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
  \(^{16}\text{O} + ^{16}\text{O},\ ^{16}\text{O} + ^{28}\text{O}\)
  spherical + deformed nuclei (\(^{16}\text{O} + ^{22}\text{Ne},\ ^{16}\text{O} + ^{34}\text{Ne}\))
  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)
  Rhoades-Brown & Oberacker, PRL 50, 1435 (1983)

- **Coupled channels calculations**

- **Time-dependent Hartree-Fock** (TDHF)
  Umar, Strayer, Wu, Dean & Guclu, PRC 44, 2512 (1991)
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)
$^{16}\text{O} + ^{28}\text{O}$ at $E_{\text{cm}} = 43$ MeV, SLy5, $b = 7.5$ fm

$\sigma_{\text{fusion}} = 1916$ mb
$^{16}\text{O} + ^{28}\text{O}$ at $E_{cm} = 43$ MeV, SLy5, $b = 7.6$ fm
Basic TDHF Equations

- Equations of motion obtained from variation of the action

\[
S = \int_{t_1}^{t_2} dt \left< \Phi(t)|H - i \hbar \partial_t|\Phi(t)\right> \quad \text{with} \quad H = \sum_i t_i + \sum_{i<j} v_{ij}
\]

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

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

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

\[
i \hbar \frac{\partial \phi_\lambda}{\partial t} = \hbar \left( \begin{smallmatrix} \phi_\mu \end{smallmatrix} \right) \phi_\lambda
\]

- Skyrme energy functional is given by the 3D integral

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

- **Basis-Spline** discretization for high accuracy

- **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)

$$\Phi_j \rightarrow \exp(ik_j \cdot R)\Phi_j$$

- Combine two determinants into a single one

For nucleus $j$:

$$R = \frac{1}{A_j} \sum_{i=1}^{A_j} r_i$$

Initial state:

$$\begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}$$

Final state:

$$\begin{pmatrix} \Lambda_1 + \Lambda_2 \end{pmatrix}$$
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
  

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

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 $\mathcal{J}_{\mu \nu}$
- Not included in the past due to numerical difficulty
Additional terms in Skyrme energy density:
spin density, spin current tensor, ...

New Terms

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

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

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

Old Term

\[ \rho \tau \vec{j}^2 \]
$^{16}$O+$^{16}$O Fusion Cross Section at $E_{cm} = 34$ MeV

<table>
<thead>
<tr>
<th>Force</th>
<th>$\sigma_{fusion} \text{ (mb)}$</th>
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<tr>
<td>BKN</td>
<td>794</td>
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<tr>
<td>Skyrme II$_Y$(*)</td>
<td>1694</td>
</tr>
<tr>
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<td>SkM*</td>
<td>1368</td>
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<td>Sly5</td>
<td>1347</td>
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<tr>
<td>Experiment(**)</td>
<td>1075</td>
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Sharp-Cutoff Approximation:

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


Time Evolution of the $J^2$ Term

$\langle J^2 \rangle$ (MeV)

$t$ (fm/c)

$^{16}\text{O} + ^{16}\text{O}$

$E_{CM} = 34$ MeV

SLy5

$b = 6.6$ fm

$b = 6.7$ fm
Evolution of the Time-Odd Energy

\[ E_{\text{odd}}(\text{MeV}) \]

- \[ ^{16}\text{O}+^{16}\text{O} \]
- \[ E_{\text{cm}} = 34 \text{MeV} \]
- SLy5
- \( b = 6.6 \text{fm} \)
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
$^{16}\text{O} + ^{22}\text{Ne}$ (alignment 1), $E_{cm} = 95\text{ MeV}, b=0\text{ fm}$

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

$^{16}\text{O} + ^{34}\text{Ne}$ (alignment 1), $E_{\text{cm}} = 115$ MeV, $b = 5$ fm
\[ ^{16}\text{O} + ^{34}\text{Ne}, \quad E_{\text{cm}} = 115 \text{ MeV} \]

<table>
<thead>
<tr>
<th>b (fm)</th>
<th>alignment</th>
<th>fusion</th>
<th>b (fm)</th>
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<td>5</td>
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<tr>
<td>8</td>
<td>Perpendicular</td>
<td>No</td>
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</table>
Dynamic Alignment of Deformed Nucleus Due to Coulomb Excitation


K=0 rotational band

E

10^+
8^+
6^+
4^+
2^+
0^+

E2 Coulex

E4

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

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

$^{64}$Ni + $^{162}$Dy

$E_{cm} = 265$ MeV

$b = 0$ fm

$R = 13.2$ fm

$R = 1363$ fm
Expression for Fusion Cross-Section

\[ \sigma_{\text{fusion}}(E_{cm}) = \int_{0}^{b_{\text{max}}} b \, db \, P_{\text{fusion}}(b, E_{cm}) \]  
(total cross-section)

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

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

\[ P_{\text{TDHF}}(b, E_{cm}; \beta, \alpha) = \begin{cases} 1 & \text{TDHF fuse} \\ 0 & \text{TDHF does not fuse} \end{cases} \]
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:**
  \[ ^{16}\text{O} + ^{16}\text{O}, \quad ^{16}\text{O} + ^{24}\text{O} \]
Conclusions and Outlook (part 2)

- TDHF fusion calculations for light spherical + deformed nuclei:
  \[ ^{16}\text{O} + ^{22}\text{Ne}, \quad ^{16}\text{O} + ^{34}\text{Ne} \]
  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. \(^{132}\text{Sn} \rightarrow ^{64}\text{Ni}, ^{96}\text{Zr}\)
  requires massively parallel supercomputers (NERSC)