MR-TDDFT for low-energy heavy ion reactions: Ideas

Kazuyuki Sekizawa

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2015. 4: I started working at WUT in collaboration with P. Magierski
2015. 3: I have finished my PhD at Univ. of Tsukuba (Supervisor: K. Yabana)
What I'd like to talk about
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“MR-TDDFT”: What I meant is “MR-TDEDF” or “TDGCM”
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I'll discuss a use of a “multi-Slater-determinant” to describe:

- multi-nucleon transfer (MNT) reaction
- sub-barrier fusion
- superheavy element (SHE) synthesis
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„Let's imagine the future of MR-DFT!!”

Any comments/questions/criticisms are welcome!!
1. Introduction: Drawbacks in "SR-TDEDF"

2. Method: "MR-TDEDF" with a multi-Slater-determinant

3. "Ideas" for MNT / subbarrier fusion / SHE synthesis

4. Summary
Outline

1. **Introduction:** Drawbacks in “SR-TDEDF”

2. **Method:** “MR-TDEDF” with a multi-Slater-determinant

3. “Ideas” for MNT / subbarrier fusion / SHE synthesis

4. **Summary**
About the “SR-TDEDF” (or TDHF)
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Action to be minimized:

\[ S = \int_{t_1}^{t_2} dt \left\langle \Phi(t) | i \hbar \partial_t - \hat{H} | \Phi(t) \right\rangle \]

\[ = \int_{t_1}^{t_2} dt \left[ i\hbar \sum_{i=1}^{N} \langle \phi_i(t) | \partial_t | \phi_i(t) \rangle - E[\rho(t)] \right) \]

Trial w.f.: a single Slater determinant

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

Single-particle wavefunctions

\[ \phi_i(x, t) \quad (i = 1, \ldots, N; \ x \equiv (r, \sigma)) \]
About the "SR-TDEDF" (or TDHF)

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Single-particle wavefunctions

\[ \phi_i(x, t) \quad (i = 1, \cdots, N; x \equiv (r, \sigma)) \]

Variation \( \frac{\delta S}{\delta \phi_i^*(t)} = 0 \) leads to:

\[ i\hbar \partial_t \phi_i(x, t) = \hat{h}[\rho(t)] \phi_i(x, t) \quad : \text{TDEDF (or TDHF, TDKS) equations} \]

One-body density

\[ \rho(r, t) = \sum_{i, \sigma} |\phi_i(x, t)|^2 \]

Single-particle Hamiltonian

\[ \hat{h}[\rho(t)] = \frac{\delta E}{\delta \rho(t)} \]
About the "SR-TDEDF" (or TDHF)

Action to be minimized:

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Single-particle Hamiltonian

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✓ No empirical parameters: Input is an EDF only

✓ Successfully applied: Giant resonances (linear response, RPA)

Heavy ion reactions (fusion, transfer, quasi-fission, fission, ...)

K. Sekizawa

MR-TDDFT for low-energy heavy ion reactions: Ideas

Thu., 25 June, 2015
“Drawback” of the SR-TDEDF (or TDHF)
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rawid1.png

😊 : Many-body dynamics is described within a *single* mean-field potential
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- MNT:
- Subbarrier fusion:
- SHE synthesis:
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- MNT: Insufficient description of transfer channels far from average
- Subbarrier fusion:
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Ex. 1: Multi-nucleon transfer (MNT) reaction

$^{40}\text{Ca}+^{124}\text{Sn}$ at $E_{\text{lab}}=170$ MeV, $b=3.96$ fm
“Drawback” of the SR-TDDED (or TDHF)

Emoji: :sob: : Many-body dynamics is described within a single mean-field potential

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✔ At most 2 neutrons/protons were transferred on average
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✔ At most 2 neutrons/protons were transferred on average

✔ Particle-number projection technique can be applied:

- Probability: $n$ nucleons are inside the volume $A$

$$P_n = \langle \Phi | \hat{P}_n | \Phi \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta \ e^{in\theta} \det \{ \langle \phi_i | \phi_j \rangle_B + e^{-i\theta} \langle \phi_i | \phi_j \rangle_A \}$$

$$\hat{P}_n = \frac{1}{2\pi} \int_0^{2\pi} d\theta \ e^{i(n-N_A)\theta} : \text{Particle-number projection op.}$$

- Cross section for a nucleus containing $N, Z$ nucleons

$$\sigma_{N,Z} = 2\pi \int db \ b P_N(b) P_Z(b)$$

PNP: C. Simenel, PRL 105(2010)192701
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✔ At most 2 neutrons/protons were transferred on average
✔ Result:
  - Reasonable description around the average
  - Underestimate many-nucleon transfer channels

K.S., K. Yabana, PRC 88(2013)064614
“Drawback” of the SR-TDDEDF (or TDHF)

\(^{40}\text{Ca} + ^{124}\text{Sn} \text{ at } E_{\text{lab}} = 170 \text{ MeV, } b = 3.96 \text{ fm}

- Reasonable description around the average
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✔ Possible reason: We don't have a mean-field for 6-proton transfer channel
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Naive picture: potential for neutrons
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: potential for neutrons

be shallower

be deeper
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Naive picture

Neutron transfer would be suppressed

: potential for neutrons

be shallower

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“Drawback” of the SR-TDEDF (or TDHF)

😊 : Many-body dynamics is described within a single mean-field potential

- MNT: Insufficient description of transfer channels far from average
- Subbarrier fusion: Absence of quantum tunneling of the many-body wavefunction
- SHE synthesis:

Ex. 2: Subbarrier fusion

$^{40}\text{Ca} + ^{40}\text{Ca}$ at $E_{\text{c.m.}} = 64$ MeV < $V_B$

✔ $P_{\text{fusion}} = 0$ when $E < V_B$
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- SHE synthesis: Deterministic nature (either fusion or non-fusion)

Ex. 2: Subbarrier fusion

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Ex. 3: SHE synthesis

\[ ^{64}\text{Ni} + ^{238}\text{U} \rightarrow ^{302}120 ? (E_{\text{lab}} = 428 \text{ MeV}, b=0 \text{ fm}) \]
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Ex. 3: SHE synthesis

$^{64}\text{Ni} + ^{238}\text{U} \rightarrow ^{302}\text{120} ?$ ($E_{\text{lab}} = 428 \text{ MeV}, b = 0 \text{ fm}$)

✔ In this case $P_{\text{fusion}} = 0$, but we would also like to have a tiny, finite fusion probability
1. Introduction: Drawbacks in “SR-TDSEDF”


3. “Ideas” for MNT / subbarrier fusion / SHE synthesis

4. Summary
1. Introduction: Drawbacks in “SR-TDEDF”


3. “Ideas” for MNT / subbarrier fusion / SHE synthesis

4. Summary
“MR-TDEDF”: Structure of the many-body wavefunction
Let's consider a many-body wavefunction of the following form:

\[ \Psi(t) = \sum_i C_i(t) \Phi_i(t) \]
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Calculated by SR-TDEDF (TDHF)
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Determined by variation

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- Determined by variation
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✓ \( \Psi(t) \) is a superposition of Slater determinants calculated by SR-TDDEDF (TDHF)
Let's consider a many-body wavefunction of the following form:

$$\Psi(t) = \sum_i C_i(t) \Phi_i(t)$$

- $\Phi_i(t)$ is already fixed, and only the coefficients $C_i(t)$ are the variables of the variation.

- $\Psi(t)$ is a superposition of Slater determinants calculated by SR-TDEDF (TDHF).

![Diagram showing the relationship between $\Phi_i(t)$ and $C_i(t)$ over time.](image)
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$$\Psi(t) = \sum_i C_i(t) \Phi_i(t)$$

- $\Phi_i(t)$ is already fixed, and only the coefficients $C_i(t)$ are the variables of the variation
- $\Psi(t)$ is a superposition of Slater determinants calculated by SR-TDEDF (TDHF)
“MR-TDEDF”: Equation for the coefficients $C_i(t)$
Action to be minimized:

\[ S = \int_{t_1}^{t_2} dt \langle \Psi(t) | i\hbar \partial_t - \hat{H} | \Psi(t) \rangle \]

\[ \Psi(t) = \sum_i C_i(t) \Phi_i(t) \quad : \text{Multi-Slater-determinant} \]
Action to be minimized:

\[
S = \int_{t_1}^{t_2} dt \left[ \langle \Psi(t) | i\hbar \partial_t - \hat{H} | \Psi(t) \rangle \right] \\
= \int_{t_1}^{t_2} dt \sum_{i,j} C_i^*(t) \langle \Phi_i(t) | \left( i\hbar \dot{C}_j(t) | \Phi_j(t) \rangle + i\hbar C_j(t) \partial_t | \Phi_j(t) \rangle - C_j(t) \hat{H} | \Phi_j(t) \rangle \right)
\]

\[\Psi(t) = \sum_i C_i(t) \Phi_i(t) : \text{Multi-Slater-determinant}\]
**“MR-TDEDF”: Equation for the coefficients $C_i(t)$**

Action to be minimized:

$$ S = \int_{t_1}^{t_2} dt \, \langle \Psi(t) | i\hbar \partial_t - \hat{H} | \Psi(t) \rangle $$

$$ = \int_{t_1}^{t_2} dt \, \sum_{ij} C_i^*(t) \langle \Phi_i(t) | \left( i\hbar \dot{C}_j(t) | \Phi_j(t) \rangle + i\hbar C_j(t) \partial_t | \Phi_j(t) \rangle - C_j(t) \hat{H} | \Phi_j(t) \rangle \right) $$

$$ = \int_{t_1}^{t_2} dt \, \sum_{ij} C_i^*(t) \left( i\hbar \dot{C}_j(t) \mathcal{N}_{ij}(t) + C_j(t) \mathcal{A}_{ij}(t) - C_j(t) \mathcal{H}_{ij}(t) \right) $$

**Norm kernel**

$$ \mathcal{N}_{ij}(t) = \langle \Phi_i(t) | \Phi_j(t) \rangle $$

**A transition matrix**

$$ \mathcal{A}_{ij}(t) = \langle \Phi_i(t) | i\hbar \partial_t | \Phi_j(t) \rangle $$

**Interaction kernel**

$$ \mathcal{H}_{ij}(t) = \langle \Phi_i(t) | \hat{H} | \Phi_j(t) \rangle $$

$$ = \det \left\{ \langle \phi_{k}^{(i)}(t) | \hat{h}^{(j)}(t) | \phi_l^{(j)}(t) \rangle \right\} $$. 

$\Psi(t) = \sum_i C_i(t) \Phi_i(t)$ : Multi-Slater-determinant
Action to be minimized:

\[
S = \int_{t_1}^{t_2} dt \langle \Psi(t) | i \hbar \partial_t - \hat{H} | \Psi(t) \rangle
\]

\[
= \int_{t_1}^{t_2} dt \sum_{ij} C_i^*(t) \langle \Phi_i(t) | \left( i \hbar \dot{\Phi}_j(t) | \Phi_j(t) \rangle + i \hbar C_j(t) \partial_t | \Phi_j(t) \rangle - C_j(t) \hat{H} | \Phi_j(t) \rangle \right)
\]

\[
= \int_{t_1}^{t_2} dt \sum_{ij} C_i^*(t) \left( i \hbar \dot{\Phi}_j(t) \mathcal{N}_{ij}(t) + C_j(t) \mathcal{A}_{ij}(t) - C_j(t) \mathcal{H}_{ij}(t) \right)
\]

Norm kernel \( \mathcal{N}_{ij}(t) = \langle \Phi_i(t) | \Phi_j(t) \rangle \)

A transition matrix \( \mathcal{A}_{ij}(t) = \langle \Phi_i(t) | i \hbar \partial_t | \Phi_j(t) \rangle \)

Interaction kernel \( \mathcal{H}_{ij}(t) = \langle \Phi_i(t) | \hat{H} | \Phi_j(t) \rangle \)

\[
\frac{\delta S}{\delta C_i^*(t)} = 0 \quad \text{leads to:}
\]

Equation for the coefficients \( \{ C_i(t) \} \)

\[
i \hbar \mathcal{N}(t) \dot{\mathcal{C}}(t) = \left( \mathcal{H}(t) - \mathcal{A}(t) \right) \mathcal{C}(t)
\]

where \( \mathcal{C}(t) \equiv \begin{pmatrix} C_1(t) \\ C_2(t) \\ \vdots \\ C_M(t) \end{pmatrix} \)
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4. Summary
Ideas: MR-TDSEDF for MNT reaction

Ex. 1: MNT

Choice of $\Phi_i(t)$?

\[ \Psi(t) = \sum_i C_i(t) \Phi_i(t) \]

- Determined by variation
- Calculated by SR-TDSEDF (TDHF)
Ideas: MR-TDEDF for MNT reaction

**Ex. 1: MNT**

**Choice of $\Phi_i(t)$?**

1. Transfer-constrained SR-TDEDF (TDHF)

\[
S' = \int_{t_1}^{t_2} dt \, \langle \Phi(t) | i\hbar \partial_t - \hat{H} - \lambda \hat{N}_A | \Phi(t) \rangle
\]

\[
\Phi_1(t_0) = \Phi_2(t_0) = \cdots = \Phi_M(t_0)
\]

\[
C_1(t_0) = C_2(t_0) = \cdots = C_M(t_0) = 1/M
\]


Calculated by SR-TDEDF (TDHF)

Determined by variation

\[
\Delta N = 0
\]

\[
\Delta N = 1
\]

\[
\Delta N = 2
\]
Ideas: MR-TDEDF for MNT reaction

Ex. 1: MNT

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$$S' = \int_{t_1}^{t_2} dt \left\langle \Phi(t) \right| i\hbar \partial_t - \hat{H} - \lambda \hat{N}_A \left| \Phi(t) \right\rangle$$

$\Phi_1(t_0) = \Phi_2(t_0) = \cdots = \Phi_M(t_0)$

$C_1(t_0) = C_2(t_0) = \cdots = C_M(t_0) = 1/M$

ΔN=0

ΔN=1

ΔN=2


2. Use different projectile / target combinations

$\Phi_1(t) = ^{40}\text{Ca}^{124}\text{Sn}$,  $\Phi_2(t) = ^{42}\text{Ca}^{122}\text{Sn}$,  $\Phi_3(t) = ^{18}\text{Ar}^{126}\text{Te}$,  

$C_1(t_0) = 1$,  $C_{i\neq1}(t_0) = 0$
Ideas: MR-TEDDF for subbarrier fusion / SHE synthesis

Ex. 2: Subbarrier fusion

\[ \Psi(t) = \sum_i C_i(t) \Phi_i(t) \]

Choice of \( \Phi_i(t) \)?

1. Modify the nucleus-nucleus potential

\[ V(R) \]

\[ R \]
**Ideas: MR-TDDEDF for subbarrier fusion / SHE synthesis**

**Ex. 2: Subbarrier fusion**

**1.** Modify the nucleus-nucleus potential

\[ V(R) \]

**2.** Put static solutions in addition to SR-TDDEDF

\[ \Phi_1(t): \text{SR-TDDEDF} \]

**Choice of \( \Phi_i(t) \):**

Determined by variation

Calculated by SR-TDDEDF (TDHF)

\[ \Psi(t) = \sum_i C_i(t) \Phi_i(t) \]
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We have considered a possible use of the multi-Slater-determinant:

$$\Psi(t) = \sum_i C_i(t) \Phi_i(t)$$

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Determined by variation

Calculated by SR-TDEDF (TDHF)

Hopefully, a bad w.f. will be automatically discarded

\[ C_k(t) \approx 0 \]
We have considered a possible use of the multi-Slater-determinant:

\[ \Psi(t) = \sum_i C_i(t) \Phi_i(t) \]

Determined by variation \hspace{2cm} Calculated by SR-TDEDF (TDHF)

Hopefully, a bad w.f. will be automatically discarded

the value of \( C_i(t) \) may tell us which channels are important
We have considered a possible use of the multi-Slater-determinant:

\[ \Psi(t) = \sum_i C_i(t) \Phi_i(t) \]

- Determined by variation
- Calculated by SR-TDDFF (TDHF)

Although there are many practical problems, we can try it in the near future!
About me:

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Thank you for your attention.