Purpose of today's presentation

✔ To clarify what is interesting to study low-energy heavy ion reactions

My short answer:

Quantum many-body dynamics!!
Time-dependent density functional theory for low-energy heavy ion reactions

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What I would like to tell you today
1. **Introduction:** Our interests for low-energy heavy ion reactions

2. **Method:** Time-dependent density functional theory (TDDFT)

3. **Example:** $^{238}\text{U} + ^{124}\text{Sn}$ reaction

4. **Proposal and conclusion**
1. **Introduction:** Our interests for low-energy heavy ion reactions


3. Example: $^{238}\text{U} + ^{124}\text{Sn}$ reaction

4. Proposal and conclusion
What is a low-energy heavy ion reaction?
What is a low-energy heavy ion reaction?

Not “high-energy” !!
What is a low-energy heavy ion reaction?

Not “high-energy” !!

RHIC
Relativistic Heavy Ion Collider
What is a low-energy heavy ion reaction?
What is a low-energy heavy ion reaction?

✔ a “gentle” collision at around the Coulomb barrier
What is a low-energy heavy ion reaction?

✔ a “gentle” collision at around the Coulomb barrier

\[ V(R): \text{Nucleus-nucleus potential} \]

\[ R: \text{Inter-nuclear distance} \]
What is a low-energy heavy ion reaction?

✔ a “gentle” collision at around the Coulomb barrier

\[ V(R) \]: Nucleus-nucleus potential

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K. Sekizawa

Time-dependent density functional theory for low-energy heavy ion reactions

Mon., May 18, 2015
What is a low-energy heavy ion reaction?

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$R$: Inter-nuclear distance

Effects of nuclear force

Coulomb potential
What is a low-energy heavy ion reaction?

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Coulomb potential

Total potential (Coulomb+Nuclear)

Effects of nuclear force
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\[ V(R): \text{Nucleus-nucleus potential} \]

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Total potential (Coulomb+Nuclear)

Coulomb barrier \( V_B \)

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\( R: \text{Inter-nuclear distance} \)
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\[ R \]

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✔ a “gentle” collision at around the Coulomb barrier

\[ V(R) : \text{Nucleus-nucleus potential} \]

\[ V_B : \text{Coulomb barrier} \]

\[ R : \text{Inter-nuclear distance} \]

at a very low energy: \[ E < V_B \]
What is a low-energy heavy ion reaction?

✔ a “gentle” collision at around the Coulomb barrier

$V(R)$: Nucleus-nucleus potential

Coulomb barrier $V_B$

$R$: Inter-nuclear distance

at around the Coulomb barrier: $E \sim V_B$
What is a low-energy heavy ion reaction?

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Coulomb barrier \( V_B \)

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at around the Coulomb barrier: \( E \sim V_B \)
Low-energy heavy ion reactions
(a “gentle” collision at around the Coulomb barrier)
contain a rich physics of many-body dynamics
What I'd like to understand: Quantum many-body dynamics

- ✔ Low-energy heavy ion reactions
  (a “gentle” collision at around the Coulomb barrier)
  contain a rich physics of many-body dynamics

- ➔ Nucleon transfer, energy dissipation, nuclear excitations, dynamical deformation, ...
What I'd like to understand: Quantum many-body dynamics

- Low-energy heavy ion reactions (a “gentle” collision at around the Coulomb barrier) contain a rich physics of many-body dynamics

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Small-\(b\)  Impact parameter \(b\)  Large-\(b\)
What I'd like to understand: Quantum many-body dynamics

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Time-dependent density functional theory for low-energy heavy ion reactions
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What I'd like to understand: Quantum many-body dynamics

- Low-energy heavy ion reactions (a “gentle” collision at around the Coulomb barrier) contain a rich physics of many-body dynamics

- Nucleon transfer, energy dissipation, nuclear excitations, dynamical deformation, ...

Impact parameter $b$

Small-$b$  
Multinucleon transfer

Impact parameter $b$

Large-$b$  
Neck formation  
Quantum tunneling  
Transfer of few nucleons
What I'd like to understand: Quantum many-body dynamics

- Low-energy heavy ion reactions (a “gentle” collision at around the Coulomb barrier) contain a rich physics of many-body dynamics

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Diagram:
- Fusion
- Neck formation
- Quantum tunneling
- Multinucleon transfer
- Transfer of few nucleons

Impact parameter $b$

Small-$b$  Impact parameter $b$  Large-$b$
What I'd like to understand: Quantum many-body dynamics

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Time-dependent density functional theory for low-energy heavy ion reactions
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Aim: To predict how to produce unstable nuclei

- Each box represents an atomic nucleus (with different \( N \) and \( Z \))
- To study unstable nuclei, we need to produce them experimentally

![Diagram](image.png)

FIG: Rept. Prog. Phys. 70, 1525 (2007)
**Aim:** To predict how to produce unstable nuclei

- Each box represents an atomic nucleus (with different $N$ and $Z$)
- To study unstable nuclei, we need to produce them experimentally

To produce objective unstable nuclei, what is the best projectile-target combination and incident energy?

We have conducted microscopic simulations based on TDDFT

![Diagram with neutron number and proton number axes](Image)

**FIG:** Rept. Prog. Phys. 70, 1525 (2007)
1. **Introduction:** Our interests for low-energy heavy ion reactions

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3. **Example:** $^{238}$U$^{+}$ $^{124}$Sn reaction

4. **Proposal and conclusion**
1. Introduction: Our interests for low-energy heavy ion reactions


3. Example: $^{238}\text{U} + ^{124}\text{Sn}$ reaction

4. Proposal and conclusion
Basic concepts of DFT: HK theorem & KS scheme
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Hohenberg-Kohn (HK) theorem

\[ \hat{H} = \hat{T} + \hat{V}_{\text{int}} + \hat{V}_{\text{ext}} : \text{interacting system of interest} \]

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**Basic concepts of DFT: HK theorem & KS scheme**

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Basic concepts of DFT: HK theorem & KS scheme

Hohenberg-Kohn (HK) theorem

\[ \hat{H} = \hat{T} + \hat{V}_{\text{int}} + \hat{V}_{\text{ext}} \] : interacting system of interest

HK theorem states: \( \hat{V}_{\text{ext}} \Leftrightarrow \Phi \Leftrightarrow \rho(\mathbf{r}) \)

\[ \Phi = \Phi[\rho(\mathbf{r})] \]

\[ \mathcal{O}[\rho] = \langle \Phi[\rho]|\hat{\mathcal{O}}|\Phi[\rho]\rangle \]
Basic concepts of DFT: HK theorem & KS scheme

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\[ \mathcal{O}[\rho] = \langle \Phi[\rho] | \mathcal{O} | \Phi[\rho] \rangle \]

\[ E[\rho] = \langle \Phi[\rho] | \hat{H} | \Phi[\rho] \rangle \]

\[ E_{\text{g.s.}} = E[\rho_{\text{g.s.}}] = \min_{\rho} E[\rho] \]
Basic concepts of DFT: HK theorem & KS scheme

Hohenberg-Kohn (HK) theorem

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Kohn-Sham (KS) scheme

\[ \hat{H} = \hat{T} + \hat{V}_{\text{ext}} : \text{non-interacting system} \]


Basic concepts of DFT: HK theorem & KS scheme

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Hohenberg-Kohn (HK) theorem

\[ \hat{H} = \hat{T} + \hat{V}_{\text{int}} + \hat{V}_{\text{ext}} \]: interacting system of interest

\[ \Phi \]

\[ \rho(\mathbf{r}) \]

Kohn-Sham (KS) scheme

\[ \hat{H} = \hat{T} + \hat{V}_{\text{ext}} \]: non-interacting system

\[ \Phi' \]

\[ \rho'(\mathbf{r}) = \rho(\mathbf{r}) \]


Basic concepts of DFT: HK theorem & KS scheme

✔ By solving the KS equation for the non-interacting system, we can get exact solution for the interacting system
By solving the KS equation for the non-interacting system, we can get exact solution for the interacting system.

\[
\rho(r) = \sum_{i=1}^{N} |\phi_i(r)|^2 \\
\Phi(r_1, \cdots, r_N) = \frac{1}{\sqrt{N!}} \det \{ \phi_i(r_j) \} : \text{Slater determinant}
\]
Basic concepts of DFT: HK theorem & KS scheme

By solving the KS equation for the non-interacting system, we can get exact solution for the interacting system

\[
\rho(r) = \sum_{i=1}^{N} |\phi_i(r)|^2
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\[
\Phi(r_1, \cdots, r_N) = \frac{1}{\sqrt{N!}} \det\{\phi_i(r_j)\} : \text{Slater determinant}
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Hohenberg-Kohn (HK) theorem
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\hat{H} = \hat{T} + \hat{V}_{\text{int}} + \hat{V}_{\text{ext}} : \text{interacting system of interest}
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Kohn-Sham (KS) scheme
\[
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\]

We solve this

Get everything!
\[
\Phi = \Phi[\rho(r)]
\]
\[
\mathcal{O}[\rho] = \langle \Phi[\rho] | \hat{O} | \Phi[\rho] \rangle
\]
Basic concepts of DFT: HK theorem & KS scheme

By solving the KS equation for the non-interacting system, we can get exact solution for the interacting system.

**Kohn-Sham equation**

\[
\frac{-\hbar^2}{2m} \nabla^2 + \nu_{KS}[\rho(r)] \phi_i(r) = \varepsilon_i \phi_i(r)
\]

\[
\rho(r) = \sum_{i=1}^{N} |\phi_i(r)|^2 \quad \Phi(r_1, \ldots, r_N) = \frac{1}{\sqrt{N!}} \det \{\phi_i(r_j)\} : \text{Slater determinant}
\]

**Time-dependent version: time-dependent density functional theory (TDDFT)**


**Time-dependent Kohn-Sham equation**

\[
i\hbar \frac{\partial \phi_i(r, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + \hat{\nu}_{KS}[\rho(r, t)] \right] \phi_i(r, t)
\]

\[
\rho(r, t) = \sum_{i=1}^{N} |\phi_i(r, t)|^2 \quad \Phi(r_1, \ldots, r_N, t) = \frac{1}{\sqrt{N!}} \det \{\phi_i(r_j, t)\}
\]
Application: Real-time/real-space simulation of heavy ion reactions
**Ground-state calculation**

Kohn-Sham eq.
\[
\hat{h}[\rho]\phi_i(r, \sigma, q) = \varepsilon_i \phi_i(r, \sigma, q)
\]

Slater determinant
\[
\Phi(x_1, \ldots, x_N, t) = \frac{1}{\sqrt{N!}} \det \left\{ \phi_i(x_j, t) \right\} \\
x \equiv \{r, \sigma, q\}
\]

Target  
Projectile

# of grid points: 30×30×30=27,000
Mesh size: 0.8 fm → \(L_{\text{box}} = 24\) fm
Imaginary time method
Kohn-Sham eq.
\[ \hat{h}[\rho] \phi_i(\mathbf{r}, \sigma, q) = \varepsilon_i \phi_i(\mathbf{r}, \sigma, q) \]

Slater determinant
\[ \Phi(x_1, \ldots, x_N, t) = \frac{1}{\sqrt{N!}} \det \{ \phi_i(x_j, t) \} \]
for \( x \equiv \{ \mathbf{r}, \sigma, q \} \)

Application: Real-time/real-space simulation of heavy ion reactions

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Ground-state calculation

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Slater determinant
\[ \Phi(x_1, \ldots, x_N, t) = \frac{1}{\sqrt{N!}} \det \{ \phi_i(x_j, t) \} \]

Reaction calculation

A large numerical box

\# of grid points: 30×30×30=27,000
Mesh size: 0.8 fm → \( L_{\text{box}} = 24 \) fm
Imaginary time method
**Ground-state calculation**

Kohn-Sham eq.

\[ \hat{h}[\rho] \phi_i(\mathbf{r}, \sigma, q) = \varepsilon_i \phi_i(\mathbf{r}, \sigma, q) \]

Slater determinant

\[ \Phi(x_1, \cdots, x_N, t) = \frac{1}{\sqrt{N!}} \det \{ \phi_i(x_j, t) \} \quad x \equiv \{ \mathbf{r}, \sigma, q \} \]

**Reaction calculation**

Put projectile/target nuclei

- # of grid points: 30×30×30 = 27,000
- Mesh size: 0.8 fm \( \rightarrow \) \( L_{\text{box}} = 24 \) fm
- Imaginary time method

*Application: Real-time/real-space simulation of heavy ion reactions*
**Application: Real-time/real-space simulation of heavy ion reactions**

**Ground-state calculation**

Kohn-Sham eq.

\[ \hat{h}[\rho] \phi_i(\mathbf{r}, \sigma, q) = \varepsilon_i \phi_i(\mathbf{r}, \sigma, q) \]

Slater determinant

\[ \Phi(x_1, \cdots, x_N, t) = \frac{1}{\sqrt{N!}} \text{det} \{ \phi_i(x_j, t) \} \]

\[ x \equiv \{ \mathbf{r}, \sigma, q \} \]

**Reaction calculation**

Give a relative momentum for c.m. motion

# of grid points: 30×30×30=27,000
Mesh size: 0.8 fm → \( L_{\text{box}} = 24 \text{ fm} \)
Imaginary time method

Target

Projectile
Application: Real-time/real-space simulation of heavy ion reactions

Ground-state calculation

Kohn-Sham eq.
\[ \hat{h}[\rho] \phi_i(\mathbf{r}, \sigma, q) = \varepsilon_i \phi_i(\mathbf{r}, \sigma, q) \]

Slater determinant
\[ \Phi(x_1, \ldots, x_N, t) = \frac{1}{\sqrt{N!}} \det \{ \phi_i(x_j, t) \} \]
\[ x \equiv \{ \mathbf{r}, \sigma, q \} \]

Reaction calculation

Time-dependent Kohn-Sham eq.
\[ i\hbar \frac{\partial}{\partial t} \phi_i(\mathbf{r}, \sigma, q, t) = \hat{h}[\rho] \phi_i(\mathbf{r}, \sigma, q, t) \]

Solve time evolution

Target

Projectile

# of grid points: 30×30×30=27,000
Mesh size: 0.8 fm \( \rightarrow L_{\text{box}} = 24 \text{ fm} \)
Imaginary time method

# of grid points: 70×70×30=147,000
Time evolution: 4th order Taylor expansion
Outline

What I would like to tell you today

1. Introduction: Our interests for low-energy heavy ion reactions


3. Example: $^{238}\text{U}+^{124}\text{Sn}$ reaction

4. Proposal and conclusion
1. Introduction: Our interests for low-energy heavy ion reactions


3. Example: $^{238}\text{U} + ^{124}\text{Sn}$ reaction

4. Proposal and conclusion
Example of TDDFT calculation: \( ^{238}\text{U}_{146} + ^{124}\text{Sn}_{74} \) at \( E_{\text{lab}} = 5.7 \text{ MeV/A} \)

➢ Reactions with different orientations of \( ^{238}\text{U} \)

Projectile (Uranium, \( ^{238}\text{U} \)): largely deformed in prolate shape

Target (Tin, \( ^{124}\text{Sn} \)): slightly deformed in oblate shape
Example of TDDFT calculation: $^{238}_{92}\text{U}_{146} + ^{124}_{50}\text{Sn}_{74}$ at $E_{\text{lab}} = 5.7$ MeV/A

Reactions with different orientations of $^{238}\text{U}$

Projectile (Uranium, $^{238}\text{U}$): largely deformed in prolate shape
Target (Tin, $^{124}\text{Sn}$): slightly deformed in oblate shape

Ex.) $b = 1$ fm

- Symm. axis of $^{238}\text{U}$: $z$-direction
- $y$-direction
- $x$-direction

# of grid points: 70×70×30 (56 fm×56 fm×24 fm), Mesh: 0.8 fm
Skyrme: SLy5, $\Delta t$: 0.2 fm/c, Calculated $b$: $0 \leq b \leq 10$ fm

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- **Reactions with different orientations of $^{238}U$**
  - **Projectile (Uranium, $^{238}U$):** largely deformed in prolate shape
  - **Target (Tin, $^{124}Sn$):** slightly deformed in oblate shape

#### Example of TDDFT calculation:
- $b = 1$ fm
- Symm. axis of $^{238}U$: $z$-direction
- Target orientation:
  - $y$-direction
  - $x$-direction

- Calculations:
  - # of grid points: $70 \times 70 \times 30$ (56 fm $\times$ 56 fm $\times$ 24 fm), Mesh: 0.8 fm
  - Skyrme: SLy5, $\Delta t$: 0.2 fm/c, Calculated $b$: $0 \leq b \leq 10$ fm

Sn $\leftrightarrow$ U, 3 nucleons
Example of TDDFT calculation: $^{238}_{92}\text{U}_{146} + ^{124}_{50}\text{Sn}_{74}$ at $E_{\text{lab}} = 5.7 \text{ MeV/A}$

Reactions with different orientations of $^{238}\text{U}$

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Ex. $b = 1 \text{ fm}$

Symm. axis of $^{238}\text{U}$: $z$-direction

\begin{align*}
\text{Skyrme: SLy5, } \Delta t: 0.2 \text{ fm/c, Calculated } b: 0 \leq b \leq 10 \text{ fm} \\
\text{# of grid points: 70×70×30 (56 fm×56 fm×24 fm), Mesh: 0.8 fm}
\end{align*}
Example of TDDFT calculation: $^{238}_{92}{\text{U}}_{146} + ^{124}_{50}{\text{Sn}}_{74}$ at $E_{\text{lab}}=5.7$ MeV/A

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Projectile (Uranium, $^{238}$U): largely deformed in prolate shape
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Ex.) $b = 1$ fm

Symm. axis of $^{238}$U: z-direction
$y$-direction
x-direction

Almost no transfer

# of grid points: 70×70×30 (56 fm×56 fm×24 fm), Mesh: 0.8 fm
Skyrme: SLy5, $\Delta t$: 0.2 fm/c, Calculated $b$: $0 \leq b \leq 10$ fm
Example of TDDFT calculation: \(^{238}\text{U}_{146} + ^{124}\text{Sn}_{74} \text{ at } E_{\text{lab}} = 5.7 \text{ MeV/A} \)

Reactions with different orientations of \(^{238}\text{U}\)

- Projectile (Uranium, \(^{238}\text{U}\)): largely deformed in prolate shape
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Ex. \( b = 1 \text{ fm} \)

Symm. axis of \(^{238}\text{U}\): \(z\)-direction

\[ \begin{align*}
\text{# of grid points: } & 70 \times 70 \times 30 \text{ (56 fm} \times 56 \text{ fm} \times 24 \text{ fm)}, \text{ Mesh: } 0.8 \text{ fm} \\
\text{Skyrme: } & \text{SLy5, } \Delta t: 0.2 \text{ fm/c, Calculated } b: 0 \leq b \leq 10 \text{ fm}
\end{align*} \]
Example of TDDFT calculation: $^{238}\text{U}_{146} + ^{124}\text{Sn}_{74}$ at $E_{\text{lab}} = 5.7 \text{ MeV/A}$

➢ Reactions with different orientations of $^{238}\text{U}$

- **Projectile (Uranium, $^{238}\text{U}$):** largely deformed in prolate shape
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Ex.) $b = 1 \text{ fm}$

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Sn ⇣ U, 17 nucleons
Example of TDDFT calculation: $^{238}\text{U}_{146} + ^{124}\text{Sn}_{74}$ at $E_{\text{lab}} = 5.7 \text{ MeV/A}$

✔ Amount of transferred nucleons depends much on orientations of $^{238}\text{U}$

Ex.) $b = 1 \text{ fm}$

symm. axis of $^{238}\text{U}$: $z$-direction

- $y$-direction
- $x$-direction

Sn $\leftrightarrow$ U, 3 nucleons

almost no transfer

Sn $\leftrightarrow$ U, 17 nucleons

# of grid points: 70×70×30 (56 fm×56 fm×24 fm), Mesh: 0.8 fm
Skyrme: SLy5, $\Delta t$: 0.2 fm/c, Calculated $b$: 0 $\leq b \leq$ 10 fm
Example of TDDFT calculation: $^{238}_{92}U_{146} + ^{124}_{50}Sn_{74}$ at $E_{\text{lab}} = 5.7$ MeV/A

Production cross sections for lighter ($^{124}$Sn-like) fragments

$$\sigma(N, Z) = 2\pi \int_0^\infty b \, P_{N,Z}(b) \, db$$

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Production cross sections for lighter \(^{124}\text{Sn-like}\) fragments

\[ \sigma(N, Z) = 2\pi \int_0^\infty b P_{N,Z}(b) \, db \]

- Measured proton flow would be contributed from the “x-direction” configuration with the neck breaking dynamics.

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Mon., May 18, 2015
1. Introduction: Our interests for low-energy heavy ion reactions


3. Example: $^{238}\text{U} + ^{124}\text{Sn}$ reaction

4. Proposal and conclusion
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4. Proposal and conclusion
Missing physics: “pairing correlation”
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I have treated nucleons as independent particles...
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FIG: http://www.hdwalls.xyz/images/welcome-to-dance-this-is-our-first-time-dancing-
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✔ To what extent, do they retain the pair?

✔ How do they affect to the dynamics (transfer, shape evolution, energy dissipation, ...)?

✔ Nuclear Josephson effect? (effect of a relative phase)
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Purpose of today's presentation

✔ To clarify what is interesting to study low-energy heavy ion reactions

My short answer:
Quantum many-body dynamics!!
To clarify what is interesting to study low-energy heavy ion reactions

My short answer:

Quantum many-body dynamics!!
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Thank you for your attention.