



*Pauli energy and dynamical contributions  
to nucleus-nucleus interaction*

Cédric Simenel

*Australian National University*

Collaborators: K. Godbey (TAMU,FRIB), A. S. Umar (Vanderbilt University)



# Goal

- **Fusion phenomenology**
- **Quantitative predictions (no free parameter)**
- **From deep sub-barrier to above barrier**
- **Isolate contributions to nucleus-nucleus potentials**
  - Pauli repulsion
  - Dynamics (shape polarisation, transfer...)

# Outline

- **Microscopic approach to nucleus-nucleus potential**  
FHF, DCFHF, DC-TDHF
- **Application to  $^{16}\text{O}+^{208}\text{Pb}$**
- **Dynamical isovector contribution to the potential**
- **Pauli energy distribution**

# Microscopic approach

## Hartree-Fock (HF)

$$\delta \langle \Phi | \hat{H} | \Phi \rangle = 0$$



Independent nucleons  
= Slater determinant (=> Pauli)

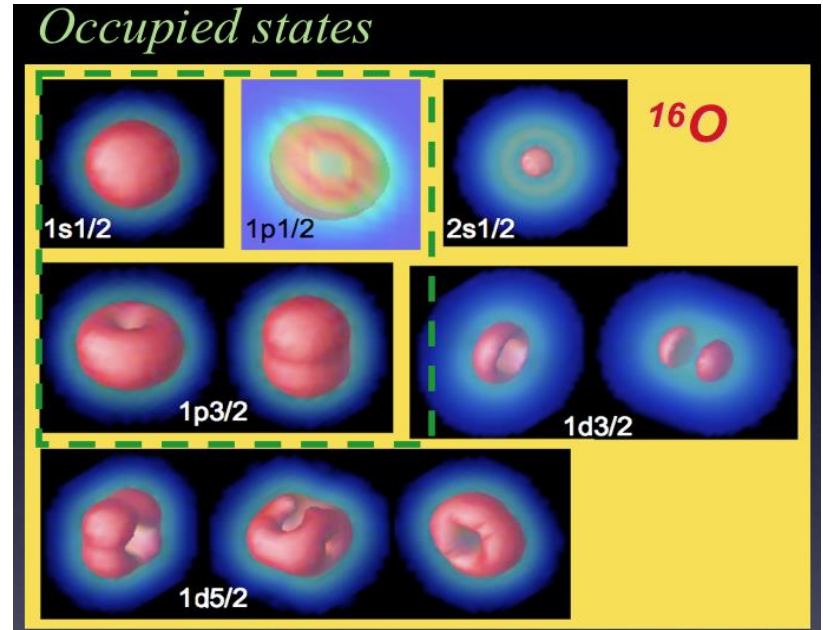
# Microscopic approach

## Hartree-Fock (HF)

$$\delta \langle \Phi | \hat{H} | \Phi \rangle = 0$$



Independent nucleons  
= Slater determinant ( $\Rightarrow$  Pauli)



# Microscopic approach

## Hartree-Fock (HF)

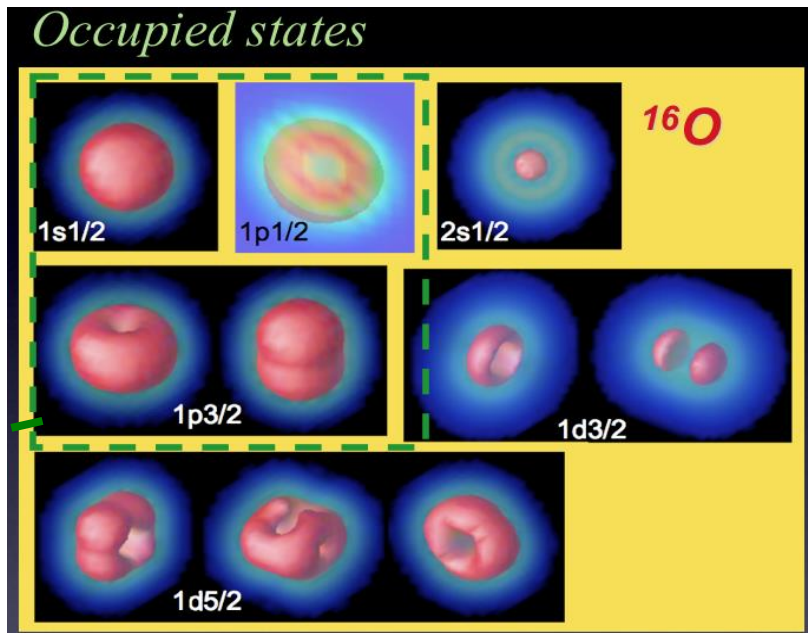
$$\delta \langle \Phi | \hat{H} | \Phi \rangle = 0$$



Independent nucleons  
= Slater determinant ( $\Rightarrow$  Pauli)



$\rho(\mathbf{r})$



$$E[\rho] = \int d^3r \mathcal{H}(\mathbf{r})$$

Skyrme SLy4d functional

# Microscopic approach

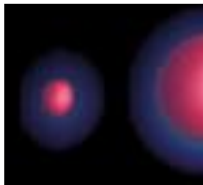
## Frozen Hartree-Fock (FHF)

Brueckner *et al.*, PR **173**, 944 (1968)

$$\delta \langle \Phi | \hat{H} | \Phi \rangle = 0$$

$$V_{FHF}(R) = E[\rho_1 + \rho_2] - E[\rho_1] - E[\rho_2]$$

(No Pauli)




$$\rho_1(\mathbf{r}) + \rho_2(\mathbf{r} - \mathbf{R})$$

# Microscopic approach

## Frozen Hartree-Fock (FHF)

Brueckner *et al.*, PR **173**, 944 (1968)

$$\delta \langle \Phi | \hat{H} | \Phi \rangle = 0$$


$$V_{FHF}(R) = E[\rho_1 + \rho_2] - E[\rho_1] - E[\rho_2]$$

(No Pauli)

## Density-Constrained Frozen Hartree-Fock (DCFHF)

Simenel *et al.*, PRC **95**, 031601 (2017)

$$\delta \langle \Phi | \left[ \hat{H} - \int d\mathbf{r} \lambda(\mathbf{r}) \rho(\mathbf{r}) \right] | \Phi \rangle = 0$$



# Microscopic approach

## Frozen Hartree-Fock (FHF)

Brueckner *et al.*, PR **173**, 944 (1968)

$$\delta \langle \Phi | \hat{H} | \Phi \rangle = 0$$

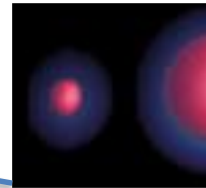
$$V_{FHF}(R) = E[\rho_1 + \rho_2] - E[\rho_1] - E[\rho_2]$$

(No Pauli)

## Density-Constrained Frozen Hartree-Fock (DCFHF)

Simenel *et al.*, PRC **95**, 031601 (2017)

$$\delta \langle \Phi | \left[ \hat{H} - \int d\mathbf{r} \lambda(\mathbf{r}) \rho(\mathbf{r}) \right] | \Phi \rangle = 0$$



$$\rho_1(\mathbf{r}) + \rho_2(\mathbf{r} - \mathbf{R})$$

$$V_{DCFHF}(R) = \langle \Phi | \hat{H} | \Phi \rangle - E[\rho_1] - E[\rho_2]$$

# Microscopic approach

## Frozen Hartree-Fock (FHF)

Brueckner *et al.*, PR **173**, 944 (1968)

$$\delta \langle \Phi | \hat{H} | \Phi \rangle = 0$$

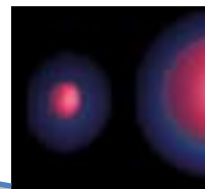
$$V_{FHF}(R) = E[\rho_1 + \rho_2] - E[\rho_1] - E[\rho_2]$$

(No Pauli)

## Density-Constrained Frozen Hartree-Fock (DCFHF)

Simenel *et al.*, PRC **95**, 031601 (2017)

$$\delta \langle \Phi | \left[ \hat{H} - \int d\mathbf{r} \lambda(\mathbf{r}) \rho(\mathbf{r}) \right] | \Phi \rangle = 0$$



$$\rho_1(\mathbf{r}) + \rho_2(\mathbf{r} - \mathbf{R})$$

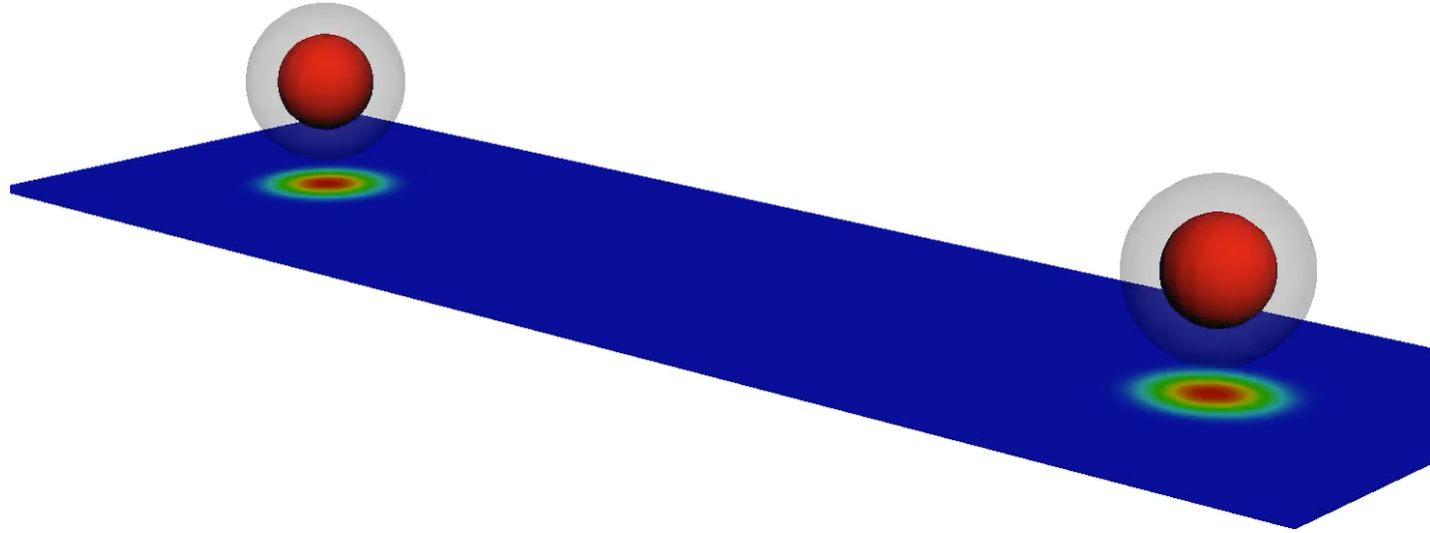
$$V_{DCFHF}(R) = \langle \Phi | \hat{H} | \Phi \rangle - E[\rho_1] - E[\rho_2]$$



# Dynamics

Time-Dependent HF

$$\delta \langle \Phi | [\hat{H} - i\partial_t] | \Phi \rangle = 0$$



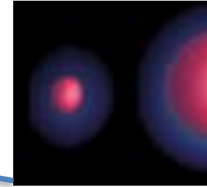
$^{12}\text{C} + ^{12}\text{C}$  at  $E \sim V_B$   
Courtesy of K. Godbey

# Microscopic approach

## Density-Constrained Time-Dependent Hartree-Fock (DC-TDHF)

Simenel *et al.*, PRC **95**, 031601 (2017)

$$\delta \langle \Phi | \left[ \hat{H} - \int d\mathbf{r} \lambda(\mathbf{r}) \rho(\mathbf{r}) \right] | \Phi \rangle = 0$$



$$\rho_{TDHF}(\mathbf{r}, t)$$

$$V_{DCTDHF}[R(t)] = \langle \Phi | \hat{H} | \Phi \rangle - E[\rho_1] - E[\rho_2]$$

$$\delta \langle \Phi | \left[ \hat{H} - i\partial_t \right] | \Phi \rangle = 0$$

# Microscopic approach

## Frozen Hartree-Fock (FHF)

Static, no Pauli

## Density-Constrained Frozen Hartree-Fock (DCFHF)

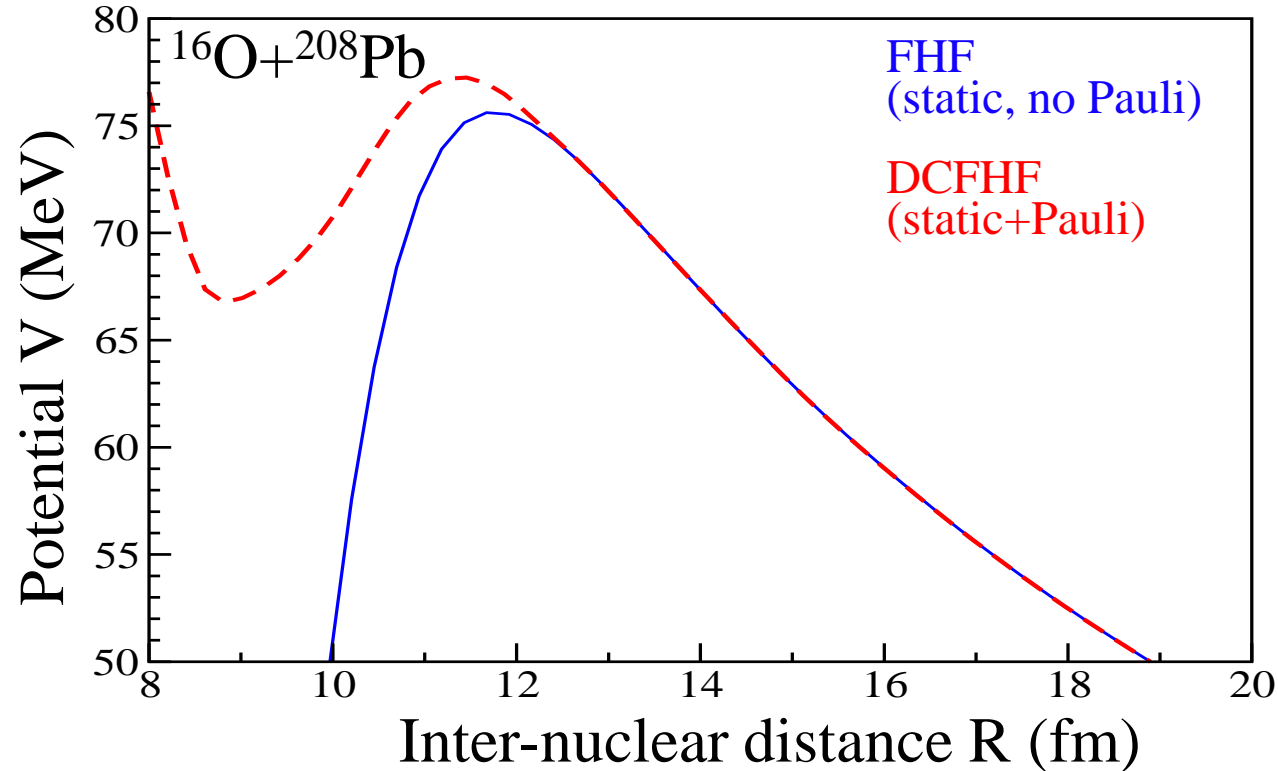
Static + Pauli

## Density-Constrained Time-Dependent Hartree-Fock (DC-TDHF)

Dynamic + Pauli

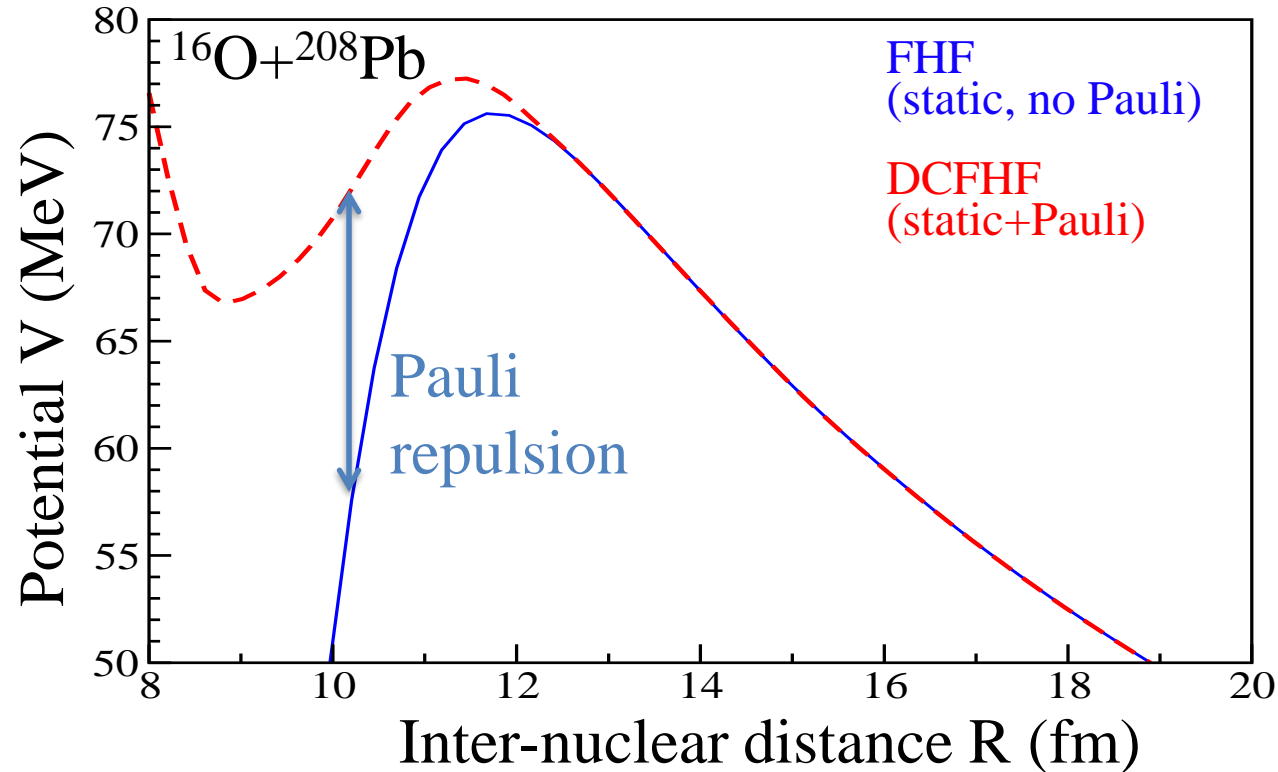
# Nucleus-nucleus potential

## Pauli repulsion from DCFHF



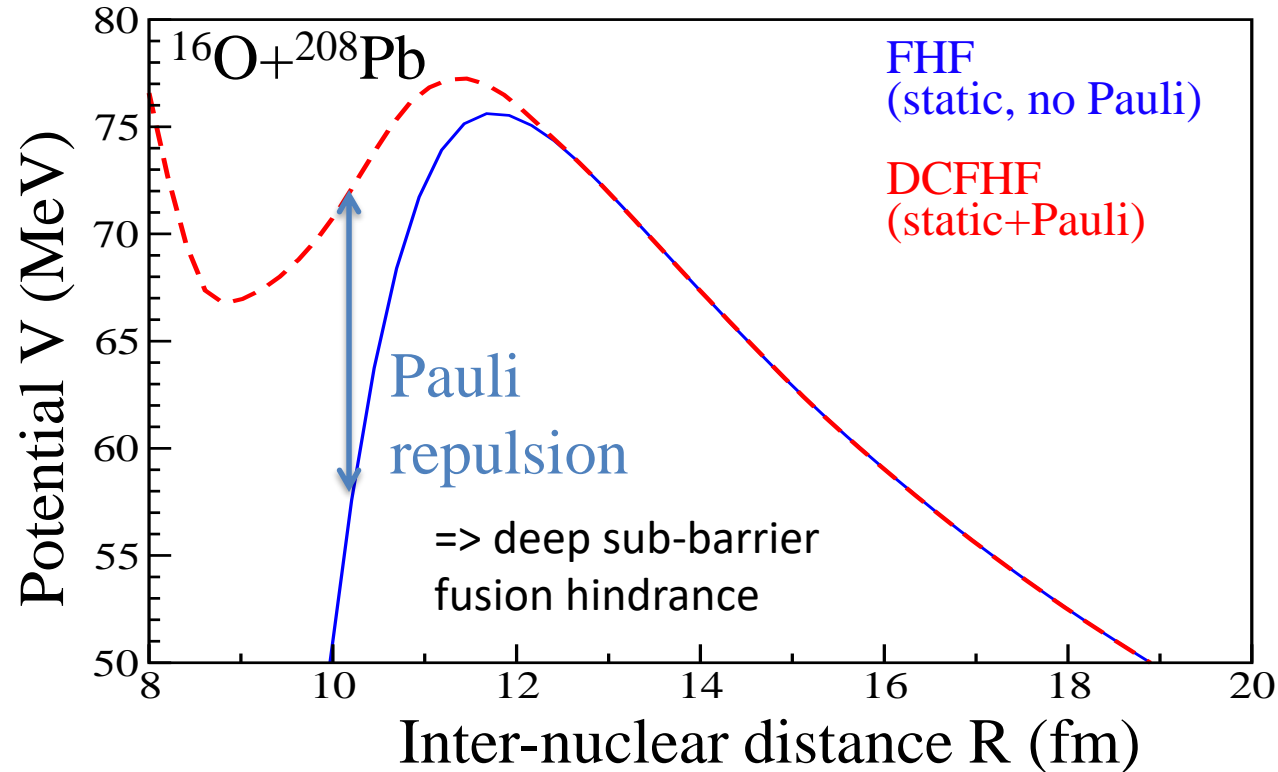
# Nucleus-nucleus potential

## Pauli repulsion from DCFHF



# Nucleus-nucleus potential

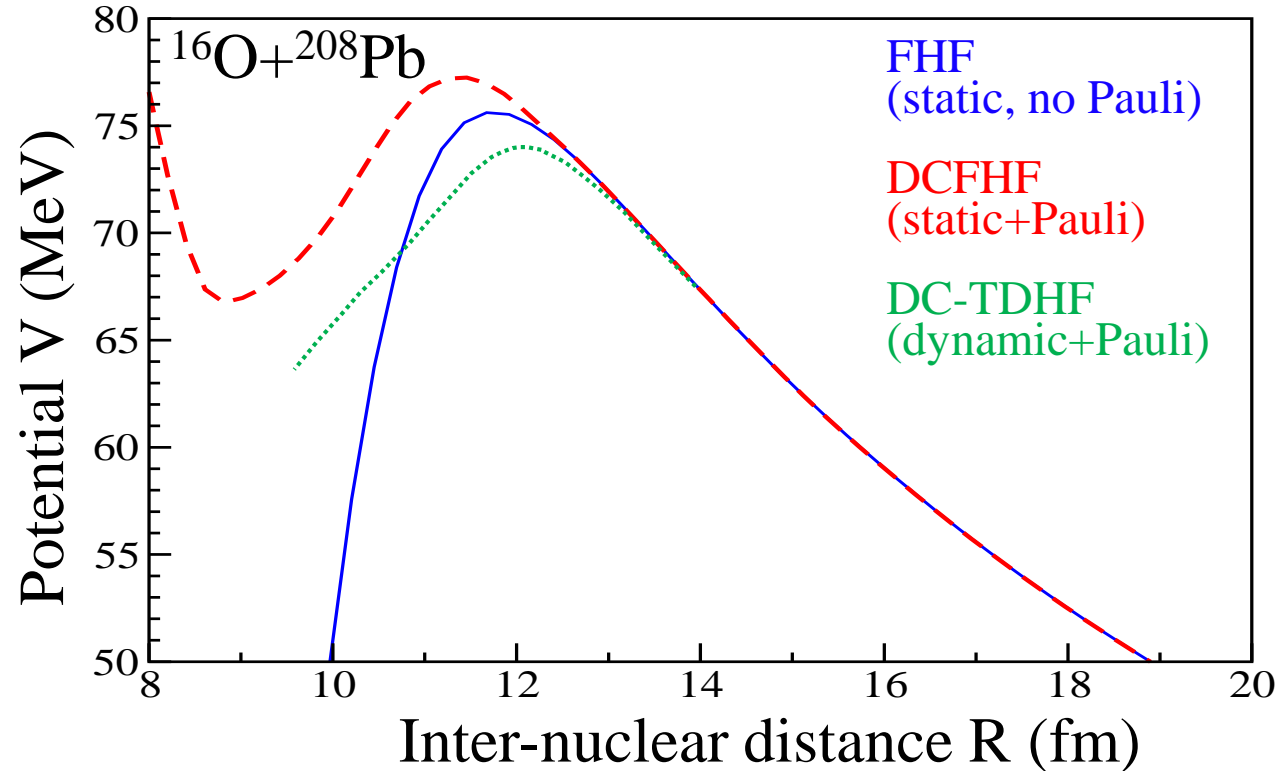
## Pauli repulsion from DCFHF





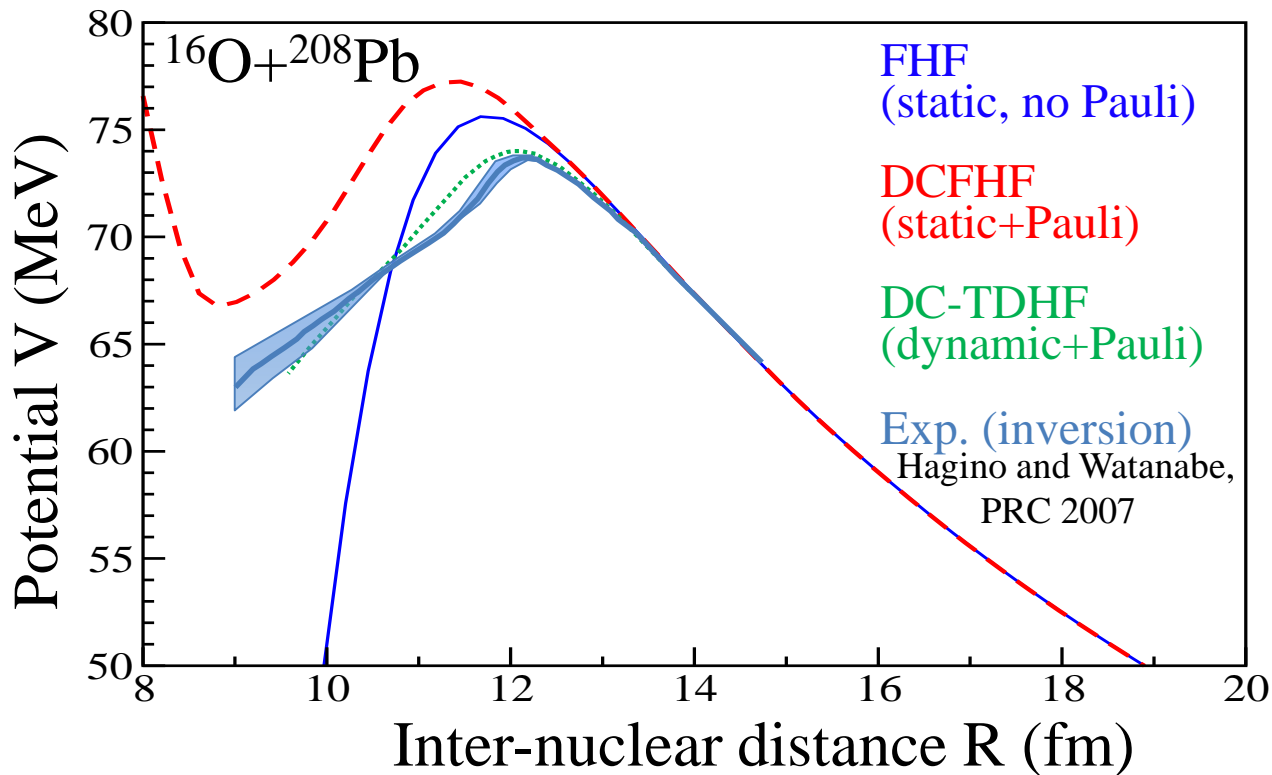
# Nucleus-nucleus potential

## Pauli repulsion from DCFHF

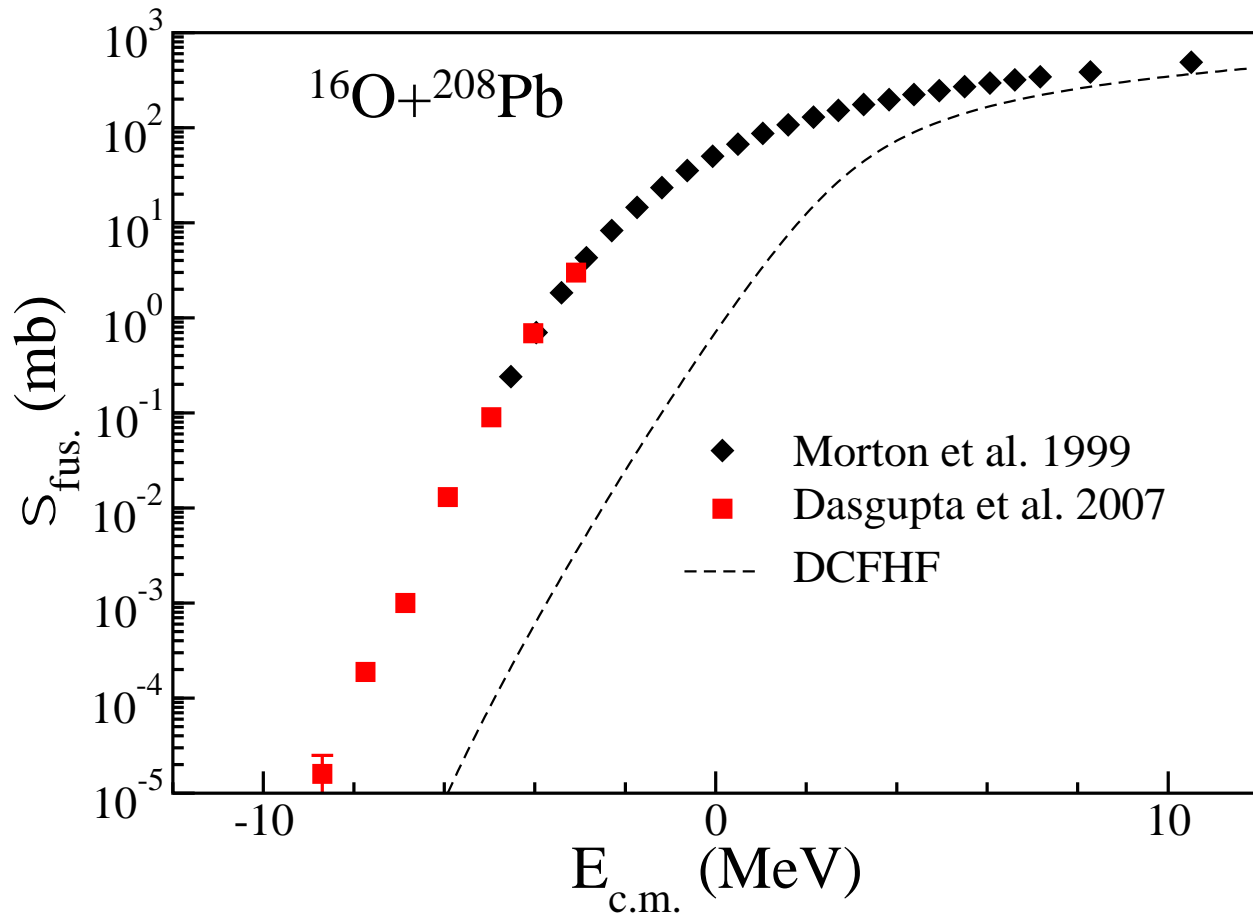


# Nucleus-nucleus potential

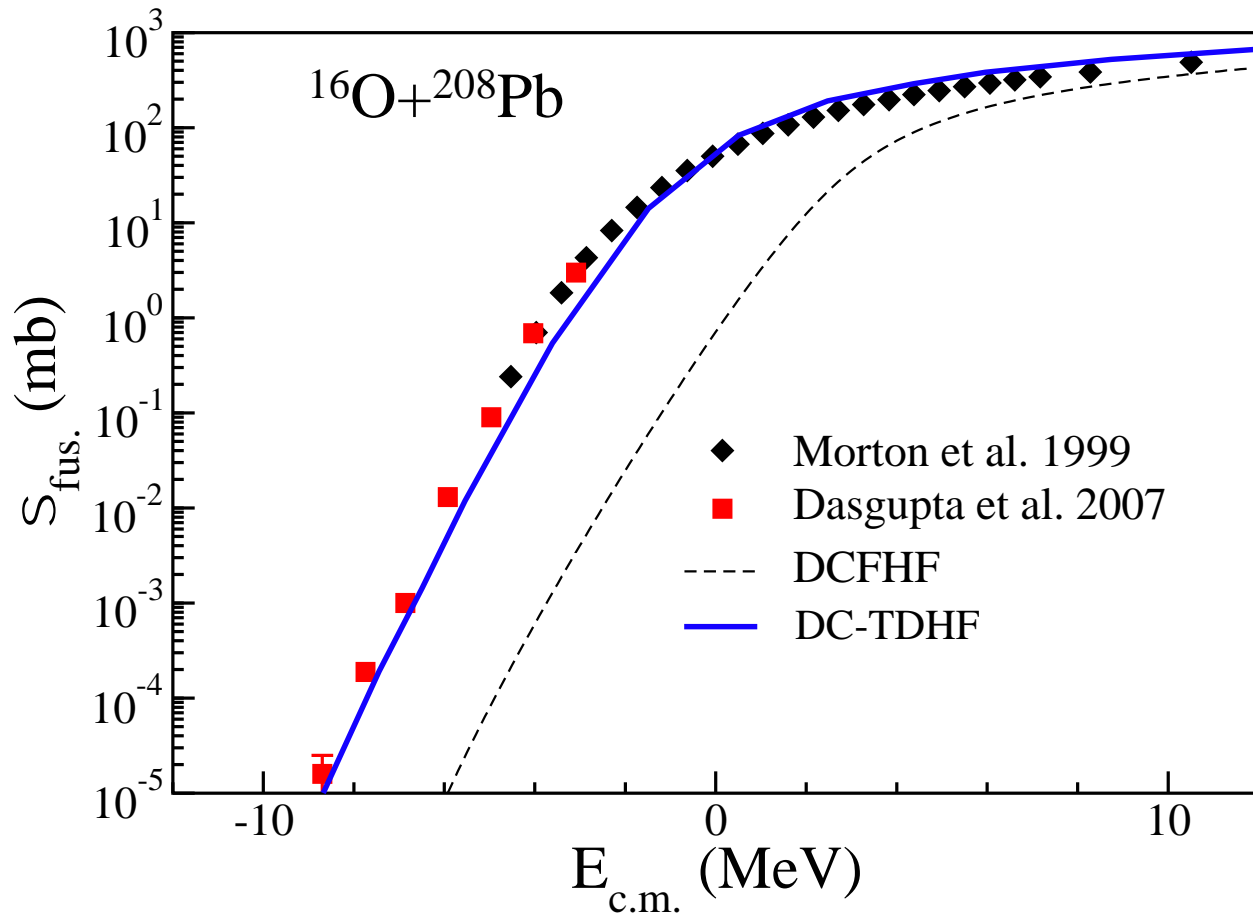
## Pauli repulsion from DCFHF



# Deep sub-barrier fusion



# Deep sub-barrier fusion



# Dynamics

## Isvector (transfer) dynamics with DCTDHF

Godbey, Umar, Simenel, PRC (R) 2017

$$H(\mathbf{r}) = \frac{\vec{r}^2}{2m} t_0 + H_0(\mathbf{r}) + H_1(\mathbf{r}) + H_C(\mathbf{r})$$


# Dynamics

## Isvector (transfer) dynamics with DCTDHF

Godbey, Umar, Simenel, PRC (R) 2017

$$H(\mathbf{r}) = \frac{\vec{r}^2}{2m} t_0 + H_0(\mathbf{r}) + H_1(\mathbf{r}) + H_C(\mathbf{r})$$

isoscalar                      isovector



# Dynamics

## Isvector (transfer) dynamics with DCTDHF

Godbey, Umar, Simenel, PRC (R) 2017

$$H(r) = \frac{\hbar^2}{2m} t_0 + H_0(r) + H_1(r) + H_C(r)$$

isoscalar                      isovector

$$\Rightarrow V(\mathbf{R}) = v_0(\mathbf{R}) + v_1(\mathbf{R}) + V_C(\mathbf{R})$$

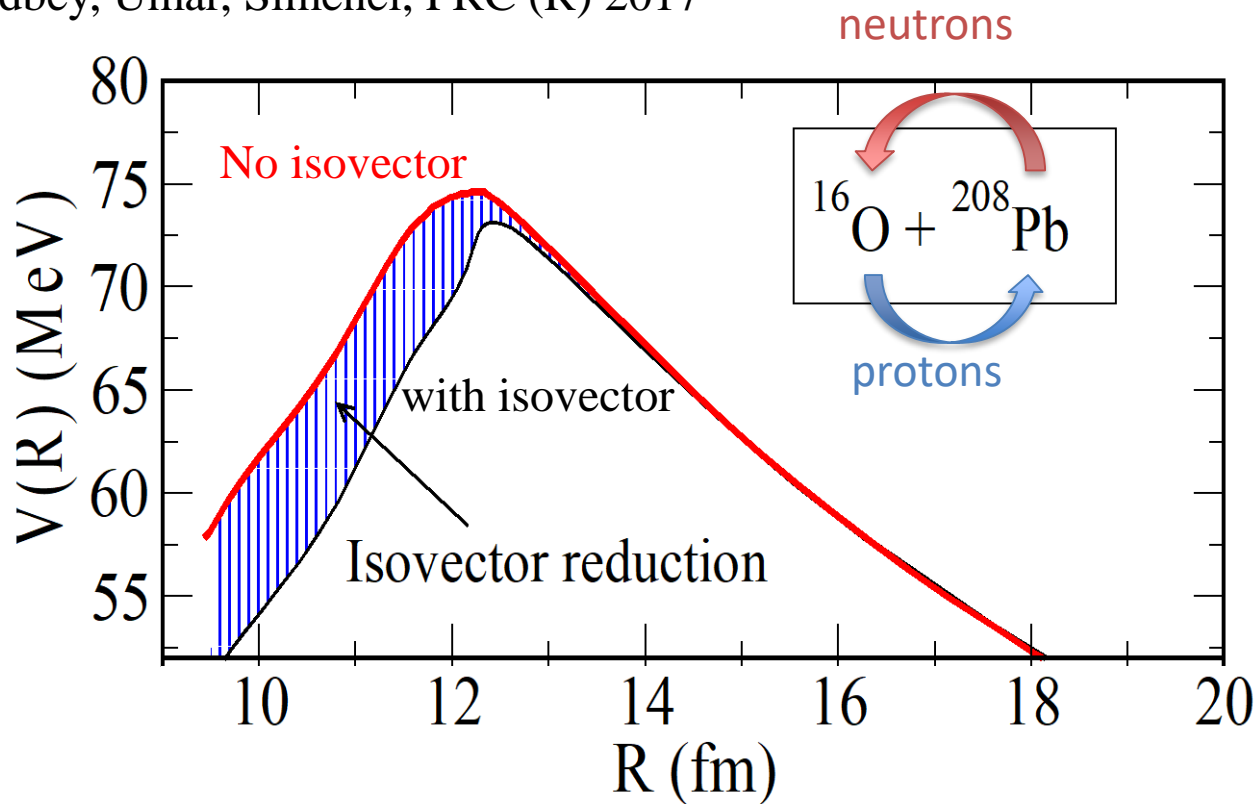
= 0 in FHF

=> purely dynamical (polarisation and transfer)

# Dynamics

## Isvector (transfer) dynamics with DCTDHF

Godbey, Umar, Simenel, PRC (R) 2017





# Pauli energy distribution

## Nucleon localisation function

Probability of finding 2 nucleons

$$P_{qs}(\mathbf{r}, \mathbf{r}') = \rho_q(\mathbf{r}s, \mathbf{r}s)\rho_q(\mathbf{r}'s, \mathbf{r}'s) - |\rho_q(\mathbf{r}s, \mathbf{r}'s)|^2$$

Short range behaviour ( $\mathbf{r} \sim \mathbf{r}'$ )  $\Rightarrow$  localisation measure

$$D_{qs_\mu} = \tau_{qs_\mu} - \frac{1}{4} \frac{|\nabla \rho_{qs_\mu}|^2}{\rho_{qs_\mu}} - \frac{|\mathbf{j}_{qs_\mu}|^2}{\rho_{qs_\mu}}$$

# Pauli energy distribution

## Nucleon localisation function

Probability of finding 2 nucleons

$$P_{qs}(\mathbf{r}, \mathbf{r}') = \rho_q(\mathbf{r}s, \mathbf{r}s)\rho_q(\mathbf{r}'s, \mathbf{r}'s) - |\rho_q(\mathbf{r}s, \mathbf{r}'s)|^2$$

Short range behaviour ( $\mathbf{r} \sim \mathbf{r}'$ )  $\Rightarrow$  localisation measure

$$D_{qs_\mu} = \tau_{qs_\mu} - \frac{1}{4} \frac{|\nabla \rho_{qs_\mu}|^2}{\rho_{qs_\mu}} - \frac{|\mathbf{j}_{qs_\mu}|^2}{\rho_{qs_\mu}}$$

## Pauli kinetic energy

$$E_{qs}^P = \frac{\hbar^2}{2m} \int d^3r D_{qs}(\mathbf{r})$$

Pauli (static) repulsion  $\Delta E_{q\mu}^{P(F)}(R) = \frac{\hbar^2}{2m} \sum_{s_\mu} \int d^3r [D_{qs_\mu}^{\text{DCFHF}}(\mathbf{r}, R) - D_{qs_\mu}^{\text{FHF}}(\mathbf{r}, R)]$

Dynamic  $\Delta E_{q\mu}^{P(D)}(R) = \frac{\hbar^2}{2m} \sum_{s_\mu} \int d^3r [D_{qs_\mu}^{\text{DC-TDHF}}(\mathbf{r}, R) - D_{qs_\mu}^{\text{DCFHF}}(\mathbf{r}, R)]$

# Pauli energy distribution

## Nucleon localisation function

Probability of finding 2 nucleons

$$P_{qs}(\mathbf{r}, \mathbf{r}') = \rho_q(\mathbf{r}s, \mathbf{r}s)\rho_q(\mathbf{r}'s, \mathbf{r}'s) - |\rho_q(\mathbf{r}s, \mathbf{r}'s)|^2$$

Short range behaviour ( $\mathbf{r} \sim \mathbf{r}'$ )  $\Rightarrow$  localisation measure

$$D_{qs\mu} = \tau_{qs\mu} - \frac{1}{4} \frac{|\nabla \rho_{qs\mu}|^2}{\rho_{qs\mu}} - \frac{|\mathbf{j}_{qs\mu}|^2}{\rho_{qs\mu}}$$

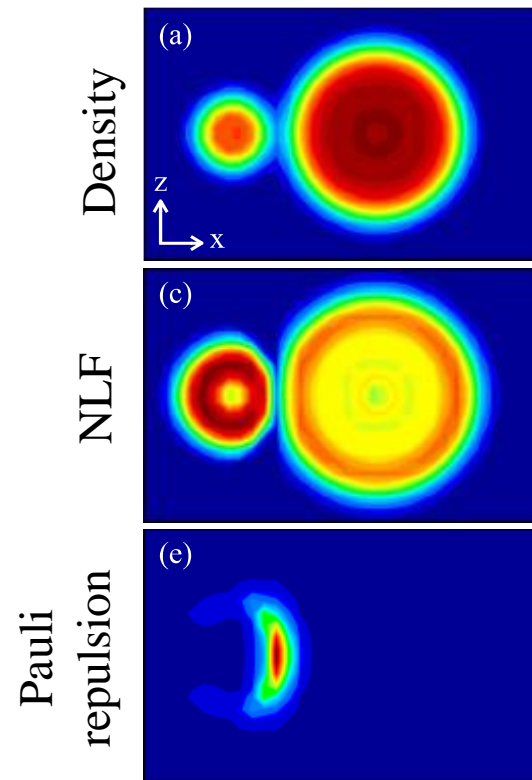
## Pauli kinetic energy

$$E_{qs}^P = \frac{\hbar^2}{2m} \int d^3r D_{qs}(\mathbf{r})$$

Pauli (static) repulsion  $\Delta E_{q\mu}^{P(F)}(R) = \frac{\hbar^2}{2m} \sum_{s\mu} \int d^3r [D_{qs\mu}^{\text{DCFHF}}(\mathbf{r}, R) - D_{qs\mu}^{\text{FHF}}(\mathbf{r}, R)]$

Dynamic  $\Delta E_{q\mu}^{P(D)}(R) = \frac{\hbar^2}{2m} \sum_{s\mu} \int d^3r [D_{qs\mu}^{\text{DC-TDHF}}(\mathbf{r}, R) - D_{qs\mu}^{\text{DCFHF}}(\mathbf{r}, R)]$

$^{16}\text{O} + ^{208}\text{Pb}$



Umar, Simenel, Godbey, PRC 2021

# Pauli energy distribution

## Nucleon localisation function

Probability of finding 2 nucleons

$$P_{qs}(\mathbf{r}, \mathbf{r}') = \rho_q(\mathbf{r}s, \mathbf{r}s)\rho_q(\mathbf{r}'s, \mathbf{r}'s) - |\rho_q(\mathbf{r}s, \mathbf{r}'s)|^2$$

Short range behaviour ( $\mathbf{r} \sim \mathbf{r}'$ )  $\Rightarrow$  localisation measure

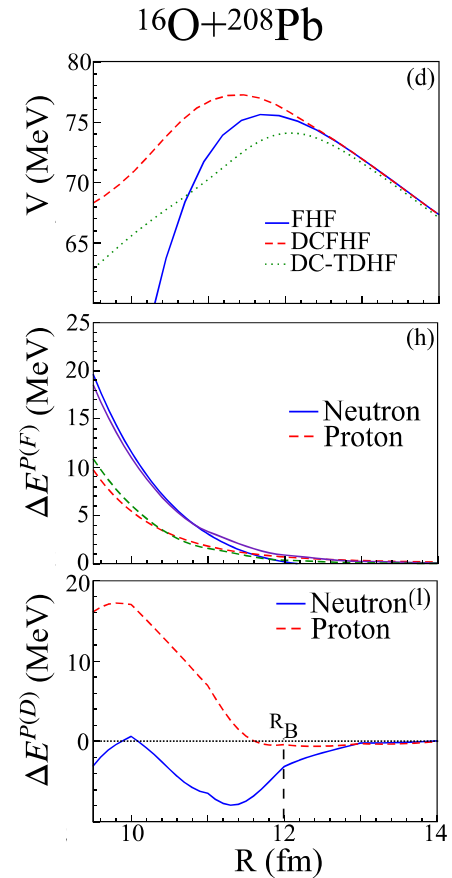
$$D_{qs\mu} = \tau_{qs\mu} - \frac{1}{4} \frac{|\nabla \rho_{qs\mu}|^2}{\rho_{qs\mu}} - \frac{|\mathbf{j}_{qs\mu}|^2}{\rho_{qs\mu}}$$

## Pauli kinetic energy

$$E_{qs}^P = \frac{\hbar^2}{2m} \int d^3r D_{qs}(\mathbf{r})$$

Pauli (static) repulsion  $\Delta E_{q\mu}^{P(F)}(R) = \frac{\hbar^2}{2m} \sum_{s\mu} \int d^3r [D_{qs\mu}^{\text{DCFHF}}(\mathbf{r}, R) - D_{qs\mu}^{\text{FHF}}(\mathbf{r}, R)]$

Dynamic  $\Delta E_{q\mu}^{P(D)}(R) = \frac{\hbar^2}{2m} \sum_{s\mu} \int d^3r [D_{qs\mu}^{\text{DC-TDHF}}(\mathbf{r}, R) - D_{qs\mu}^{\text{DCFHF}}(\mathbf{r}, R)]$



Umar, Simenel, Godbey, PRC 2021

# Conclusions

- Microscopic predictions (no free parameters)
- FHF, DCFHF, and DC-TDFHF to isolate Pauli repulsion and dynamics
- Applications to  $^{16}\text{O}+^{208}\text{Pb}$
- Pauli repulsion inside the fusion barrier => Deep sub-barrier fusion hindrance
- Isovector dynamics (transfer)
- NLF => Pauli energy
- Pauli repulsion in the neck
- Different dynamical effects for protons and neutrons