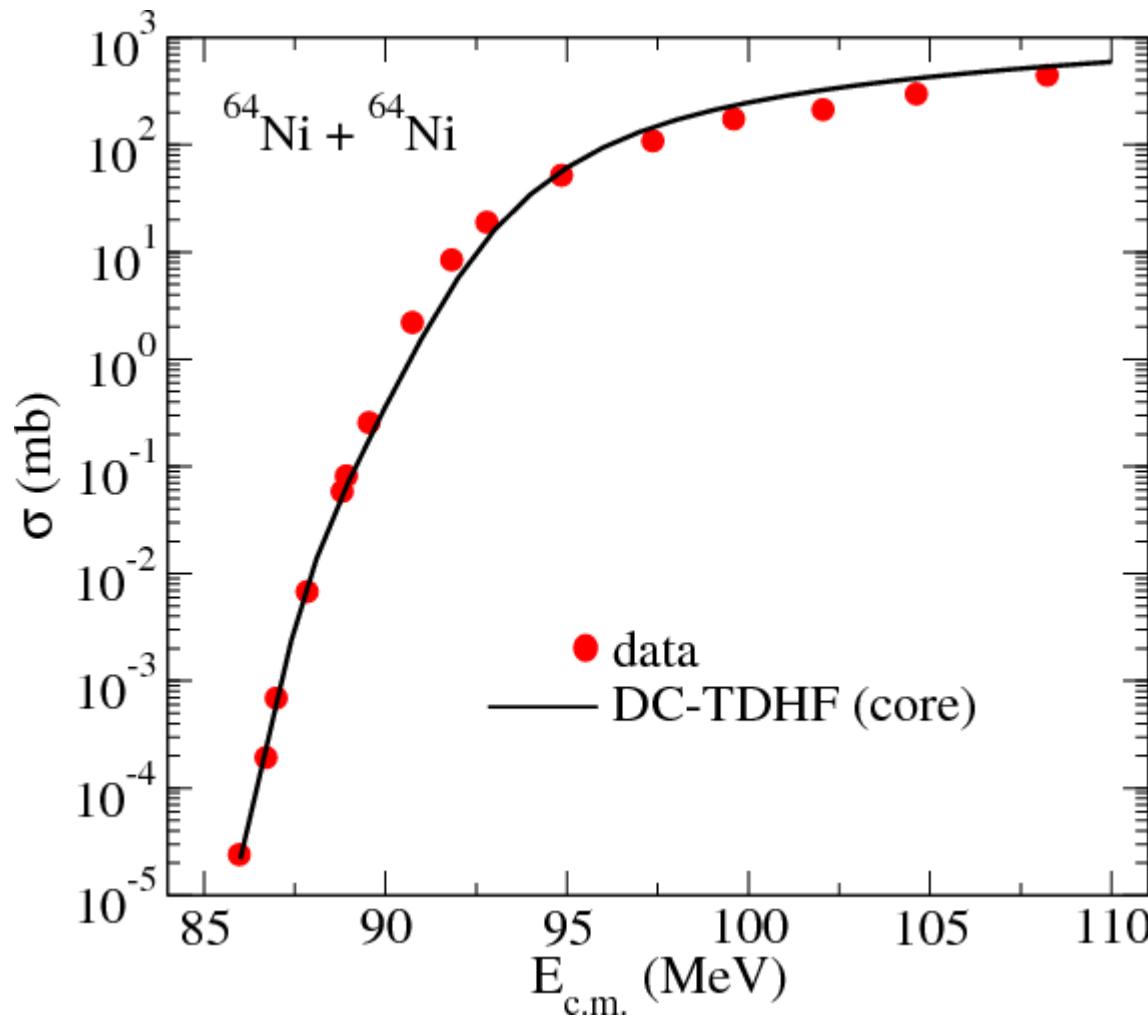
Conjecture - Skin versus Core Orientation

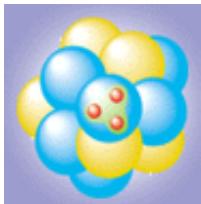
- Neutron rich systems have extended outer skins
- Orientation of core in ^{64}Ni perpendicular to outer surface
- Top of the barrier primarily determined by outer surface
- Lower energies imply larger overlaps for inner turning point
- Ambiguity in which orientation to choose in angle averaging



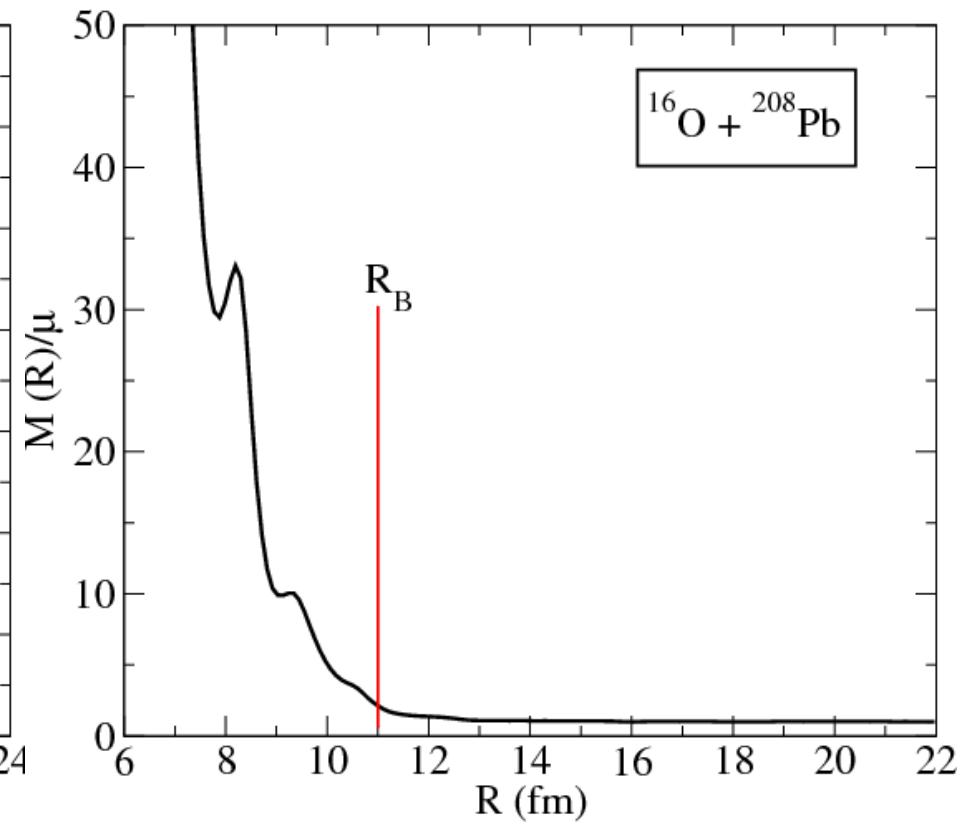
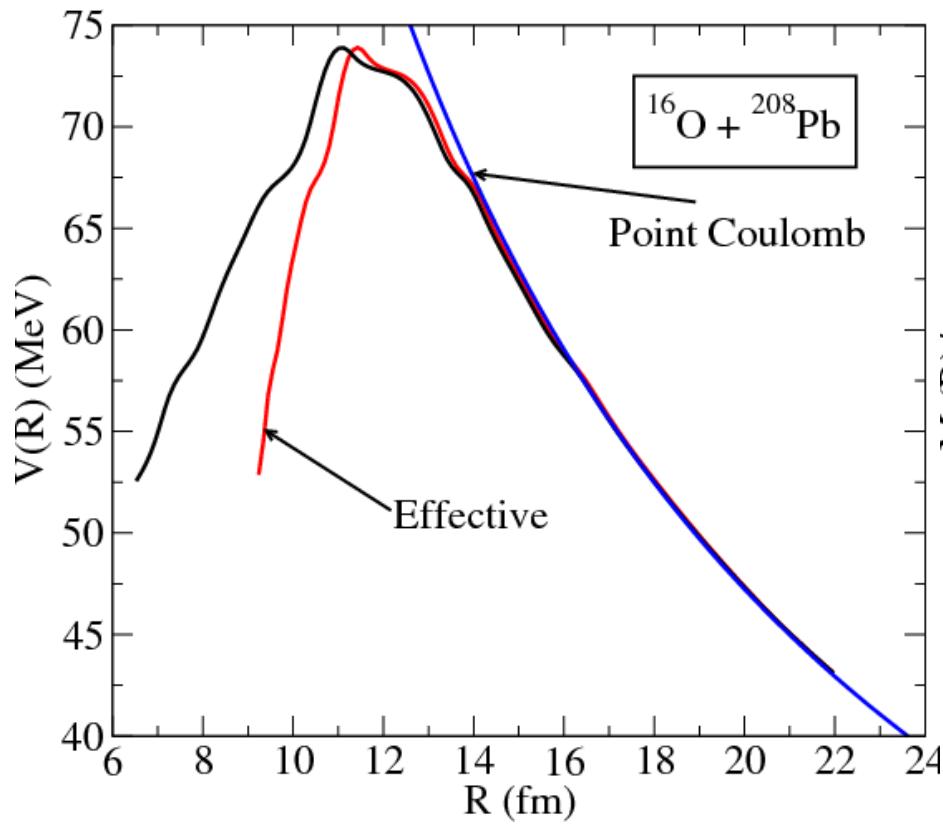


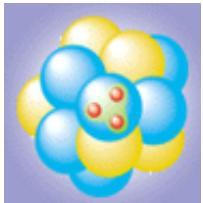
For Low Energies use Core Orientation



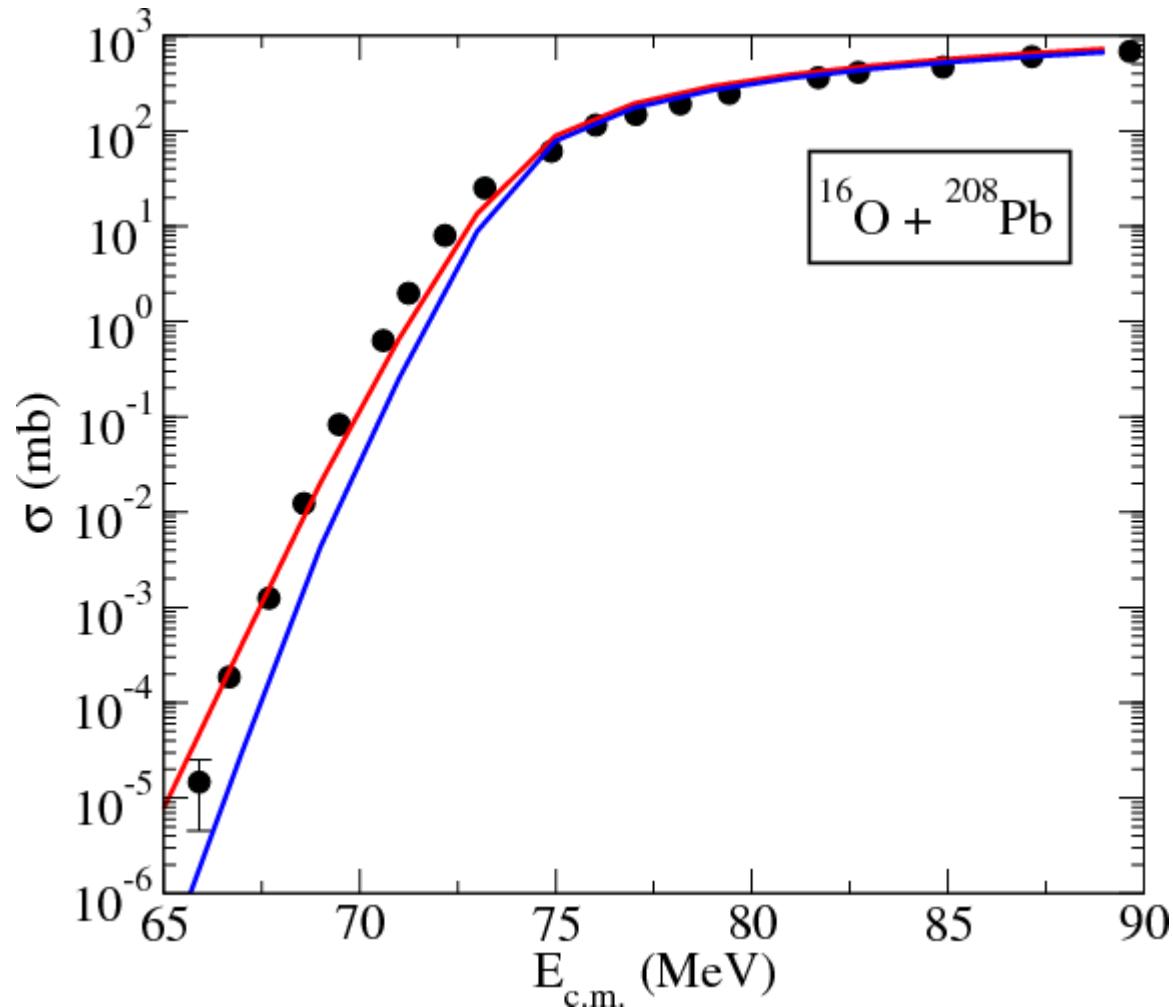


$^{16}\text{O} + ^{208}\text{Pb}$ Fusion Barrier - Preliminary





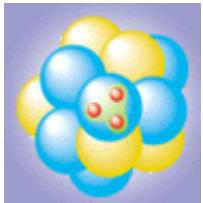
$^{16}\text{O} + ^{208}\text{Pb}$ Fusion Cross - Section



M. Dasgupta et al., PRL 99, 192701 (2007)

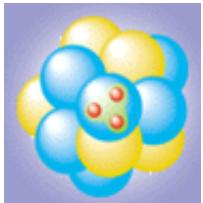
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Summary and Conclusions

- Density-constrained TDHF provides a microscopic method for extracting ion-ion potentials that incorporates the mean-field dynamics
- The method is not limited to TDHF, can be used in any dynamical approach (TDHFB, time-dependent DFT, and beyond)
- Use is limited by the extent of how well the nucleus is described by Hartree-Fock and the effective interaction.



TDHF and C.M. Corrections - I

- Initial state has no cross-channel coupling



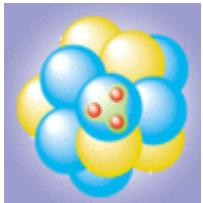
- Each nucleus is boosted by multiplying with a phase factor

$$\Phi_j \rightarrow \exp(i\mathbf{k}_j \cdot \mathbf{R}_j) \Phi_j \quad \text{and} \quad \mathbf{R}_j = \frac{1}{A_j} \sum_{i=1}^{A_j} \mathbf{r}_i$$

- They are placed in the center-of-mass of the entire system

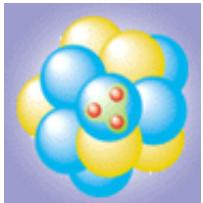
$$A_1 \mathbf{R}_1 + A_2 \mathbf{R}_2 = 0$$

- Total initial momentum has expectation zero and relative momentum is $2\hbar\mathbf{k}$
- Physics of the collision is determined by relative momenta



TDHF and C.M. Corrections - II

- Initial states are interpreted as wave packets whose centers of momentum are shifted by \mathbf{k} , and travel without spreading
- We are not free to change the intrinsic wave packet contained in the Slater determinant
- Various estimates for the uncertainties/spread is available
- Calculations most accurate for early stages of time-evolution
- DC-TDHF is not sensitive to spread in beam-energy
- We have already shown agreement with point Coulomb and double-folding potential for O+O



TDHF and C.M. Corrections - III

- Run TDHF with simple c.m. Corrections included in static and dynamic
- Perform DC-TDHF calculation – result is mostly a constant shift

