TDHF – Basic Facts

Advantages

- Fully microscopic, parameter-free description of nuclear collisions
- Use same microscopic interaction used in static calculations
- Successful in describing low-energy fusion, deep-inelastic collisions, nuclear molecules, and collective phenomena
- Provides a method for linear response calculations (RPA)

Shortcomings

- Semi-classical (no reaction channels, describes dominant channel)
- Does not include pairing
- Only one-body dissipation (collisions with “walls” of mean field)

TDHF Equations

- Equations of motion obtained from variation of the action

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

- Many-body state is a single time-dependent Slater determinant

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

- TDHF equations for single-particle states

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

- Skyrme energy functional is given by the 3D integral

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

Skyrme Hamiltonian Density

$$
\begin{aligned}
H_S(\boldsymbol{r}) =\; & \frac{\hbar^2}{2\mathrm{m}}\tau + \frac{1}{2}t_0\left(1+\frac{1}{2}x_0\right)\rho^2 - \frac{1}{2}t_0\left(\frac{1}{2}+x_0\right)\left[\rho_p^2+\rho_n^2\right] + \frac{1}{4}\left[t_1\left(1+\frac{1}{2}x_1\right)+t_2\left(1+\frac{1}{2}x_2\right)\right](\rho\tau-\boldsymbol{j}^2) \\
& -\frac{1}{4}\left[t_1\left(\frac{1}{2}+x_1\right)-t_2\left(\frac{1}{2}+x_2\right)\right]\left(\rho_p\tau_p+\rho_n\tau_n-\boldsymbol{j}_p^2-\boldsymbol{j}_n^2\right) - \frac{1}{16}\left[3\mathrm{t}_1\left(1+\frac{1}{2}x_1\right)-t_2\left(1+\frac{1}{2}x_2\right)\right]\rho\nabla^2\rho \\
& +\frac{1}{16}\left[3\mathrm{t}_1\left(\frac{1}{2}+x_1\right)+t_2\left(\frac{1}{2}+x_2\right)\right]\left(\rho_p\nabla^2\rho_p+\rho_n\nabla^2\rho_n\right) \\
& +\frac{1}{12}t_3\left[\rho^{\alpha+2}\left(1+\frac{1}{2}x_3\right)-\rho^{\alpha}\left(\rho_p^2+\rho_n^2\right)\left(x_3+\frac{1}{2}\right)\right] \\
& +\frac{1}{4}t_0x_0\boldsymbol{s}^2-\frac{1}{4}t_0(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2)+\frac{1}{24}\rho^{\alpha}t_3x_3\boldsymbol{s}^2-\frac{1}{24}t_3\rho^{\alpha}(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2) \\
& +\frac{1}{32}(t_2+3\mathrm{t}_1)\sum_q \boldsymbol{s}_q\cdot\nabla^2\boldsymbol{s}_q-\frac{1}{32}(t_2x_2-3t_1x_1)\boldsymbol{s}\cdot\nabla^2\boldsymbol{s} \\
& +\frac{1}{8}(t_1x_1+t_2x_2)(\boldsymbol{s}\cdot\boldsymbol{T}-\boldsymbol{J}_{\mu\nu}^2)+\frac{1}{8}(t_2-t_1)\sum_q(\boldsymbol{s}_q\cdot\boldsymbol{T}_q-\boldsymbol{J}_{q\mu\nu}^2) \\
& -\frac{t_4}{2}\sum_{qq'}(1+\delta_{qq'})[\boldsymbol{s}_q\cdot\nabla\times\boldsymbol{j}_{q'}+\rho_q\boldsymbol{\nabla}_{\mu\nu}\cdot\boldsymbol{J}_{\mu\nu}]
\end{aligned}
$$

Time-odd terms come in pairs!
Total is TR invariant

(s,j,T) time-odd, vanish for static HF calculations of even-even nuclei
non-zero for dynamic calculations, odd mass nuclei, cranking, etc.

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: brief summary

Umar and Oberacker, PRC 73, 054607 (2006)

- Modern Skyrme forces with all terms (time-even /-odd)
- Unrestricted 3-D Cartesian lattice
- Coded in Fortran-95 and OpenMP
- Basis-Spline discretization for high accuracy

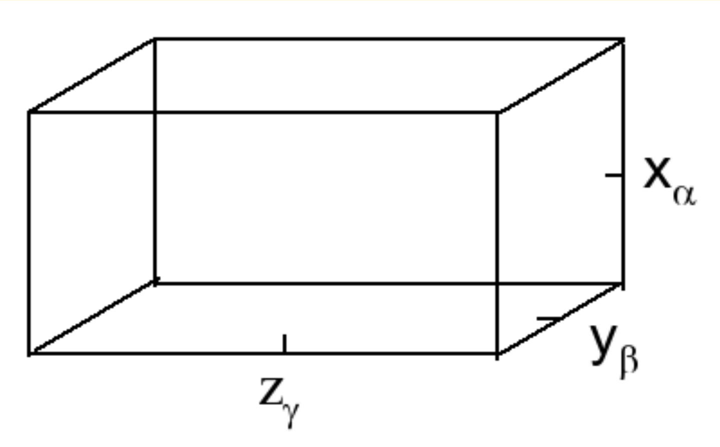
Umar *et al.*, J. Comp. Phys. 93, 426 (1991)

- Other TDHF codes:

Simenel, Chomaz, and de France, PRL 93, 102701 (2004)
Washiyama and Lacroix, PRC 78, 024610 (2008)
Guo, Maruhn, Reinhard and Hashimoto, PRC 77, 041301(R) (2008)

Numerical implementation

Represent wave functions for all A nucleons on 3-D Cartesian lattice



Grid points:

$$x_\alpha \quad (\alpha = 1, ..., N_x)$$
$$y_\beta \quad (\beta = 1, ..., N_y)$$
$$z_\gamma \quad (\gamma = 1, ..., N_z)$$

$$\psi(x, y, z; \sigma_z, t_z) \rightarrow \psi(x_\alpha, y_\beta, z_\gamma; \sigma_z, t_z)$$

Wave function on the lattice becomes a complex-numbered array of dimension

$$psi(N_x, N_y, N_z, 2, 2)$$

Heavy-ion reactions as function of impact parameter b

impact
parameter b

large	Elastic collision, inelastic collision (Coulomb excitation)
	Coulomb + nuclear inelastic excitation few-nucleon transfer
medium	
	Multi-nucleon transfer
	Deep-inelastic collisions ($E^* \approx 30$ MeV), 2 fragments emerge
small	Fusion reactions, 1 fragment in exit channel

Heavy-ion fusion experiments: current frontiers

- Use RIBs to create new neutron-rich nuclei
  accelerators at HRIBF, NSCL, ATLAS, RIKEN

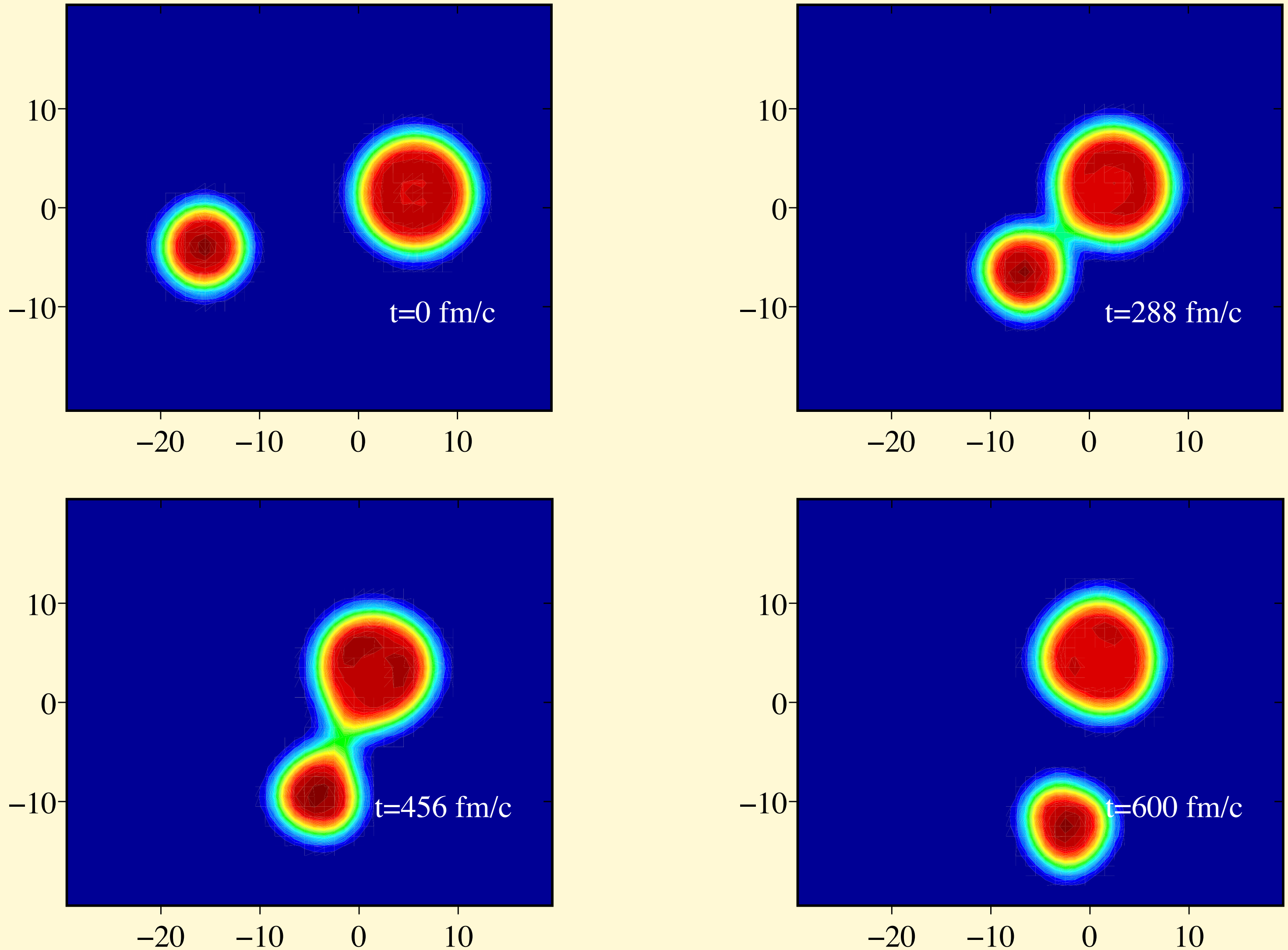
  J.F. Liang et al., PRC 78, 047601 (2008)
  Vinodkumar et al., PRC 78, 054608 (2008)

- Synthesis of superheavy elements (Z=110-116,...)
  accelerators at GSI, JINR, RIKEN

  W. Loveland, PRC 76, 014612 (2007)
  Oganessian et al., PRC 74, 044602 (2006)
  Hofmann et al., Eur. Phys. J. A14, 147 (2002)

$^{48}Ca + {}^{132}Sn$, E_{cm} = 130 MeV, b = 4.6 fm (deep-inelastic)

TDHF, SLy4 interaction, 3-D lattice (50*42*30 points)



Structure of Slater determinant in TDHF

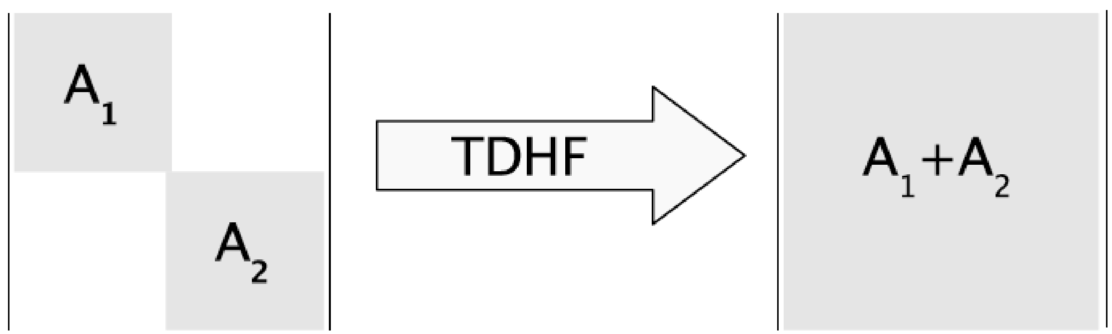
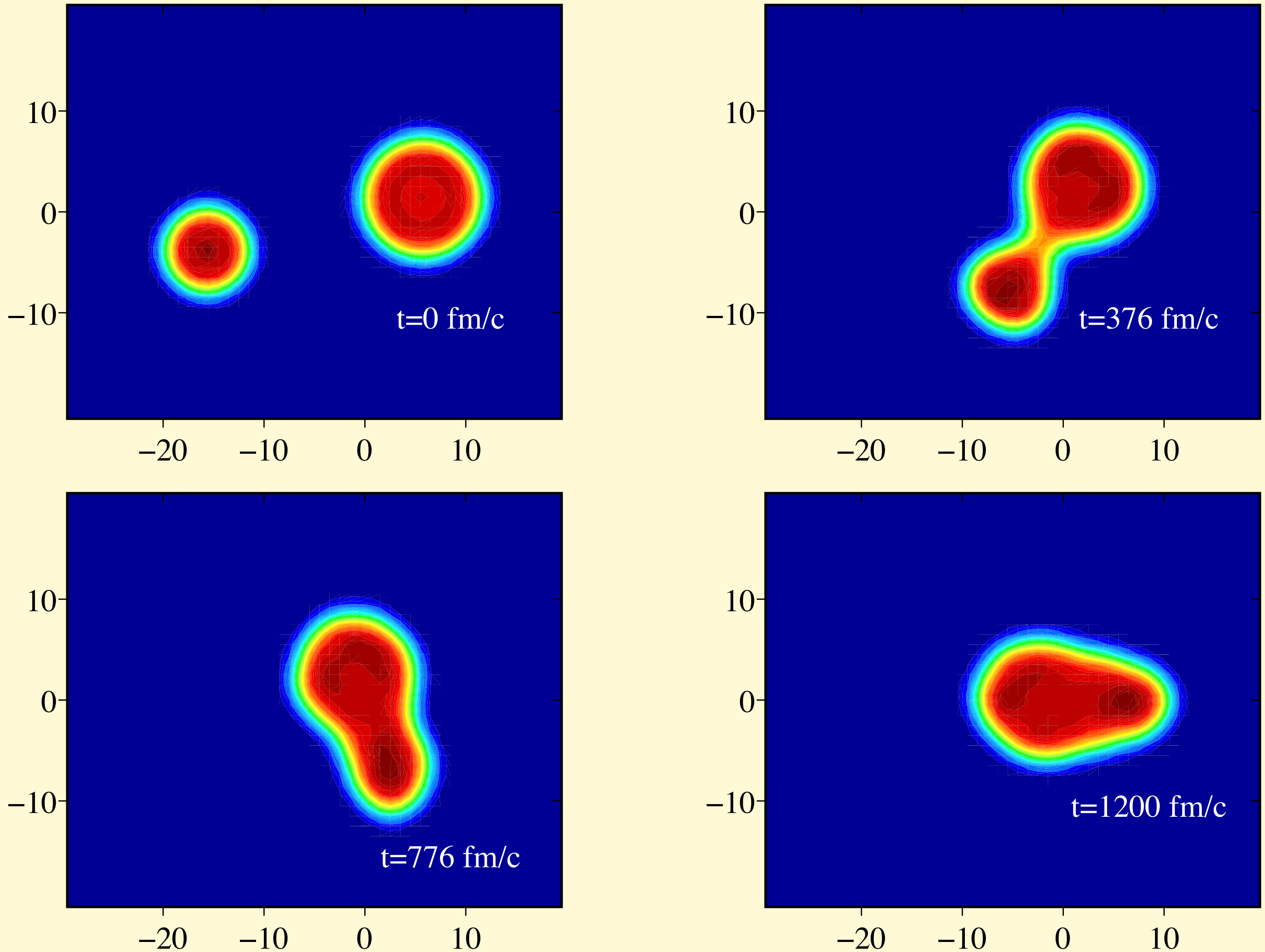


FIG. 1. Schematic illustration of the initial and final many-body states. The initial state is block diagonal whereas the final state is a full Slater determinant.

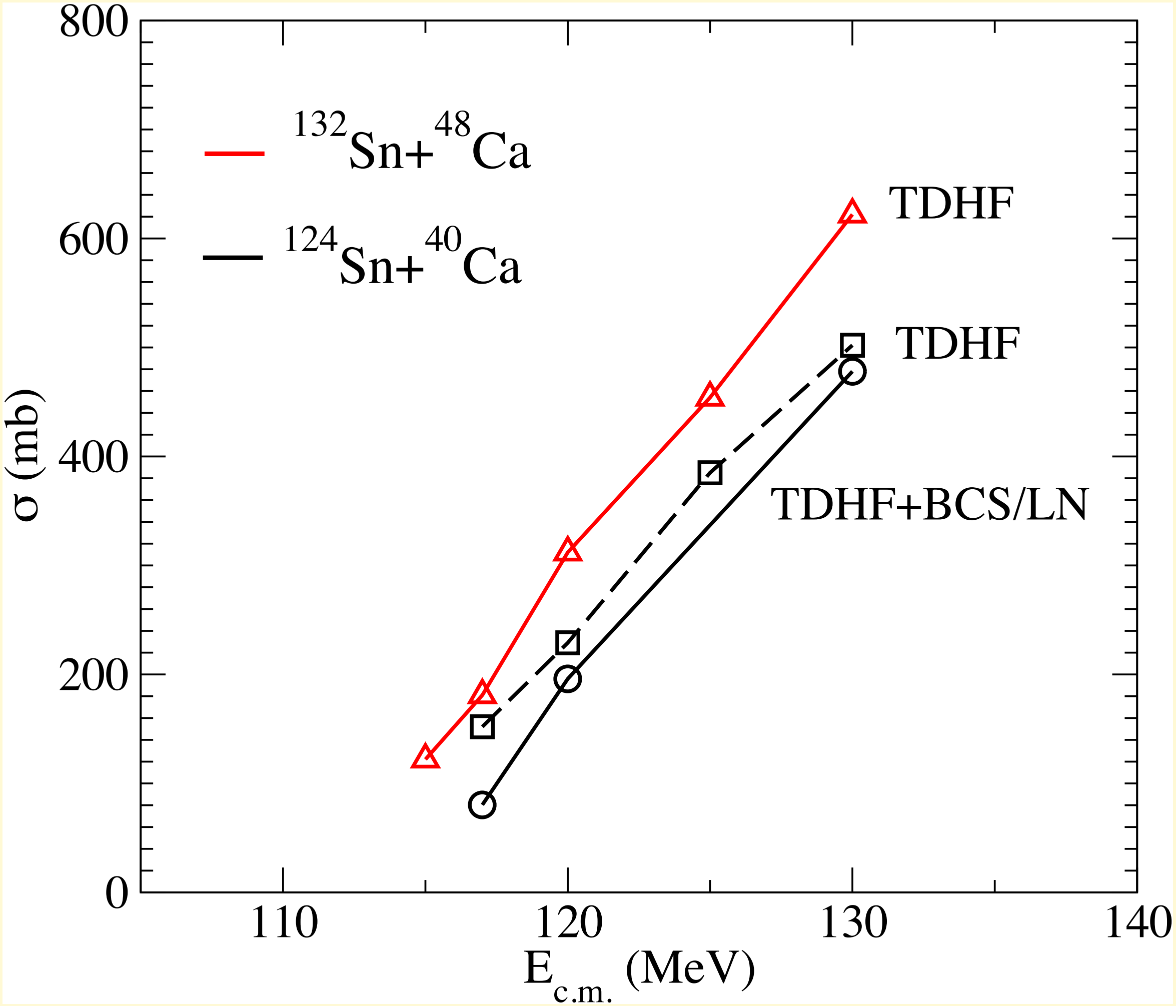
^{48}Ca + ^{132}Sn, E_{cm} = 130 MeV, b = 4.45 fm (fusion)

TDHF, SLy4 interaction, 3-D lattice (50*40*30 points)



Fusion above the potential barrier (unrestricted TDHF)

Oberacker, Umar, Maruhn, and Reinhard, Phys. Rev. C 85, 034609 (2012)



sharp cutoff model

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