# 3-d unrestricted TDHF fusion studies of neutron-rich nuclei using the full Skyrme interaction

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# Outline of talk

- Introduction: theoretical descriptions of fusion
- Brief review of TDHF theory
- new TDHF code (Fortran-95):
  3-D lattice (no symmetry restrictions), B-Splines,
  full Skyrme interaction (additional time-odd terms in TDHF mean field Hamiltonian)
- TDHF fusion studies of spherical nuclei
  $^{16}O + ^{16}O$, $^{16}O + ^{28}O$
  spherical + deformed nuclei ($^{16}O + ^{22}Ne$, $^{16}O + ^{34}Ne$)
  discussion of dynamic alignment due to Coulex
- Conclusions and outlook

# Some theoretical descriptions of heavy-ion fusion

- Barrier penetration models
  Balantekin & Takigawa, Rev. Mod. Phys. 70, 77 (1998)
  Takigawa & Bertsch, PRC 29, 2358 (1984)
  Rhoades-Brown & Oberacker, PRL 50, 1435 (1983)

- Coupled channels calculations
  Esbensen, Prog. Theor. Phys. Suppl. 154, 11 (2004)
  Hagino, Rowley & Kruppa, Comp. Phys. Comm. 123, 143 (1999)
  Landowne & Pieper, PRC 29, 1352 (1984)

- Time-dependent Hartree-Fock (TDHF)
  Umar & Oberacker, Eur. Phys. J. A25, s01, 553 (2005)
  Umar, Strayer, Wu, Dean & Guclu, PRC 44, 2512 (1991)

# TDHF – Basic Facts

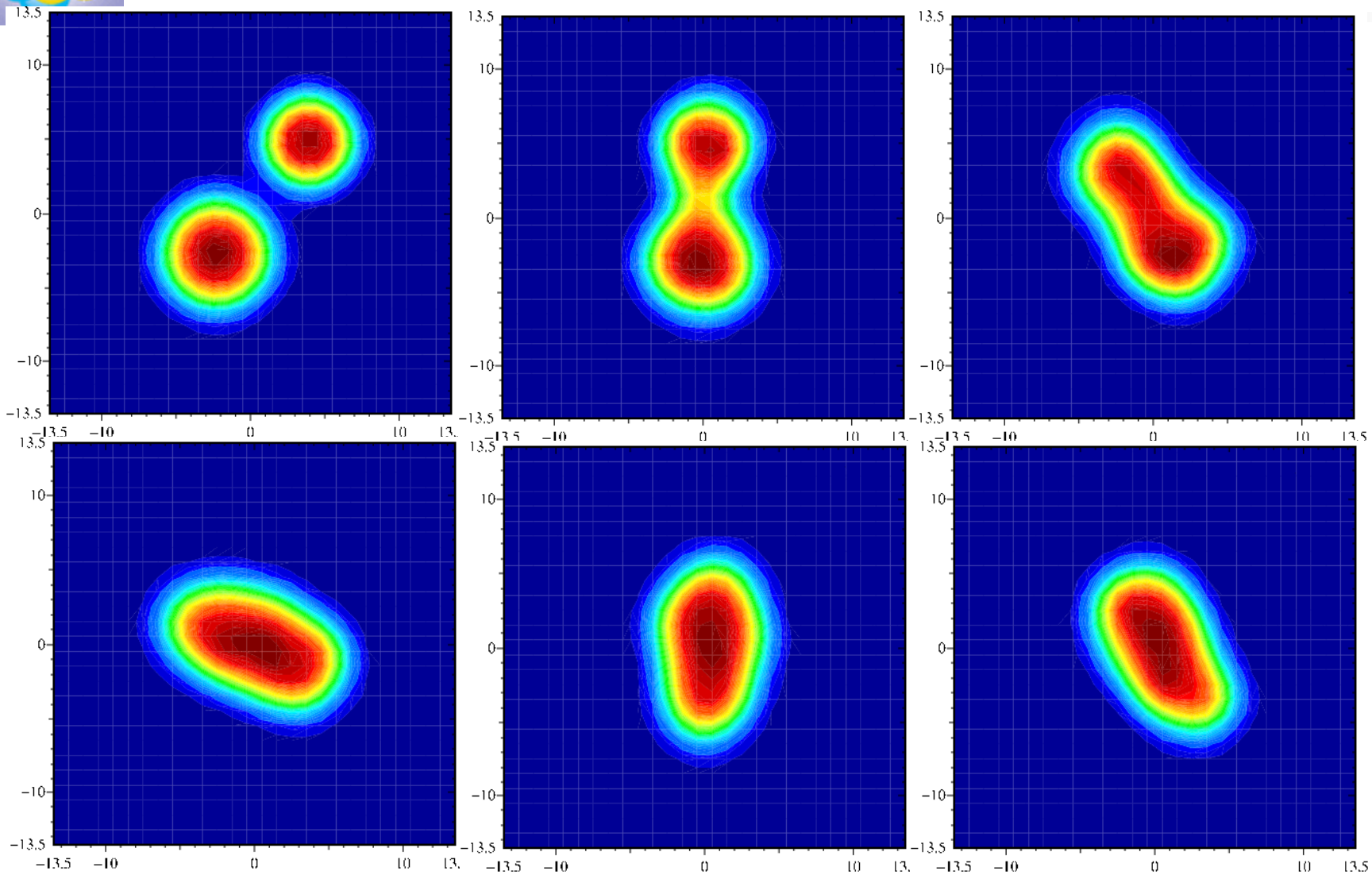
Advantages

- Fully microscopic, parameter-free description of nuclear collisions
- One can follow the time-evolution of the nuclear density distribution during collision (neck formation, surface vibrations, rotation, ...) --> fusion and fission become “visible”
- Use same microscopic interaction used in static HF calculations
- Successful in describing low-energy fusion, deep-inelastic collisions, nuclear molecules, and collective phenomena
- Provides a method for linear response calculations (e.g. for giant resonances)

Shortcomings

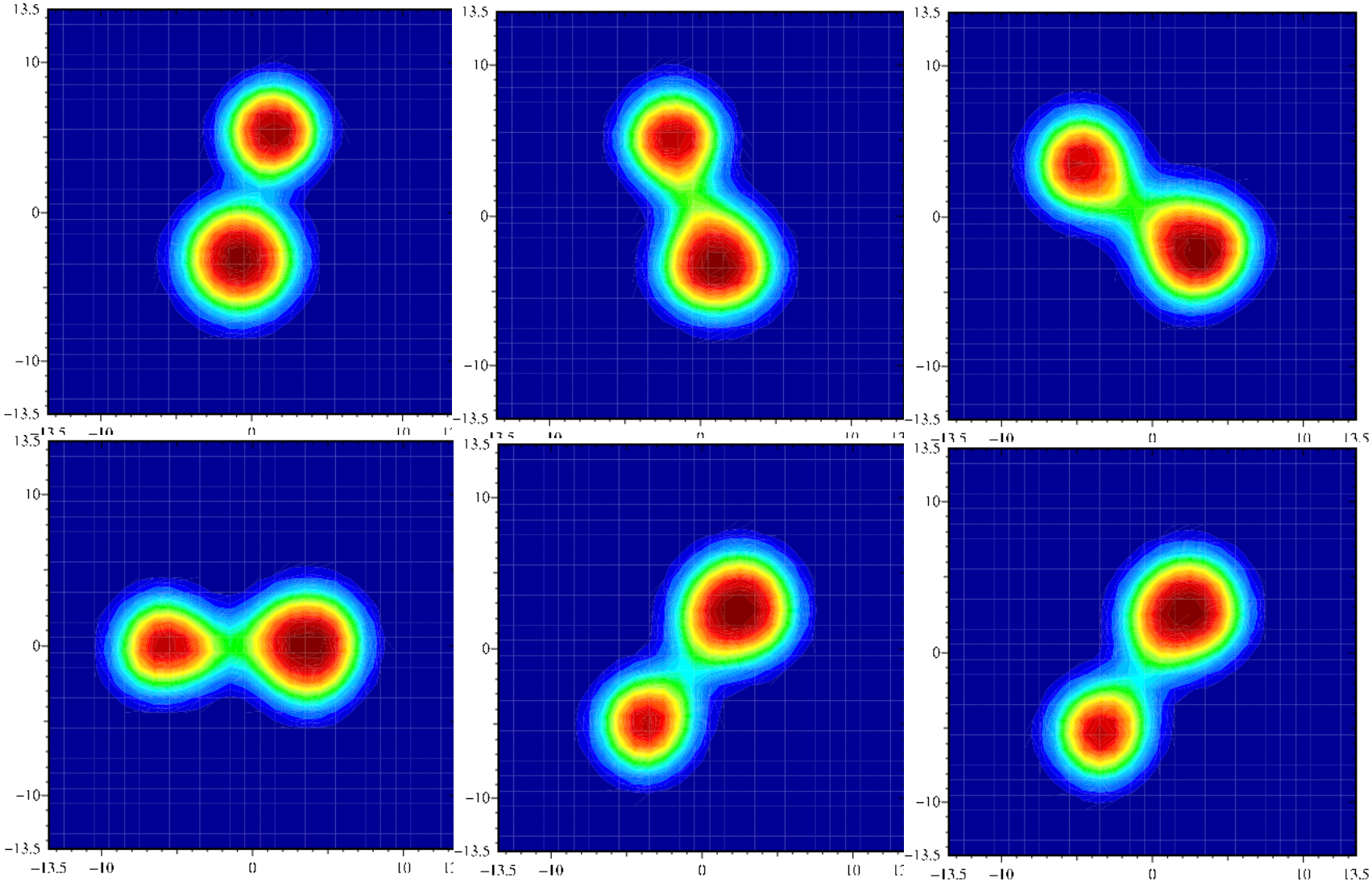
- Only one-body dissipation (collision with walls of mean field)
- Semiclassical (represents dominant reaction channel)
- Does not include pairing (--> need TDHFB)

# $^{16}O+^{28}O$ at $E_{cm}$ = 43 MeV, SLy5, b = 7.5 fm




$\sigma_{fusion}$ = 1916 mb

# $^{16}O+^{28}O$ at $E_{cm}$ = 43 MeV, SLy5, b = 7.6 fm



# Basic TDHF Equations

- Equations of motion obtained from variation of the action

$$S=\int_{t_1}^{t_2} dt \langle \Phi(t)|H-i\hbar\partial_t|\Phi(t)\rangle \quad \text{with} \quad H=\sum_i^A t_i+\sum_{i<j}^A v_{ij}$$

Skyrme

- Many-body state is a Slater determinant at all times

$$\Phi(r_1\cdots r_A;t)=\frac{1}{\sqrt{A!}}det|\phi_\lambda(r_i,t)|$$

- Time-dependence of the single-particle states are governed by

$$i\hbar\frac{\partial\phi_\lambda}{\partial t}=h(\{\phi_\mu\})\phi_\lambda$$

- Skyrme energy functional is given by the 3D integral

$$E=\int d^3r \;\; \mathcal{H}(\rho,\tau,\vec{j},\vec{s},\vec{T},J_{\mu\nu}\;;\vec{r})$$

# History of TDHF Codes

1970-1985

- Axially symmetric. Impact parameter simulated via the rotating frame approximation
- Reflection symmetry with respect to fixed reaction plane and z-parity symmetry for identical systems
- Simple forms of Skyrme interaction used. Certain terms of the interaction replaced by Yukawa terms (without fit)
- No spin-orbit term
- Low order finite-difference discretization

1985-1991

- Spin-orbit term included

1991-2004

- 3D with reflection symmetry
- Modern Skyrme forces, but not all the dynamical terms
- High order finite-difference methods

# 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)
  - F77/BKN version: Umar et al, Phys. Rev. C44, 2512 (1991)

- Basis-Spline discretization for high accuracy
  - Umar et al, J. Comp. Phys., 93, 426 (1991)

- Damped gradient iteration for static solution

- Time-evolution by Taylor expansion of propagator for small time step

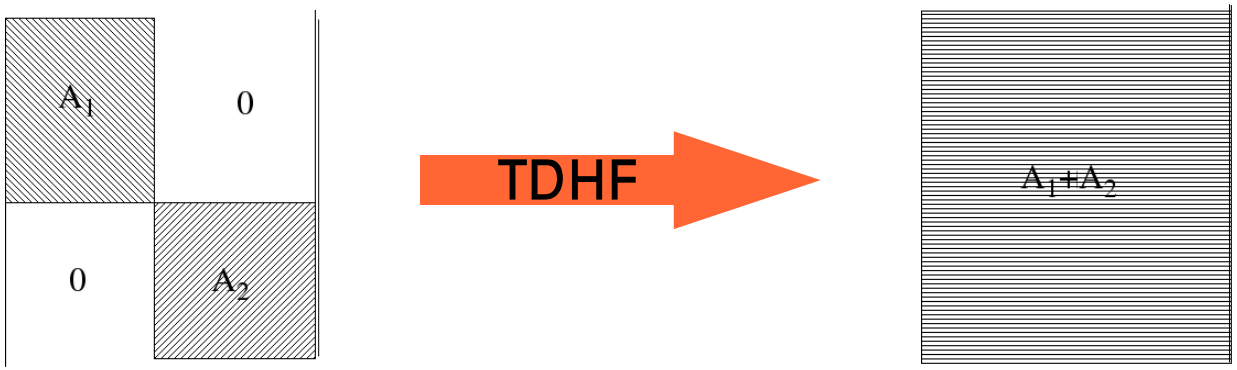
$$\phi_\lambda(t+\tau)=\exp[-i\tau h(\tau)]\phi_\lambda(t)$$

# Initial TDHF Setup

- Generate HF Slater determinants for each nucleus
- Multiply each determinant by a boost, determined from Coulomb trajectory and the asymptotic $E_{cm}$, at the initial nuclear separation (above the Coulomb barrier)

for nucleus $j$ $\quad \Phi_j \rightarrow \exp(i\boldsymbol{k}_j \cdot \boldsymbol{R})\Phi_j \quad$ and $\quad \boldsymbol{R} = \frac{1}{A_j}\sum_{i=1}^{A_j} r_i$

- Combine two determinants into a single one

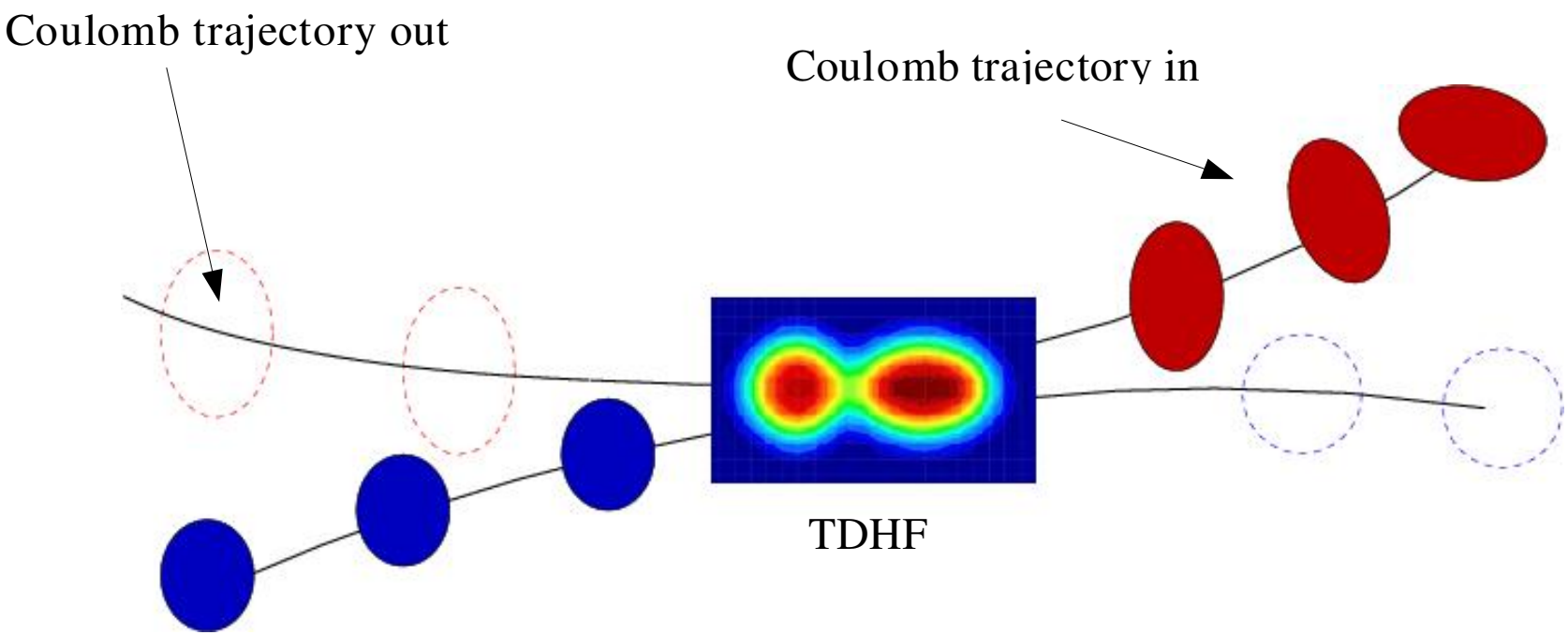



initial state

final state

# TDHF Collision Process

- If final stage contains a single fragment – FUSION
- If final stage contains two fragments – DEEP INELASTIC SCATTERING
- Initial approach is determined by Coulomb interaction only



# Full Skyrme Interaction

- Without time-reversal invariance Skyrme has many extra terms
  - They come in pairs/products such that Hamiltonian density is time-even

    *Engel, Brink, Goeke, Krieger, and Vautherin, Nucl. Phys. A249, 215 (1975)*

- These terms are zero while fitting the force parameters
  - To properties of static even-even nuclei

    *Chabanat, Bonche, Haensel, Meyer, and Schaeffer, Nucl. Phys. A635, 231 (1998)*

- They are all non-zero for dynamical calculations (also for odd-A)

- The extra terms are required to satisfy (no new parameters)
  - Galilean invariance
  - Local gauge invariance *(Dobaczewski and Dudek, Phys. Rev. C52, 1827 (1995))*

- In addition, we have a time-even spin-current tensor $J_{\mu\nu}$
  - Not included in the past due to numerical difficulty

# Additional terms in Skyrme energy density: spin density, spin current tensor, ...

## New Terms

$t_0, t_3$ →

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

$t_1, t_2$ →

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

$t_4$ →

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

## Old Term

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

# $^{16}O+^{16}O$ Fusion Cross Section at $E_{cm}$ = 34 MeV

| Force | $\sigma_{fusion}$ *(mb)* |
|---|---|
| BKN | 794 |
| Skyrme $II_Y^{(*)}$ | 1694 |
| $SkM^*_Y{}^{(*)}$ | 1822 |
| SkM* | 1368 |
| Sly5 | 1347 |
| Experiment$^{(**)}$ | 1075 |

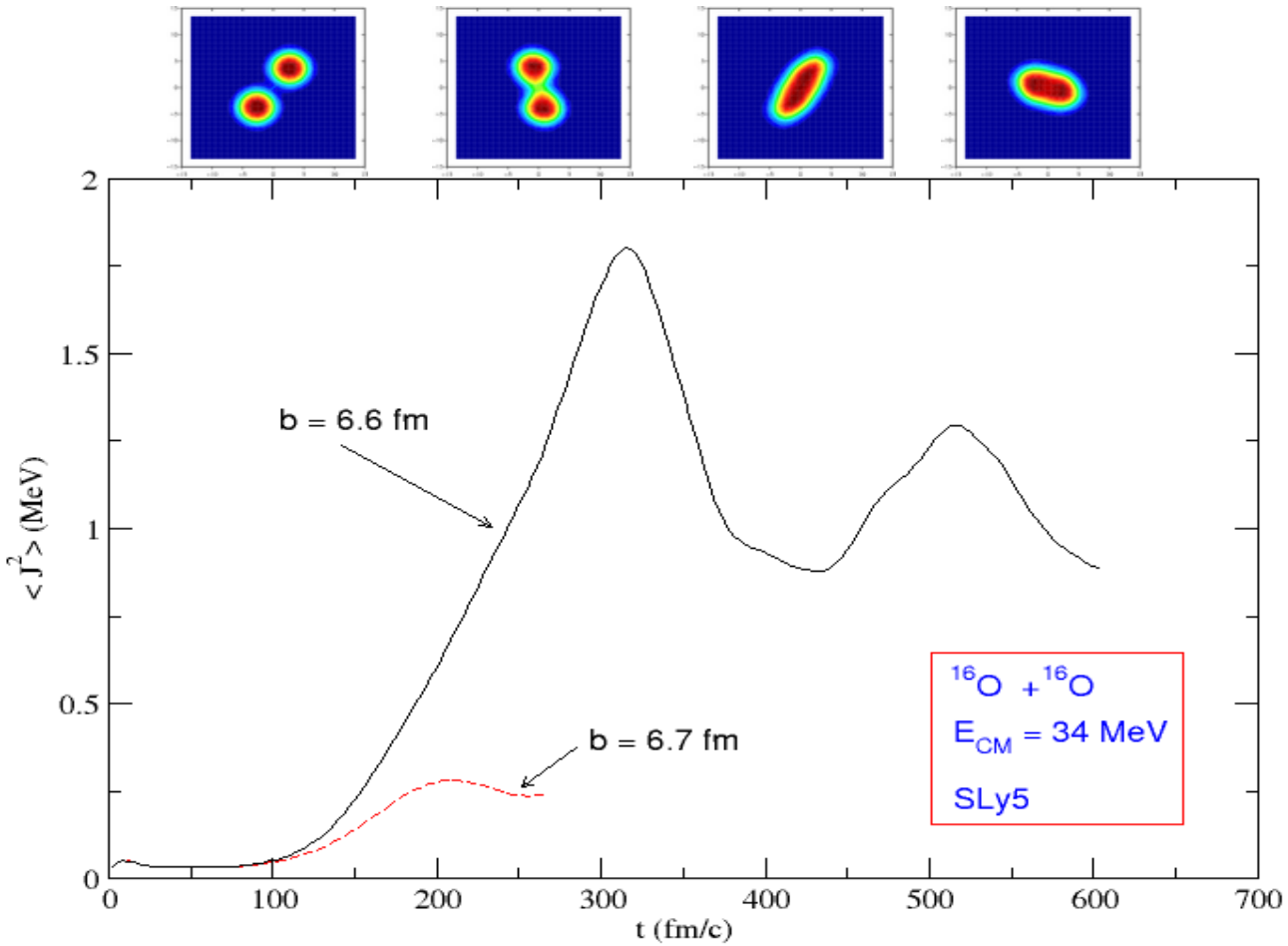
Sharp-Cutoff Approximation:

$$\sigma_{fusion} = \frac{\pi \hbar^2}{2 \mu E_{cm}} (l_{max} + 1)^2$$

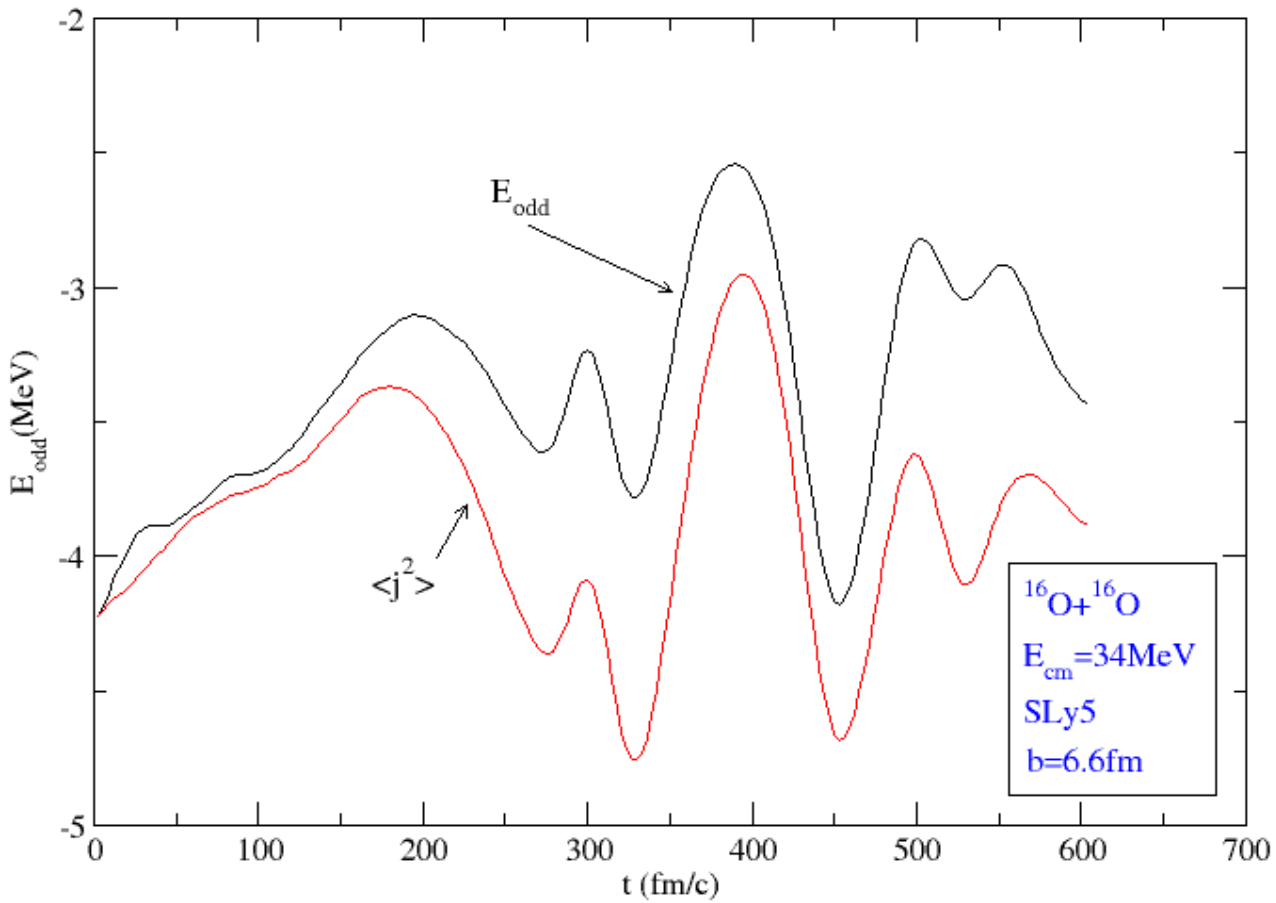
(*) Umar et al., Phys. Rev. Lett. 56, 2793 (1986)

(**) Birkelund, Tubbs, Huizenga, De, and Sperber, Phys. Rep. 56, 107 (1979)

# Time Evolution of the $J^2$ Term



# Evolution of the Time-Odd Energy

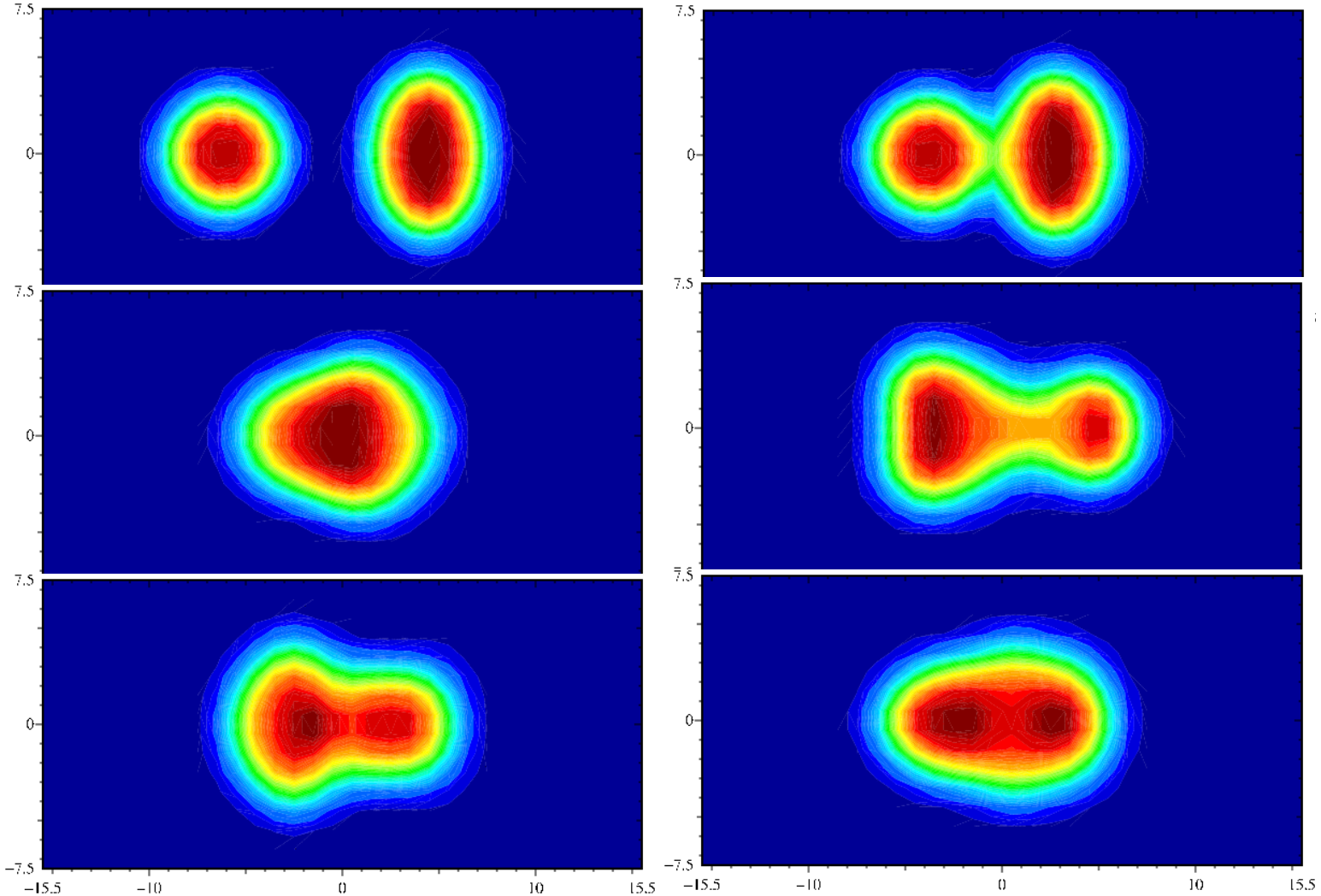


# TDHF fusion studies of spherical + deformed nuclei including dynamic alignment

- step 1: TDHF calculations for several orientations of deformed nucleus
- step 2: semi-quantal time-dependent Coulex calculation, determine orientation probability near distance of closest approach
- step 3: take average of weighted orientations to determine fusion cross section

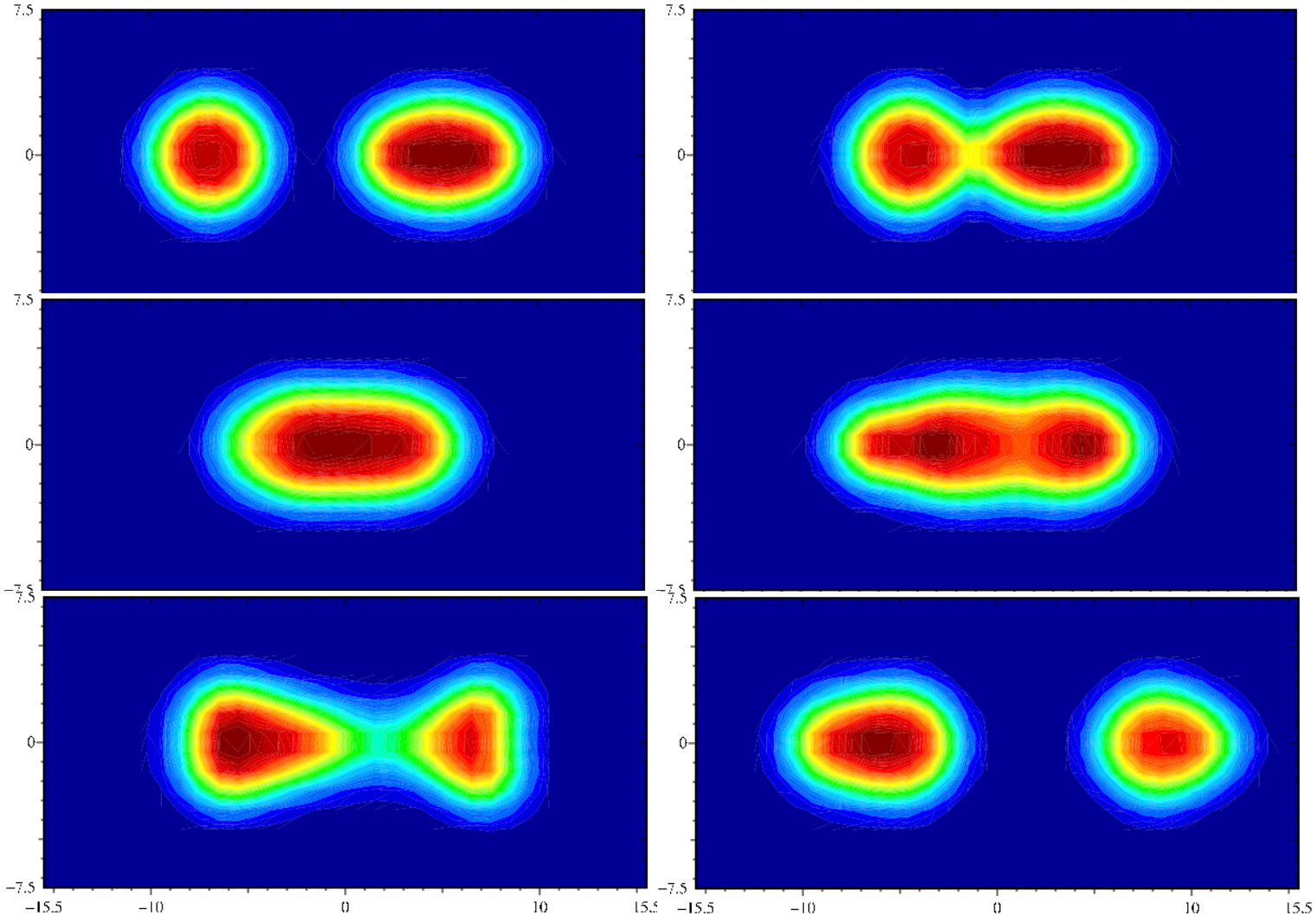
# $^{16}O + ^{22}Ne$ (alignment 1), $E_{cm}$ = 95 MeV, b=0 fm

Umar & Oberacker, Eur. Phys. J. A25, s01, 553 (2005)

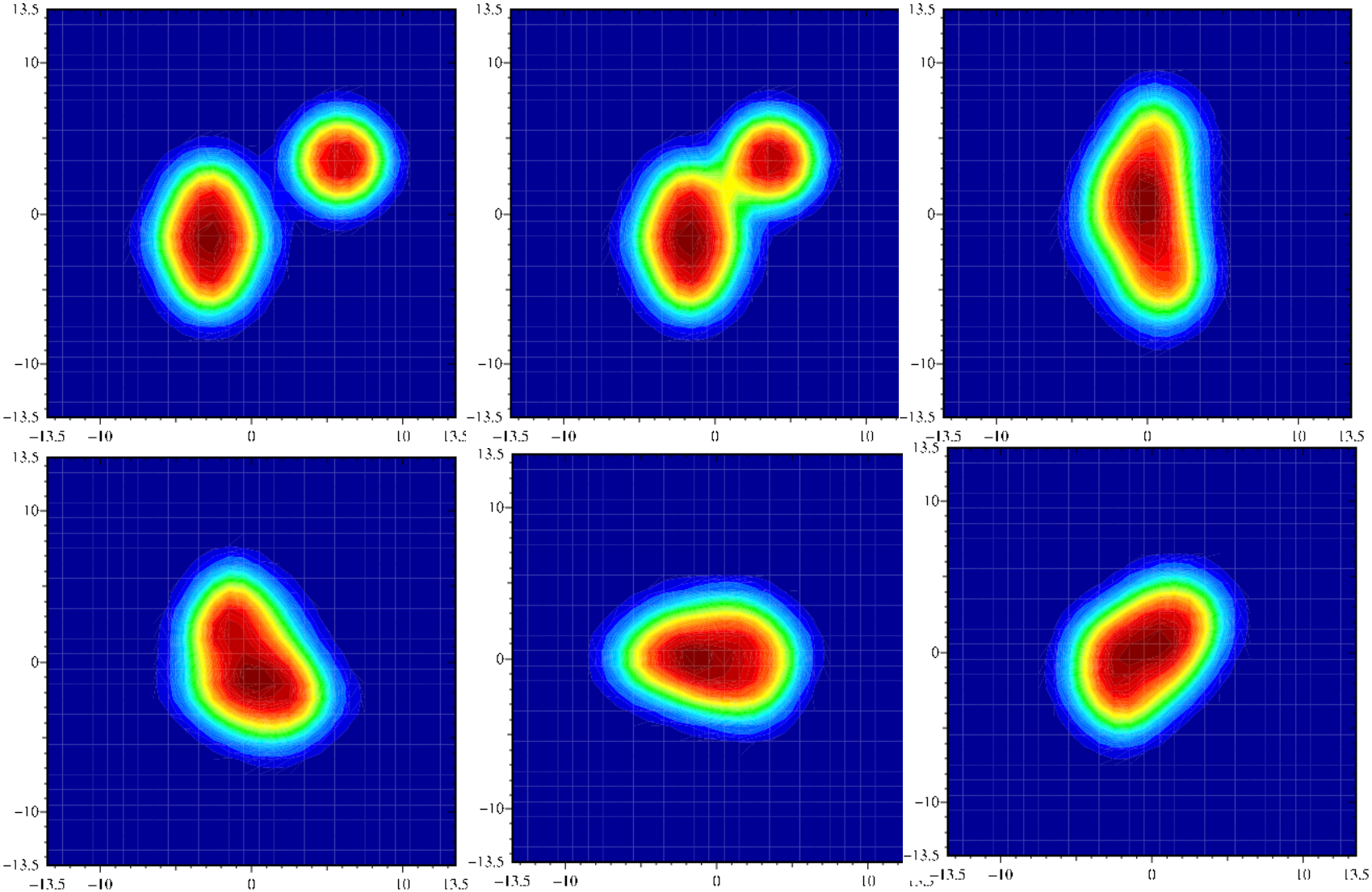


# $^{16}O + ^{22}Ne$ (alignment 2), $E_{cm}$ = 95 MeV, b=0 fm

Umar & Oberacker, Eur. Phys. J. A25, s01, 553 (2005)



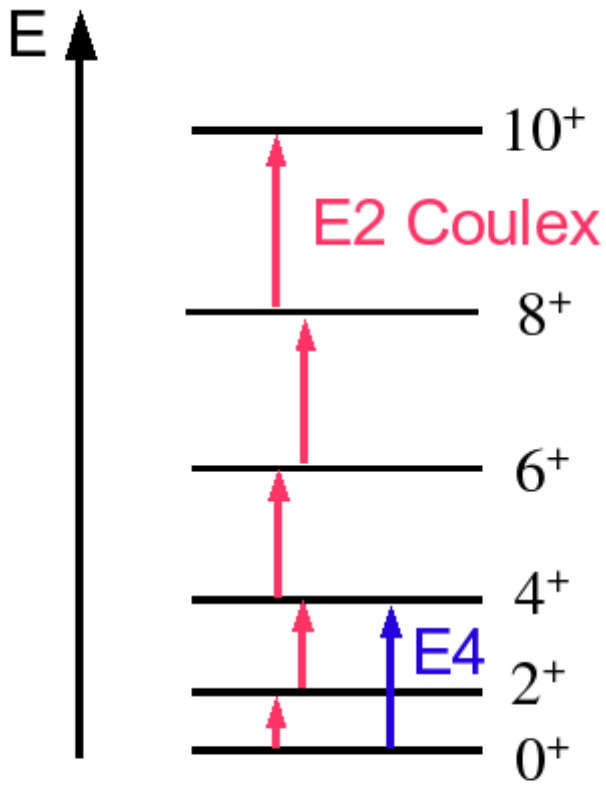
# $^{16}O+^{34}Ne$ (alignment 1), $E_{cm}$ = 115 MeV, b= 5 fm



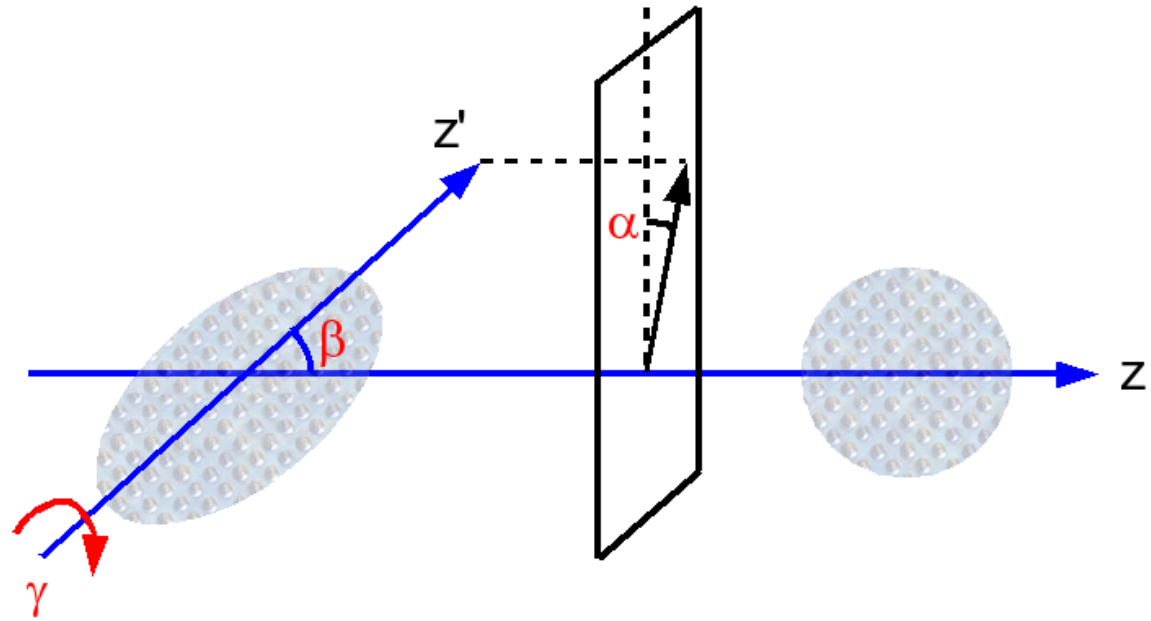
# $^{16}O + ^{34}Ne$ , $E_{cm} = 115$ MeV

| b (fm) | alignment | fusion | | b (fm) | alignment | fusion |
|---|---|---|---|---|---|---|
| | | | | | | |
| 0 | Perpendicular | Yes | | 0 | Parallel | No |
| | | | | | | |
| 2 | Perpendicular | Yes | | 2 | Parallel | No |
| | | | | | | |
| 5 | Perpendicular | Yes | | | | |
| | | | | | | |
| 7 | Perpendicular | Yes | | | | |
| | | | | | | |
| 8 | Perpendicular | No | | | | |

# Dynamic Alignment of Deformed Nucleus Due to Coulomb Excitation



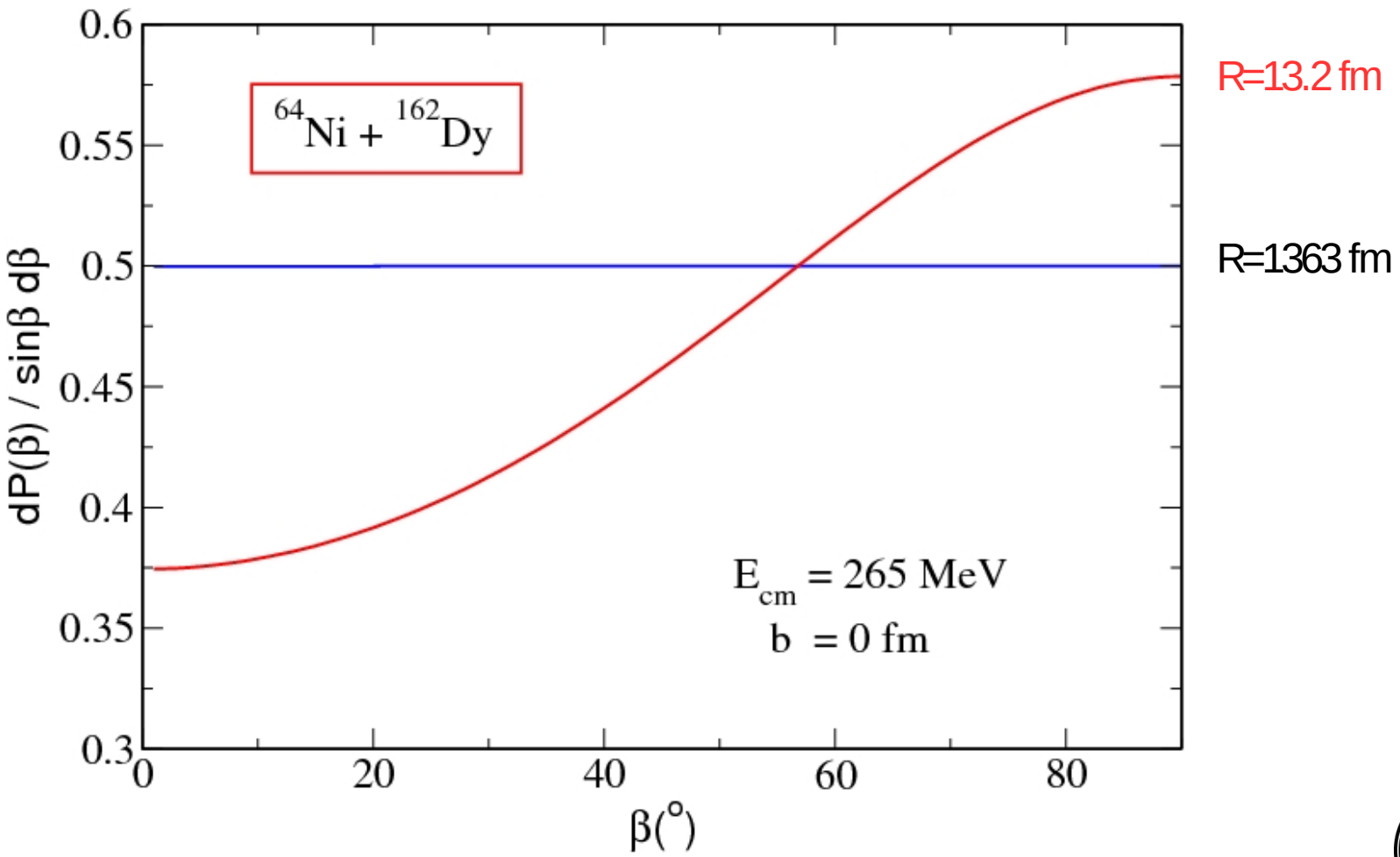

K=0 rotational band




V.E. Oberacker, Phys. Rev. C32, 1793 (1985)

# Dynamic Alignment Due to Coulomb Excitation of $^{162}$Dy

ratio of orientation prob. ($90^0$ / $0^0$ ) = 1.54



# Expression for Fusion Cross-Section

$$\sigma_{fusion}(E_{cm}) = \int_0^{b_{max}} b\,db\,P_{fusion}(b, E_{cm})$$ ← total cross-section

$$P_{fusion}(b, E_{cm}) = \int d\Omega \frac{dP_{fusion}(b, E_{cm}; \beta, \alpha)}{d\Omega}$$ ← fusion probability

$$\frac{dP_{fusion}(b, E_{cm}; \beta, \alpha)}{d\Omega} = \frac{dP_{orientation}(b, E_{cm}; \beta, \alpha)}{d\Omega} \cdot P_{TDHF}(b, E_{cm}; \beta, \alpha)$$

$$P_{TDHF}(b, E_{cm}; \beta, \alpha) = \begin{cases} 1 & \text{TDHF fuse} \\ 0 & \text{TDHF does not fuse} \end{cases}$$

# Conclusions and Outlook (part 1)

- stable and n-rich nuclei, spherical and deformed
- New TDHF code: 3-D lattice (no symmetry restrictions), B-Spline collocation method
- Modern Skyrme forces (Sly4,SLy5), full energy density functional, including spin-currents and tensors
- Studied effects of time-odd parts of TDHF mean field and influence on fusion
- Study impact parameter dependence and total fusion cross section for light spherical systems:

  $^{16}O + ^{16}O$, $^{16}O + ^{24}O$

# Conclusions and Outlook (part 2)

- TDHF fusion calculations for light spherical + deformed nuclei:

  $^{16}O + {}^{22}Ne$, $^{16}O + {}^{34}Ne$

  studied dependence on impact parameter and orientation angle

- dynamic alignment (due to Coulex) important for heavier systems (e.g. Ni + Dy): ratio of orientation prob. ($90^0$ / $0^0$ ) of about 1.5

- In future, study heavy n-rich systems e.g. $^{132}Sn$ --> $^{64}Ni$, $^{96}Zr$ requires massively parallel supercomputers (NERSC)