Macroscopic properties in low-energy nuclear reactions by microscopic TDDFT



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### Nucleus-nucleus potential

• Low-energy nuclear reactions E/A < 10 MeV



# Macroscopic, Microscopic picture



#### Aim

Study the property of macroscopic quantities by TDHF

# Time-dependent Hartree-Fock (TDHF)

$$i\hbar \frac{\partial}{\partial t}\phi_i(\mathbf{r},t) = \hat{h}[\rho(\mathbf{r},t)]\phi_i(\mathbf{r},t)$$

*h*: self-consistent single-particle Hamiltonian

(static case 
$$\hat{h}[
ho]\phi_i=\epsilon_i\phi_i$$
 )

- Self-consistent description for both static and dynamical properties
- Single-particle: **Quantum**, Collective motion: **Classical**
- Low energy: mean-field approximation
  - 3D-TDHF code by P. Bonche (Kim, Otsuka, Bonche, J. Phys. G23(1997)1267)
     Input:
    - ✓ Skyrme SLy4d parameterization
    - ✓ 3D, dx = 0.8 fm, dt = 0.45 fm/c

- Bonche et al., PRC 13 (1976)
- Flocard et al., PRC 17 (1978)
- Kim et al., J. Phys. G 23 (1997)
- Simenel et al., PRL 86 (2001)
- Nakatsukasa, Yabana, PRC 71 (2005)
- Umar, Oberacker, PRC 73 (2006)
- Maruhn et al., PRC 74 (2006)

# Energy density functional

Skyrme energy density functional

$$\mathcal{E}_{Sk} \equiv \int d^3 r \sum_{t=0,1} \mathcal{H}_t(\mathbf{r}) \qquad \begin{array}{l} \rho_{t=0} = \rho_n + \rho_p \\ \rho_{t=1} = \rho_n - \rho_p \end{array}$$

$$\mathcal{H}_{t} = C_{t}^{\rho} \rho_{t}^{2} + C_{t}^{\Delta \rho} \rho_{t} \Delta \rho_{t} + C_{t}^{\tau} \rho_{t} \tau_{t} + C_{t}^{\nabla \cdot J} \rho_{t} \nabla \cdot \boldsymbol{J}_{t} - C_{t}^{T} \sum_{\mu,\nu=x,y,z} \boldsymbol{J}_{t,\mu\nu} \boldsymbol{J}_{t,\mu\nu} \cdots$$
$$+ C_{t}^{s} \boldsymbol{s}_{t}^{2} + C_{t}^{\Delta s} \boldsymbol{s}_{t} \cdot \Delta \boldsymbol{s}_{t} - C_{t}^{\tau} \boldsymbol{j}_{t}^{2} + C_{t}^{\nabla \cdot J} \boldsymbol{s}_{t} \cdot \nabla \times \boldsymbol{j}_{t} + C_{t}^{T} \boldsymbol{s}_{t} \cdot \boldsymbol{T}_{t} + \cdots$$

$$\rho_q(\boldsymbol{r}) = \rho_q(\boldsymbol{r}, \boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}, \quad \tau_q(\boldsymbol{r}) = \nabla \cdot \nabla' \rho_q(\boldsymbol{r}, \boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}, \quad J_{q,\mu\nu}(\boldsymbol{r}) = -\frac{i}{2} (\nabla_\mu - \nabla'_\mu) s_{q,\nu}(\boldsymbol{r}, \boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}$$
$$s_q(\boldsymbol{r}) = s_q(\boldsymbol{r}, \boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}, \quad \boldsymbol{T}_q(\boldsymbol{r}) = \nabla \cdot \nabla' s_q(\boldsymbol{r}, \boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}, \quad \boldsymbol{j}_q(\boldsymbol{r}) = -\frac{i}{2} (\nabla - \nabla') \rho_q(\boldsymbol{r}, \boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}$$

$$\rho_q(\boldsymbol{r}, \boldsymbol{r}') = \sum_{\sigma=\pm 1} \rho_q(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma) = \sum_{\sigma=\pm 1} \sum_k n_k \phi_k(\boldsymbol{r}\sigma q) \phi_k^*(\boldsymbol{r}'\sigma q)$$
$$\boldsymbol{s}_q(\boldsymbol{r}, \boldsymbol{r}') = \sum_{\sigma, \sigma'=\pm 1} \rho_q(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma') \langle \sigma' | \hat{\boldsymbol{\sigma}} | \sigma \rangle$$

Bender, Heenen, Reinhard, Rev. Mod. Phys. 75 (2003) 121

# Numerical method for solving TDHF

$$\begin{cases} \{\phi_i^{(n)}\} \\ \{\phi_i^{(n+1)}\} \end{cases} \qquad \rho^{(n)} \\ \hat{\phi}_i^{(n+1)} = \exp[-i\frac{\Delta t}{\hbar}\hat{h}^{(n+\frac{1}{2})}] \phi_i^{(n)} \\ \hat{h}^{(n+\frac{1}{2})} = \hat{h}[\rho^{(n+\frac{1}{2})}] \\ \rho^{(n+\frac{1}{2})} = \frac{1}{2}[\rho^{(n)} + \tilde{\rho}^{(n+1)}] \qquad \tilde{\rho}^{(n+1)} \end{cases}$$

# Recent applications of TDHF



<sup>238</sup>U + <sup>238</sup>U central collision Golabek, Simenel, PRL103(2009)042701 time Sekizawa, Yabana, Transfer reaction PRC88(2013)014614



## Frozen density approximation: Sudden

$$V_{\rm FD}(R) = \mathcal{E}[\rho_{P+T}](R) - \mathcal{E}[\rho_P] - \mathcal{E}[\rho_T]$$
$$\rho_{P+T} = \rho_P + \rho_T$$

Denisov, Norenberg, EPJA15(2002)375



Approximate that densities are *frozen* to be their ground state densities during time evolution

## Density-constrained TDHF: "Adiabatic"

$$V_{\rm DC}(R) = \mathcal{E}_{\rm DC}[\rho_{\rm TDHF}](R) - \mathcal{E}[\rho_P] - \mathcal{E}[\rho_T]$$
  
with minimization  $\left\langle H - \int d^3 r \lambda(r) \hat{\rho}(r) \right\rangle \rho = \rho_{\rm TDHF}(t)$ 

Umar, Oberacker, PRC74(2006)021601



 Energy is obtained by minimization with a constraint on the density from TDHF time evolution

# Method: Extract potential and dissipation

Washiyama, Lacroix, PRC78 (2008) 024610



1. 
$$\rho(t) \Rightarrow R(t), P(t), \frac{dR}{dt}, \frac{dP}{dt}$$
  
2.  $\frac{dP}{dt} = -\frac{dV(R)}{dR} - \gamma(R)\frac{dR}{dt}$   
3.  $\frac{dP}{dt}, \frac{dR}{dt} \Longrightarrow \gamma(R), V(R)$ 

Central collisions Mass

- *R*: Relative distance
- *P*: Momentum
- V: Potential
- $\gamma$ : Friction coefficient

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Washiyama, Lacroix, PRC78 (2008) 024610



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Central collisions Mass

 Two trajectories (R<sub>1</sub>, P<sub>1</sub>), (R<sub>2</sub>, P<sub>2</sub>) at slightly different energies (E<sub>1</sub>, E<sub>2</sub>)

$$\Rightarrow \gamma(R) = \frac{\frac{dP_1}{dt} - \frac{dP_2}{dt}}{\frac{dR_1}{dt} - \frac{dR_2}{dt}} \Big|_{R_1, R_2 = R}$$

## Result: Comparison of potentials

$$\frac{dP}{dt} = -\frac{dV(R)}{dR} - \gamma(R)\frac{dR}{dt}$$



Washiyama, Lacroix, PRC78 (2008) 024610

Agree with each model

Validation of our model

## Energy dependence of potential

Washiyama, Lacroix, PRC78 (2008) 024610

$$\frac{dP}{dt} = -\frac{dV(R)}{dR} - \gamma(R)\frac{dR}{dt}$$



# Energy dependence of potential

Washiyama, Lacroix, PRC78 (2008) 024610

$$\frac{dP}{dt} = -\frac{dV(R)}{dR} - \gamma(R)\frac{dR}{dt}$$



- High E<sub>cm</sub> = Frozen density
- Decrease of the barrier: from high E<sub>cm</sub> to low E<sub>cm</sub>

# Energy dependence of potential

Washiyama, Lacroix, PRC78 (2008) 024610

$$\frac{dP}{dt} = -\frac{dV(R)}{dR} - \gamma(R)\frac{dR}{dt}$$



#### Systematics of potentials



$$\frac{dP}{dt} = -\frac{dV(R)}{dR} - \gamma(R)\frac{dR}{dt}$$

$$F_{cm} = \frac{P^2}{2\mu} + V + E_{dissipation}$$

 $\gamma$ : friction coefficient

$$\frac{dP}{dt} = -\frac{dV(R)}{dR} - \frac{\gamma(R)}{\eta(R)}\frac{dR}{dt}$$

 $\gamma$ : friction coefficient



Washiyama, Lacroix, Ayik, PRC79(2009)024609

$$\frac{dP}{dt} = -\frac{dV(R)}{dR} - \frac{\gamma(R)}{\eta(R)}\frac{dR}{dt}$$

 $\gamma$ : friction coefficient



Washiyama, Lacroix, Ayik, PRC79(2009)024609



Washiyama, Lacroix, Ayik, PRC79(2009)024609

### How about heavy systems ?

Heavy: Charge product > 1600 - 1800

 $^{124}$ Sn +  $^{96}$ Zr,  $E_{cm}$  = 228 MeV,

Charge product =  $50 \times 40 = 2000$ 



#### How about heavy systems ?

Heavy: Charge product > 1600 - 1800

 $^{124}$ Sn +  $^{96}$ Zr, E<sub>cm</sub> = 228 MeV, Charge product = 50 x 40 = 2000



## Fusion hindrance in heavy systems

• Fusion probability decreases in  $Z_P Z_T > 1600$  systems



### Fusion hindrance in heavy systems



## Fusion threshold energy from TDHF



Simenel et al., J.Phys.Conf.Ser. 420 (2013) 012113

Guo, Nakatsukasa, EPJ.Conf. 38 (2012) 09003

#### Results: Comparison of potentials

Heavy system

VS.

#### Light system



## Results: Comparison of potentials

Heavy system

VS.

#### Light system



Vanish the potential barrier

• Energy dependence is less around the "barrier"

### Results: Comparison of potentials

Our model

V.S.

#### . Density-constrained TDHF



#### Potentials of heavy systems





- Same order of magnitude
- Energy dependence is less



Heavy system

VS.

Light system



Same order of magnitude

# Origin of fusion hindrance?

Potential

#### **Dissipated energy**



• 
$$E_{thres} - V_{FD} = 228.4 - 214.4 = 14$$
 MeV

•  $\Delta V + E_{diss} = 7.7 + 3.7 = 11.4 \text{ MeV}$  at  $R_{stop}$ 

A part of the origin comes from more inside of the "barrier"

# Summary

- Macroscopic reduction from TDHF in low-energy reactions
- Nucleus-nucleus potential and energy dissipation are extracted
- Energy dependence

- Fusion hindrance
- Change the property of the barrier



