Fusion and other applications of density-constrained TDDFT

Volker E. Oberacker and A. Sait Umar
Vanderbilt University
Nashville, Tennessee, USA


Research supported by US Department of Energy, Division of Nuclear Physics
standard TDHF: fusion above the barrier

DC-TDHF: fusion below and above the barrier

Observables:
- fusion cross section $\sigma(E)$ for neutron-rich systems (RIB facilities)
- average multi-nucleon transfer $\Delta N(R), \Delta Z(R)$
- pre-equilibrium excitation energy $E^*(R)$
- pre-equilibrium GDR excitation and dipole spectrum $dP/dE_\gamma$

Capture cross sections for superheavy element formation
Fusion above the barrier: standard TDHF
Equations of motion obtained from variational principle

\[ \delta S = \delta \int_{t_1}^{t_2} dt < \Phi(t)|H - i\hbar \frac{\partial}{\partial t}|\Phi(t) >= 0 \]

main approximation: many-body state is assumed to be a single time-dependent Slater determinant

\[ \Phi(r_1, \ldots, r_A; t) = (A!)^{-1/2} \det |\phi_\lambda(r_i, t)| \]

TDHF equations for time-dependent single-particle states

\[ h(\{\phi_\mu\}) \phi_\lambda(r, t) = i\hbar \frac{\partial}{\partial t} \phi_\lambda(r, t) \quad (\lambda = 1, \ldots, A) \]

HF mean-field Hamiltonian \[ h = \frac{\partial E}{\partial \rho} \]
A new generation TDHF Code: brief summary


- 3-D Cartesian lattice
- Modern Skyrme forces with all terms (time-even /-odd)
- Coded in Fortran-95 and OpenMP
- Basis-Spline discretization for high accuracy
  Umar et al., J. Comp. Phys. 93, 426 (1991)
$^{48}\text{Ca} + ^{132}\text{Sn}, \quad E_{\text{cm}} = 130 \text{ MeV}, \quad b = 4.45 \text{ fm (fusion)}$

TDHF, SLy4 interaction, 3-D lattice (50*40*30 points)
animation: $^{48}\text{Ca} + ^{132}\text{Sn}$, $E_{cm} = 130$ MeV, $b = 4.45$ fm (fusion)
$^{48}\text{Ca} + ^{132}\text{Sn}, \ E_{cm} = 130 \ \text{MeV}, \ b = 4.6 \ \text{fm} \ (\text{deep-inelastic})$

TDHF, SLy4 interaction, 3-D lattice (50*42*30 points)
animation: $^{48}\text{Ca} + ^{132}\text{Sn}$, $E_{cm} = 130$ MeV, $b = 4.60$ fm (deep-inel)
Fusion above the potential barrier (unrestricted TDHF)


$\sigma_{fus} = \pi b_{max}^2$

sharp cutoff model

\[ \sigma_{fus} = \pi b_{max}^2 \]
Fusion below and above the barrier: Density-Constrained TDHF (DC-TDHF)
Theoretical Description of Sub-Barrier Fusion

- No ab-initio many-body theory for sub-barrier fusion exists. Usual approach involves several steps:

  a) Calculate internuclear potential $V(R)$
     - Woods-Saxon potential, proximity potential
       double-folding model with frozen densities (Esbensen)
     - macroscopic-microscopic (Möller, Sierk)
     - two-center shell model + liquid drop (Zagrebaev)
     - microscopic: Skyrme + extended Thomas-Fermi (Wang, Scheid, …)
       constrained HF/HFB (Dobaczewski, Nazarewicz, …)
     - our goal: time-dependent density functional theory, extract $V(R)$

  b) Quantum tunneling (either WKB-HW, or solve Schrödinger equation for relative motion $R$ with Incoming Wave Boundary Condition)

  c) Incorporate inelastic and transfer channels
     coupled channels approach (Esbensen, Hagino, …)
Brief review of standard constrained HF / HFB

\[ \delta < \Phi_0 | H - \lambda_2 Q_{20} - \lambda_3 Q_{30} | \Phi_0 | \geq 0 \] \rightarrow \text{potential energy surface } E(Q_{20}, Q_{30})

Staszczak, Baran, Dobaczewski & Nazarewicz, PRC 80, 014309 (2009)

INT-13-3 Website
Density constrained TDHF (DC-TDHF): formalism

1. Run TDHF code at energy $E_{cm}$ above potential barrier

2. Stop run at given internuclear distance $R(t)$

3. Take TDHF density

$$\rho_{TDHF}(r, t) = \langle \Phi(t) | \rho | \Phi(t) \rangle$$

and perform static HF energy minimization

$$\delta < \Phi_\rho | H - \int d^3r \lambda(r) \rho(r) | \Phi_\rho > = 0 \quad \rightarrow \quad | \Phi_\rho >$$

subject to density constraint

$$\langle \Phi_\rho | \rho | \Phi_\rho > = \rho_{TDHF}(r, t)$$

This takes out excitation energy $E^*(R)$.

4. Define density-constrained energy

$$E_{DC}(R) = \langle \Phi_\rho | H | \Phi_\rho >$$

$R = 10.4$ fm
DC-TDHF: calculate internuclear potential $V(R)$

Internuclear potential $V(R)$ is equal to density-constrained energy $E_{DC}(R)$ minus binding energies of the two nuclei

\[ V(R) = E_{DC}(R) - E_{A_1} - E_{A_2} \]
DC-TDHF fusion calculations for $^{132,124}$Sn + $^{48,40}$Ca

Detailed discussion of the following quantities:

- Internuclear potential $V(R)$
- Coordinate-dependent mass $M(R)$
- Fusion cross section $\sigma(E)$
- Pre-equilibrium excitation energy $E^*(R)$
- Multi-nucleon transfer $\Delta N(R), \Delta Z(R)$
- Pre-equilibrium GDR excitation and dipole spectrum $dP/dE_\gamma$
Calculation of internuclear potential with DC-TDHF method

\[ V(R) = E_{DC}(R) - E_{A1} - E_{A2} \]


\[ ^{48}\text{Ca}+^{132}\text{Sn} \]
\[ E_{cm}=140 \text{ MeV} \]

V(R) contains dynamical entrance channel effects (neck formation, particle transfer, surface vibrations, giant resonances)

R = 22.0 fm
R = 11.8 fm
R = 10.4 fm
R = 9.66 fm
Internuclear potential: strong $E_{\text{c.m.}}$-dependence

Mass parameter: strong $E_{\text{cm}}$-dependence

Scale transformation to constant reduced mass $\mu$


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

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

scaled distance

integrate

$$\bar{R} = f(R) \quad \leftrightarrow \quad R = f^{-1}(\bar{R})$$

$$V(R) = V(f^{-1}(\bar{R})) = U(\bar{R})$$

original potential \hspace{1cm} transformed potential
Transformed internuclear potential

Total fusion cross section for two spherical nuclei

\[
\sigma_{\text{fus}}(E_{\text{c.m.}}) = \frac{\pi \hbar^2}{2\mu E_{\text{c.m.}}} \sum_{\ell=0}^{\infty} (2\ell + 1) T_\ell(E_{\text{c.m.}})
\]

Schrödinger equation for transformed radial coordinate

\[
\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{d\bar{R}^2} + \frac{\hbar^2 \ell(\ell + 1)}{2\mu \bar{R}^2} + U(\bar{R}) - E_{\text{c.m.}} \right] \psi_\ell(\bar{R}) = 0
\]

solve Schrödinger equation numerically, with Incoming Wave Boundary Condition (IWBC)

\[ \rightarrow T_\ell(E_{\text{c.m.}}) \]
**Theory:** Oberacker, Umar, Maruhn & Reinhard, PRC 85, 034609 (2012)
Oberacker & Umar, PRC 87, 034611 (2013)

Anomaly in sub-barrier fusion cross sections for $^{132}\text{Sn} + ^{40,48}\text{Ca}$

$Q_{gg}$ ($^{40}\text{Ca}$ fusion) = -52.1 MeV, $Q_{gg}$ ($^{48}\text{Ca}$ fusion) = -76.2 MeV

Explanation of fusion anomaly in $^{132}\text{Sn} + ^{40,48}\text{Ca}$

The width of the DC-TDHF potential barrier for $^{40}\text{Ca}$ is substantially smaller than for $^{48}\text{Ca}$, resulting in enhanced sub-barrier fusion

Ref: Oberacker & Umar, PRC 87, 034611 (2013)
Multi-nucleon transfer in $^{132}\text{Sn}+^{40,48}\text{Ca}$

Ref: Oberacker & Umar, PRC 87, 034611 (2013)

$E_{cm}=120$ MeV, $b=0$

$^{132}\text{Sn}+^{40}\text{Ca}$
Q (n-pickup) > 0
Q (p-stripping) > 0

$^{132}\text{Sn}+^{48}\text{Ca}$
Q (n-pickup) < 0
Q (p-stripping) < 0
Dynamic excitation energy $E^*(R(t))$

Ref: Umar, Oberacker, Maruhn & and Reinhard, PRC 80, 041601(R) (2009)

Collective energy

$$E_{\text{coll}}(t) = E_{\text{kin}}(\rho(t), j(t)) + E_{\text{DC}}(\rho(t))$$

Excitation energy

$$E^*(R(t)) = E_{\text{TDFH}} - E_{\text{coll}}(t)$$

Approximate expression for collective kinetic energy

$$E_{\text{kin}}(\rho(t), j(t)) \approx \frac{m}{2} \int d^3r \frac{j^2(t)}{\rho(t)} \quad \rightarrow \quad \frac{\mu}{2} \dot{R}^2$$

large $R$
Dynamic excitation energy $E^*(R(t))$

![Graph showing dynamic excitation energy $E^*(R(t))$ for different collision energies and systems.](image)

- **$^{132}\text{Sn} + ^{48}\text{Ca}$**
  - DC-TDHF
  - $E_{\text{c.m.}} = 180$ MeV
  - $E_{\text{c.m.}} = 140$ MeV
  - $E_{\text{c.m.}} = 125$ MeV
  - $E_{\text{c.m.}} = 114$ MeV
  - $E_{\text{c.m.}} = 111$ MeV
$^{132}$Sn + $^{48}$Ca

DC-TDHF

$E_{c.m.} = 114$ MeV

$b = 0$ fm

Energy (MeV)

R (fm)
Pre-equilibrium GDR excitation and dipole radiation in heavy-ion fusion reactions

Goal: info about early stages of heavy-ion fusion reaction, elongated shape ($\beta_2=0.6$) during pre-equilibrium phase.

Unrestricted TDHF: $^{132}\text{Sn}+^{48}\text{Ca}$ ($E_{cm}=130$ MeV, $b=0$ fm)
Compare to $^{124}\text{Sn}+^{40}\text{Ca}$

Study dynamical density oscillations as function of time
Compute dynamical dipole moment $D(t)$ and EM radiation

• Umar & Oberacker, PRC 76, 014614 (2007)
• Simenel, Chomaz & de France, PRC 76, 024609 (2007)
• Baran, Rizzo, Colonna, Di Toro & Pierroutsakou, PRC 79, 021603(R) (2009)
• Oberacker, Umar, Maruhn & Reinhard, PRC 85, 034609 (2012)
• Keser, Umar & Oberacker, PRC 85, 044606 (2012)
Animation: dynamic giant resonance excitation:

$^{48}\text{Ca} + ^{132}\text{Sn}, \ E_{cm} = 130 \ \text{MeV}, \ b = 0 \ (\text{fusion})$

TDHF, SLy4 interaction, $t_{\text{final}} = 7,200 \ \text{fm/c}$
Pre-equilibrium GDR Excitation
dipole moment as a function of time (TDHF)

\[ D(t) = \frac{NZ}{A} \left[ \frac{1}{Z} \sum_{p=1}^{Z} x_p(t) - \frac{1}{N} \sum_{n=1}^{N} x_n(t) \right] \]

Power spectrum of electric dipole radiation

\[ \frac{dP}{dE_\gamma} = \frac{2\alpha}{3\pi E_\gamma} \left| \frac{1}{c} D''(\omega) \right|^2 \]

\[ \alpha = \frac{e^2}{\hbar c} \approx 1/137 \]

Pre-equilibrium GDR is stronger for systems with larger initial N/Z differential of the two ions:

- \( 1.48 : 1.0 \) for \(^{124}\text{Sn} + ^{40}\text{Ca}\),
- \( 1.64 : 1.4 \) for \(^{132}\text{Sn} + ^{48}\text{Ca}\)

Ref: Oberacker, Umar, Maruhn & Reinhard, PRC 85, 034609 (2012)
DC-TDHF fusion calculations for other systems

(about 25 fusion reactions studied between 2006-2013)
DC-TDHF fusion calculations for light systems

\[ ^{16,24}\text{O} + ^{16,24,28}\text{O} \text{ and } ^{16,18,19,20,24}\text{O} + ^{12}\text{C} \]

Sub-barrier fusion: relevant for neutron star crust!

- Umar, Oberacker & Horowitz, PRC 85, 055801 (2012)
- deSouza, Hudan, Oberacker & Umar, PRC 88, 014602 (2013)
$V(R)$ for light systems: weak dependence on $E_{cm}$

Ref: Umar, Oberacker, Maruhn & Reinhard, PRC 80, 041601(R) (2009)
total fusion cross sections for oxygen isotopes

Ref: Umar, Oberacker & Horowitz, PRC 85, 055801 (2012)
\( {}^{16}\text{O} + {}^{16}\text{O} \) fusion at higher energies (up to \( E=3.5 \ E_{\text{coul}} \))

Ref: Simenel, Keser, Umar & Oberacker, PRC 88, 024617 (2013)

We need new experiments!

excellent test case for current and future microscopic theories:
- \( {}^{16}\text{O} \) in most Skyrme force fits
- doubly magic (no pairing issues)
- light system (small CPU time)

Similar results and conclusions: Esbensen, PRC 77, 054608 (2008)
$^{12}\text{C} + ^{16,24}\text{O}$ fusion
Ref: Umar, Oberacker & Horowitz, PRC 85, 055801 (2012)

Barrier heights (MeV)
7.77
6.64
DC-TDHF predictions for $^{18,19,20}\text{O}+^{12}\text{C}$

Fusion experiments are scheduled for Fall 2013 / Spring 2014 at Florida State Univ. (deSouza et al.)
Sub-barrier fusion of $^{40,48}$Ca + $^{40,48}$Ca

Keser, Umar, and Oberacker, PRC 85, 044606 (2012)
Sub-barrier fusion of \(^{48}\text{Ca} + ^{48}\text{Ca}\)

Keser, Umar, and Oberacker, PRC 85, 044606 (2012)

used two Skyrme forces: SLy4 and UNEDF1
$^{16}\text{O} + ^{208}\text{Pb}$ fusion

Spherical + deformed (oblate) nucleus: $^{132}$Sn + $^{64}$Ni

Umar & Oberacker, PRC 76, 014614 (2007)

Heavy-ion potential depends on initial orientation angle $\beta$ of deformed nucleus
$^{64}$Ni + $^{132}$Sn sub-barrier fusion: first reaction studied with DC-TDHF

DC-TDHF theory
Umar and Oberacker,
PRC 76, 014614 (2007)

Exp. Data (HRIBF, ORNL)
J.F. Liang et al.,
PRC 75, 054607 (2007)
PRC 78, 047601 (2008)
**Fusion hindrance in $^{64}\text{Ni} + ^{64}\text{Ni}$**


\[ \sigma (\text{mb}) \]

\[ \text{E}_{\text{c.m.}} (\text{MeV}) \]

\[ \text{R(fm)} \]

\[ (\beta_1 = 0^\circ, \beta_2 = 90^\circ) \]

\[ (\beta_1 = 90^\circ, \beta_2 = 90^\circ) \]

\[ (\beta_1 = \beta_2 = 0^\circ) \]

\[ \text{data} \]

\[ \text{DC-TDHF (Core)} \]
Heavy-ion fusion leading to superheavy element Z=112

spherical + spherical: “cold fusion” (E* small)
spherical + deformed: “hot fusion” (E* large)
Factors Influencing Superheavy Formations

- Excitation energy
  - high excitation at the capture configuration → quasi-fission
  - high excitation of compound nucleus → fusion-fission
- Nuclear deformation and alignment
- Shell effects
- Mass asymmetry in the entrance channel
- Impact parameter dependence
- ..... 

\[ \sigma_{ER} = \sigma_{\text{capture}} \cdot P_{CN} \cdot P_{\text{survival}} \]

- Capture in ion-ion potential pocket
- Form compound system
- Survive FF process
$^{48}\text{Ca} + ^{238}\text{U}$ internuclear potential

Umar, Oberacker, Maruhn & Reinhard, PRC 81, 064607 (2010)

\[ E_{\text{c.m.}} = 250 \text{ MeV} \]
\[ E_{\text{c.m.}} = 220 \text{ MeV} \]
\[ E_{\text{c.m.}} = 200 \text{ MeV} \]
\[ E_{\text{c.m.}} = 185 \text{ MeV} \]

\[ \beta = 45^\circ \]

Exp. Energies

DC-TDHF

Point Coulomb

\[ V(R) \text{ (MeV)} \]

\[ R \text{ (fm)} \]
Dynamic alignment (due to Coulex) of $^{238}\text{U}$ in hot fusion

Umar, Oberacker, Maruhn & Reinhard, PRC 81, 064607 (2010)

$^{48}\text{Ca} + ^{238}\text{U}$

$E_{\text{c.m.}} = 220\text{ MeV}$

$b = 0\text{ fm}$

$\frac{dP(\beta)}{\sin \beta d\beta}$

$0.52$

$0.5$

$0.48$

$0.46$

$0$ 20 40 60 80

$\beta$ (deg)
$^{48}$Ca + $^{238}$U capture cross section

Umar, Oberacker, Maruhn & Reinhard, PRC 81, 064607 (2010)

$$\sigma_{capt}(E_{cm}) = \int_0^\pi \sin \beta d\beta \frac{dP(\beta)}{\sin \beta d\beta} \sigma_{capt}(E_{cm}, \beta)$$

dynamic alignment

- $\sigma(\beta)$ decreases rapidly for $\beta > 10^\circ$
- $\sin(\beta)$ multiplies small angles
- $dP(\beta)$ is in the range 0.46 - 0.52

$^{48}$Ca + $^{238}$U

DC-TDHF

Comparison: internuclear potentials for $^{48}$Ca, $^{50}$Ti + $^{249}$Bk

exp: DGFRS Dubna  
$\sigma$ (Z=117) = 1.1-2.4 pb  
50 times larger!

exp: TASCA GSI  
$\sigma$ (Z=119) < 50 fb
• DC-TDHF: time-dependent density functional theory for fusion below and above the barrier
  - only input: Skyrme N-N interaction, no adjustable parameters

• DC-TDHF output:
  - internuclear potential $V(R)$, mass $M(R)$, fusion cross section $\sigma(E)$,
  - excitation energy $E^*(R)$, average multi-nucleon transfer,
  - pre-equilibrium GDR excitation and dipole radiation

• Quantitative sub-barrier fusion calculations are now possible,
  - detailed comparison with experimental data (about 25 fusion reactions studied with DC-TDHF between 2006-2013)

• Grand Challenge: include pairing into DC-TDHF
  - develop TDHFB code on 3D lattice for nuclear reactions
Current research projects

- Neutron star crust: fusion reactions \((\text{C+O}, \text{O+O})\) in the presence of a neutron gas with variable density collaboration with Charles Horowitz and P.-G. Reinhard

- Fusion of light systems \((^{18,19,20}\text{O}+^{12}\text{C})\): DC-TDHF calculations finished, fusion experiments in Fall 2013 / Spring 2014 at Florida State, collaboration with experimentalists at Indiana University (Romualdo deSouza et al.)

- Studies in connection with superheavy element formation:
  a) DC-TDHF capture cross sections for \(^{48}\text{Ca},^{50}\text{Ti} + ^{249}\text{Bk}\)
  b) Quasifission in \(^{50}\text{Ti} + ^{208}\text{Pb}, ^{48}\text{Ca} + ^{248}\text{Cm}, \ldots\) unrestricted TDHF, possible collaboration with Cedric Simenel experimental guidance by Zach Kohley and Walt Loveland