Time-Dependent Hartree-Fock Theory for Multinucleon Transfer Reactions

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Nobel role of pairing: soliton-like excitation

\[ \Delta \varphi = \pi \]

- TDSLDA equation:

\[
\begin{pmatrix}
    u_{k\uparrow} \\
    u_{k\downarrow} \\
    v_{k\uparrow} \\
    v_{k\downarrow}
\end{pmatrix}

\begin{pmatrix}
    h_{\uparrow\uparrow} & h_{\uparrow\downarrow} & 0 & \Delta \\
    h_{\downarrow\uparrow} & h_{\downarrow\downarrow} & -\Delta & 0 \\
    0 & -\Delta^* & -h_{\uparrow\uparrow} & -h_{\uparrow\downarrow} \\
    \Delta^* & 0 & -h_{\downarrow\uparrow} & -h_{\downarrow\downarrow}
\end{pmatrix}

\begin{pmatrix}
    u_{k\uparrow} \\
    u_{k\downarrow} \\
    v_{k\uparrow} \\
    v_{k\downarrow}
\end{pmatrix}
\]

Pairing may hinder energy dissipation and fusion

Poster session C  17:20-18:30

Thursday, Aug. 1

Pairing effects in

\(^{96}\text{Zr} + ^{96}\text{Zr}\) and \(^{48}\text{Ca}, ^{50}\text{Ti} + ^{252}\text{Cf}\)

will be presented by M.C. Barton

Warsaw
University of Technology

G. Wlazłowski  P. Magierski

University of Washington

A. Bulgac  S. Jin  I. Abdurrahman

Collisions of heavy nuclei, as well as fission

Nuclear Reactions A  14:10-14:25

“Fission dynamics from saddle to scission and beyond” by A. Bulgac
How can we create yet-unknown neutron-rich nuclei?

- New magic numbers?
- Impact on r-process?
- Heaviest element?
- Island of stability?

- Theory: \(~7,000\)
- Expt.: \(~3,200\)

Remarks on TDHF (or TDDFT, TDEDF)

- There is no adjustable parameter on reaction dynamics

\[
S = \int_{t_0}^{t_1} dt \left( i\hbar \sum_i \langle \phi_i(t) | \frac{\partial}{\partial t} | \phi_i(t) \rangle - \left[ E[\rho(t)] \right] \right)
\]

\[
i\hbar \frac{\partial \phi_i(\mathbf{r}\sigma q, t)}{\partial t} = \hat{h}[\rho(t)] \phi_i(\mathbf{r}\sigma q, t) \quad : \text{TDHF eq.}
\]

Effective interaction

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

Energy Density Functional (EDF)
How to compute production cross sections?

We have developed: **TDHF + PNP + GEMINI**

**TDHF**
- Reaction dynamics
  - $(10^{-21}-10^{-20} \text{ sec})$

**GEMINI++**
- De-excitation
  - $(10^{-18}-10^{-16} \text{ sec})$
  - Evaporation, fission and $\gamma$-rays
  - $n, p, \gamma, ...$
  - Or fission

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How to compute production cross sections?

We have developed: TDHF + PNP + GEMINI


Other groups also adopted GEMINI for TDHF:
- Z. Wu and Lu Guo, PRC 100(2019)014612
Typical example: $^{64}\text{Ni} + ^{238}\text{U} (E_{c.m.} = 307 \text{ MeV})$

Production cross section for lighter fragments

**Message 1**

- **✓** TDHF can reproduce overall trends without empirical parameters other than the EDF
- **➢** However, it underestimates cross sections for channels far from the average values (well known problem of the mass width)

We should improve the description of fluctuations and correlations.

*Typical example: $^{64}\text{Ni} + ^{238}\text{U} \ (E_{c.m.} = 307 \text{ MeV})$*

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Expt.: L. Corradi et al., PRC 59 (1999) 261

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We put one step forward along this direction:

EXPLORING ZEPTOSECOND QUANTUM EQUILIBRATION DYNAMICS: FROM DEEP-INELASTIC TO FUSION-FISSION OUTCOMES IN $^{58}\text{Ni} + ^{60}\text{Ni}$ REACTIONS

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Method: Variational principle of Balian and Vénéroni

Variational space can be controlled by both “state” and “observable”

- The action-like quantity proposed by Balian and Vénéroni

\[ J = \text{Tr} \left[ \hat{A}(t_1) \hat{D}(t_1) \right] - \int_{t_0}^{t_1} \text{Tr} \left[ \hat{A}(t) \left( \frac{d\hat{D}(t)}{dt} + i[\hat{H}(t), \hat{D}(t)] \right) \right] dt \]

\( \hat{D}(t) \): describes the state of the system
\( \hat{A}(t) \): describes the evolution of the observable in the Heisenberg picture


- **Unrestricted variation** (w.r.t. either \( A \) or \( D \))

- **Slater determinant** & **one-body observable**

- **Slater determinant** & **fluctuations of one-body observable**
Numerical implementation of TDRPA for the mass width

Forward TDHF

$t_0$ → $t_1$

$\sigma_A^2 = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2$

TDHF: $\sigma_A \sim 1.5$
Experiment: $\sigma_A \sim 7.1$

Initial state: $t_0$

After collision: $t_1$

Numerical implementation of TDRPA for the mass width

The Balian-Vénéroni prescription (TDRPA):

\[
\sigma^2_{X}(t_1) = \lim_{\varepsilon \to 0} \frac{\text{Tr}\{[\rho(t_0) - \rho_X(t_0, \varepsilon)]^2\}}{2\varepsilon^2}
\]

\[
\rho_X(t_1, \varepsilon) = e^{i\varepsilon \hat{X}} \rho(t_1) e^{-i\varepsilon \hat{X}}
\]

Backward TDHF

\[
\sigma^2_A = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2
\]

TDHF: \(\sigma_A \sim 1.5\)

Experiment: \(\sigma_A \sim 7.1\)

TDRPA: \(\sigma_A \sim 7.5\)


TDRPA quantitatively reproduced the experimental mass width

Width of the mass ratio distribution, $\sigma_{\text{MR}}$: Expt. vs Theory

$58_{\text{Ni}}^60_{\text{Ni}} + 60_{\text{Ni}}^60_{\text{Ni}}$ at $E/V_B = 1.4$

TDRPA quantitatively reproduced the experimental mass width

 ✓ The results indicate that the one-body dissipation and fluctuations are sufficient

 ➢ However, the TDRPA formula can not be applied for asymmetric reactions

One needs to extend the derivation of the TDRPA formula or use alternative approaches, e.g., stochastic extensions
Then, what would be the next step?

Stochastic extensions
**Stochastic Mean-Field (SMF) approach**

✓ In the small fluctuation limit, SMF approach formally reproduces the TDRPA formula

Multinucleon transfer processes are described as diffusion processes through the neck:

\[
\begin{align*}
\frac{\partial \sigma^2_{NN}}{\partial t} &= 2 \frac{\partial \nu_n}{\partial N_1} \sigma^2_{NN} + 2 \frac{\partial \nu_n}{\partial Z_1} \sigma^2_{NZ} + 2D_{NN} \\
\frac{\partial \sigma^2_{ZZ}}{\partial t} &= 2 \frac{\partial \nu_p}{\partial Z_1} \sigma^2_{ZZ} + 2 \frac{\partial \nu_p}{\partial N_1} \sigma^2_{NZ} + 2D_{ZZ} \\
\frac{\partial \sigma^2_{NZ}}{\partial t} &= 2 \frac{\partial \nu_p}{\partial N_1} \sigma^2_{NN} + 2 \frac{\partial \nu_n}{\partial Z_1} \sigma^2_{ZZ} + \left( \frac{\partial \nu_n}{\partial N_1} + \frac{\partial \nu_p}{\partial Z_1} \right) \sigma^2_{NZ}
\end{align*}
\]

\[
\sigma^2_{XY} = \langle \hat{X} \hat{Y} \rangle - \langle \hat{X} \rangle \langle \hat{Y} \rangle
\]

✓ Drift and diffusion coefficients can be obtained with occupied single-particle orbitals in TDHF

For details of the latest formulation, see, e.g.:

S. Ayik, B. Yilmaz, O. Yilmaz, and A.S. Umar
Stochastic Mean-Field (SMF) approach

SMF has been successfully applied also for asymmetric systems

Data: E.M. Kozulin et al., PRC 85(2012)044611

SMF: B. Yilmaz et al., PRC 98(2018)034604

TDRPA: E. Williams et al., PRL 120(2018)022501
Mean-field evolution is augmented with fluctuations and dissipation:

\[ i\hbar \psi_k(r, t) = \hbar[n] \psi_k(r, t) + \gamma[n] \dot{\psi}_k(r, t) \psi_k(r, t) \]
\[ - \frac{1}{2} \left[ \mathbf{u}(r, t) \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{u}(r, t) \right] \psi_k(r, t) \]
\[ + u_0(r, t) \psi_k(r, t), \]

TKE & mass distributions in $^{258}$Fm → comparable to experimental data

Summary

**TDHF**
- **✓** TDHF can describe overall trends of MNT processes
- It underestimates cross sections far from the average values
- Needs better description of fluctuations and correlations

**TDRPA**
- **✓** TDRPA quantitatively reproduced the experimental mass width
- It can not be applied for asymmetric systems
- Needs to approaches applicable to asymmetric systems

**Next step**
- **✓** Stochastic extensions may be helpful to construct a predictable microscopic theory for the multinucleon transfer reactions
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