Microscopic approaches to large-amplitude collective motion

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Time-dependent simulation with the density-functional theory

- Microscopic description of nuclear collective & non-collective dynamics
- TDHF equations

\[ i \frac{\partial}{\partial t} \left| \psi_i(t) \right\rangle = \hbar \left[ \rho(t) \right] \psi_i(t) \left\rangle \right\rangle \]

\[ i = 1, \ldots, A \]


Flocard, Koonin, Weiss, PRC17(1978)1682.
Electron-ion dynamics

- Coulomb explosion by a strong laser
Description of Electron-Ion dynamics


\[ i \frac{\partial}{\partial t} \psi_i(\vec{r}, t) = \left\{ \hbar_{KS}[\rho(\vec{r}, t), \{\vec{R}_a\}] + V_{\text{ext}}(\vec{r}, t) \right\} \psi(\vec{r}, t) \]

Real-time propagation

\[ \psi_i(t_0 + \Delta t) \simeq e^{-i(\hbar_{KS}(t_0) + V_{\text{ext}}(t_0))\Delta t} \psi_i(t_0) \]

Ions: Classical equation of motion

\[ M_a \frac{\partial^2}{\partial t^2} \vec{R}_a = \vec{F}_{a}^{\text{elec-ion}} + \vec{F}_{a}^{\text{ion-ion}} + \vec{F}_{a}^{\text{ext-ion}} \]

\[ \vec{F}_{a}^{\text{elec-ion}} = -\sum_{i}^{N} \langle \psi_i | \frac{\partial V_{\text{ion}}(\vec{r}, \{\vec{R}_a\})}{\partial \vec{R}_a} | \psi_i \rangle \]

(Ehrenfest’s Theorem)

Laser-induced molecular motion

Ionization

Coulomb explosion
Real-space, real-time TDDFT


Time-dependent Kohn-Sham equation

\[ i \frac{\partial}{\partial t} \psi_i(r, t) = \left( -\frac{1}{2m} \nabla^2 + V_H[\rho(r, t)] + \mu_{xc}[\rho(r, t)] + V_{\text{ext}}(r, t) \right) \psi_i(r, t) \]

3D mesh representation

\[ \varphi_i(r, t) = \{ \varphi_i(r_k, t_n) \}^{n=1,\cdots, Mt}_{k=1,\cdots, Mr}, \quad i = 1, \cdots, N \]

N: Particle number

Mr: # of mesh points

Mt: # of time slices

1. Use of Green’s function

2. Use of the absorbing boundary

Coulomb explosion by a strong laser pulse

- Intensity: $I=3.35 \times 10^{15} \text{[W/cm}^2\text{]}$
- Energy: $\hbar \omega = 1.55 \text{[eV]}$
- Pulse length: $T=26 \text{[fs]}$

1. Multiple electrons are emitted by intense laser pulse
2. Multiply charged ions explode by Coulomb repulsion force

Calculated by Kawashita (Tsukuba)

Electron density calculated by TDDFT

$N_2$ molecule
Real-time simulation

I = 3.35 \times 10^{15} \text{[W/cm}^2\text{]} \quad \lambda = 800 \text{[nm]} \quad T = 26 \text{[fs]}

Direction of polarization

Coulomb force between two ions

\[ 2e^2 \frac{p \times q}{R(t)^2} \text{[eV/Å]} \]
N^{2+} : Kinetic energy of ions

Exp. fact
Pulse of 55 fs produces 29 eV (56%)

Calculation
TKE of ions 32.3[eV] (66%)

4.1 \times 10^{15}[W/cm^2], 30[fs]

33.2[eV] (64%)

Scission takes place at an elongated configuration
Consistent with experiments
Nuclear dynamics

- TDDFT (TDHF) simulation of nuclear fusion
  - Barrier energy
- Adiabatic mean-field theory
  - Collective manifold (path)
  - Collective mass, with inclusion of time-odd terms
  - Application toward the spontaneous fission
Real-time simulation of nuclear fusion

- Fusion energy threshold & Barrier height
- Comparison with experimental data
- Skyrme SLy5 functional

\[
\begin{align*}
16\ O^{(40,48}\ Ca,\ 90\ Zr,\ 100,132\ Sn,\ 208\ Pb) &+ 16\ O \\
16\ O^{(40,48}\ Ca,\ 90\ Zr,\ 100,132\ Sn,\ 208\ Pb) &+ 40,48\ Ca \\
16\ O^{(40,48}\ Ca,\ 90\ Zr,\ 100,132\ Sn,\ 208\ Pb) &+ 90\ Zr \\
16\ O^{(40,48}\ Ca,\ 90\ Zr,\ 100,132\ Sn,\ 208\ Pb) &+ 100,132\ Sn \\
16\ O^{(40,48}\ Ca,\ 90\ Zr,\ 100,132\ Sn,\ 208\ Pb) &+ 208\ Pb
\end{align*}
\]
Fusion threshold energy

Guo and T.N.  

cf) Simenel et al, arXiv:0904.2635

\[ E_{th} \leq B_{FD} \]

\[ E_{th} > B_{FD} \]
Adiabatic theories of LACM

• Baranger-Veneroni, 1972-1978
  \[ \rho(t) = e^{i\chi(t)} \rho_0 e^{-i\chi(t)} \]
  • Expansion with respect to \( \chi \)

• Villars, 1975-1977
  • Eq. for the collective subspace
    (zero-th and first-order w.r.t. momenta)
    \[
    \delta \langle \Phi(q) | H - \frac{\partial V}{\partial q} Q(q) | \Phi(q) \rangle = 0
    \]
    \[
    \delta \langle \Phi(q) | [H, Q(q)] + i M(q)^{-1} \frac{\partial}{\partial q} | \Phi(q) \rangle = 0
    \]
    Goeke, Reinhard, Rowe, NPA359 (1981) 408

• Non-uniqueness problem
  “Validity condition”
  Reinhard, 1978-
Non-adiabatic theories of LACM

- Rowe-Bassermann, Marumori, Holzwarth-Yukawa, 1974-
  - Local Harmonic Approach (LHA)
  - Curvature problem
  - Correspondence between, Q,P ↔ Infinitesimal generator, is not guaranteed.

\[
\delta \langle \Phi(q) | H - \frac{\partial V}{\partial q} Q(q) | \Phi(q) \rangle = 0 \\
\delta \langle \Phi(q) | [H, Q(q)] + i M(q)^{-1} P(q) | \Phi(q) \rangle = 0 \\
\delta \langle \Phi(q) | [H, P(q)] - i C(q) Q(q) | \Phi(q) \rangle = 0
\]

- Marumori et al, 1980-
  - Self-consistent collective coordinate (SCC) method
  - The problems of LHA are solved.
  - The SCC equation is solved by the expansion with respect to (q,p).

\[
\delta \langle \Phi(q, p) | H - \frac{\partial \mathcal{H}}{\partial q} Q - \frac{\partial \mathcal{H}}{\partial p} P | \Phi(q) \rangle = 0 \\
\mathcal{H} \equiv \langle \Phi(q, p) | H | \Phi(q, p) \rangle
\]

- “Adiabatic” approx. → LACM (Matsuo, TN, Matsuyanagi, 2000)
Microscopic derivation of the collective sub-manifold

Determination of

Canonical variables \((q,p)\)
Collective potential \(V(q)\)
Mass parameters \(B(q), J_k(q)\)

Collective Hamiltonian

\[
\{ \hat{T}[B,J](q) + \hat{V}(q) \} \Psi(q) = E \Psi(q)
\]

\[
\delta \langle \phi(q) | \hat{H}_M | \phi(q) \rangle = 0, \quad \hat{H}_M = H - \lambda(q) \hat{N} - (\partial V / \partial q) \hat{Q}(q)
\]

\[
\delta \langle \phi(q) \left[ \hat{H}_M(q), i \hat{Q}(q) \right] - B(q) \hat{P}(q) | \phi(q) \rangle = 0
\]

\[
\delta \langle \phi(q) \left[ \hat{H}_M, \hat{P}(q)/i \right] - C(q) \hat{Q}(q)
\]

\[
- \frac{1}{2B(q)} \left[ \left[ \hat{H}_M, (\partial V / \partial q) \hat{Q}(q) \right], \hat{Q}(q) \right] - (\partial \lambda / \partial q) \hat{N} | \phi(q) \rangle = 0
\]
**Q(q) is more than just a constraint**

- The decoupling from the spurious modes requires \( Q(q) \) to be a **full one-body operator**, containing \((a^+a)\) terms
  - TN, DoDang, Walet, PRC 61 (1999) 014302
- This is associated with a **gauge invariance**

\[
\text{(mf - HFB)} \quad \delta \langle \phi(q) | \hat{H}_M | \phi(q) \rangle = 0, \quad \hat{H}_M = H - \lambda(q) \hat{N} - (\partial V / \partial q) \hat{Q}(q)
\]

\[
\text{(LHE)} \quad \delta \langle \phi(q) | \left[ \hat{H}_M(q), i \hat{Q}(q) \right] - B(q) \hat{P}(q) | \phi(q) \rangle = 0
\]

\[
\delta \langle \phi(q) | \left[ \hat{H}_M, \hat{P}(q) / i \right] - C(q) \hat{Q}(q) - \frac{1}{2B(q)} \left[ \left[ \hat{H}_M, \left( \partial V / \partial q \right) \hat{Q}(q) \right], \hat{Q}(q) \right] - \left( \partial \lambda / \partial q \right) \hat{N} | \phi(q) \rangle = 0
\]

Gauge fixing
Model of protons and neutrons

T.N. & Walet, PRC58 (1998) 3397

\[ H = H_n + H_p + H_{np}, \]

\[ H_n = \sum_{i \in n, m_i} \epsilon_i c_{j_i m_i}^{\dagger} c_{j_i m_i} - G_n P_{n}^\dagger P_n - \frac{1}{2} \kappa Q_n^2, \]

\[ H_p = \sum_{i \in p, m_i} \epsilon_i c_{j_i m_i}^{\dagger} c_{j_i m_i} - G_p P_{p}^\dagger P_p - \frac{1}{2} \kappa Q_p^2, \]

\[ H_{np} = -\kappa Q_n Q_p, \]

Neutrons

Protons

Upper orbital has a larger quadrupole moment
Adiabatic vs Diabatic Dynamics

The problem has been discussed since the paper by Hill and Wheeler (1953).

The pairing interaction plays a key role for configuration changes at level crossings.
Specialization energy

• Spontaneous fission life times in odd nuclei are larger by several orders than even-even nuclei.

• Suggest importance of pairing correlation in nuclear fission

Swiatecki, PR100 (1955) 937
Pairing + Quadrupole Model ($^{68}$Se)

Microscopic Hamiltonian

SP energy + Pairing (Monopole, Quadrupole) + Quadrupole interaction

Model Space

two major shells ($N_{sh}=3,4$) ($^{40}$Ca core)

Parameters

sp energy: Modified Oscillator
interaction strength

**monopole pairing and quadrupole int. strength:**
adjusted to the pairing gaps and deformations of Skyrme-HFB
(Yamagami et al. NPA693(2001))

**quadrupole pairing strength $G_2$:**

- $G_2 = 0$
- $G_2 = (G_2)_{self}$ (self-consistent value) Sakamoto and Kishimoto PLB245 (1990) 321.

$(G_2)_{self}$ restores the Galilean invariance in RPA order, which was broken by the monopole pairing.
Energy spectra of $^{68}$Se

- Two rotational bands
- $0^+_2$ state
- Quadrupole pairing reduces excitation energy

$B(E2)$ $e^2$ fm$^4$

Effective charge: $e_{pol} = 0.904$

Collective Wavefunctions of $^{68}$Se

- $l = 0$: oblate and prolate shapes are strongly mixed via a triaxial degree of freedom
- ground band: mixing of different $K$ states, excited band: $K=0$ dominant
- oblate-prolate mixing: strong in $0^+$ states, reduced as angular momentum increases

$G_2 = 0$

$G_2 = G_2^{\text{self}}$

localization
Spectra in $^{68}$Se

1-dim. ASCC

2-dim. L-QRPA

Exp

$\langle \ldots \rangle \ldots \text{B(E2)} \ e^2 \ \text{fm}^4$

effective charge: $e_{\text{pol}} = 0.4$

Hinohara et al., PRC 82 (2010), 064313.
Skyrme CHFB

The coordinate-space Hartree-Fock-Bogoliubov theory

\[
\begin{pmatrix}
    \hat{h}^q(r, \sigma) - \lambda^q & \tilde{h}^q(r, \sigma) \\
    \tilde{h}^q(r, \sigma) & \hat{h}^q(r, \sigma) - \lambda^q
\end{pmatrix}
\begin{pmatrix}
    \varphi^q_{1,i}(r, \sigma) \\
    \varphi^q_{2,i}(r, \sigma)
\end{pmatrix}
= E_i
\begin{pmatrix}
    \varphi^q_{1,i}(r, \sigma) \\
    \varphi^q_{2,i}(r, \sigma)
\end{pmatrix}
\]

- Mean-field Hamiltonian

\[ h = \frac{\delta \mathcal{E}}{\delta \bar{\varrho}} - \mu \hat{q}_{20} \]

- Pairing field

\[ \tilde{h} = \frac{\delta \mathcal{E}}{\delta \tilde{\varrho}} \]

HFB equations solved directly on the 2D lattice.

- 13-point formula for derivative

\[ \rho_{\text{max}} \times z_{\text{max}} = 12.3 \text{fm} \times 16.8 \text{fm} \]
Collective inertia on fission pathway in $^{256}\text{Fm}$

✓ Local QRPA mass

$$M_\beta = \frac{dq^\beta}{d\hat{Q}_{20}} \frac{dq^\beta}{d\hat{Q}_{20}}$$

$$\frac{d\hat{Q}_{20}}{dq^\beta} = \langle \phi | [\hat{Q}_{20}, \frac{P_\beta}{i}] | \phi \rangle$$

✓ Cranking mass:

$$M_{\beta\beta}^{C} = \frac{1}{2} (S_1^{-1} S_3 S_1^{-1})$$

$$S_{(n)} = \sum_{\mu\nu} \frac{|\langle \mu\nu | \hat{Q}_{20} | \phi \rangle|^2}{(E_\mu + E_\nu)^n}$$

✓ ATDHFB-C:

A. Baran et al., PRC 84 (2011) 054321

Cranking approx. for ATDHFB mass

Calculated by Yoshida (Niigata)
Summary

• Electron-ion dynamics simulation with TDDFT +MD
  – Reduction of the total kinetic energy
  – Consistent with experiment (for a long pulse)

• TDDFT (TDHF) simulation of nuclear fusion
  – Barrier energy

• Adiabatic mean-field theory
  – Collective manifold (path)
  – Collective mass, with inclusion of time-odd terms
  – Application toward the spontaneous fission