Configuration-interaction time-dependent density functional theory and its application

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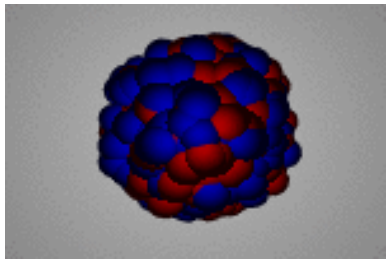
Outline

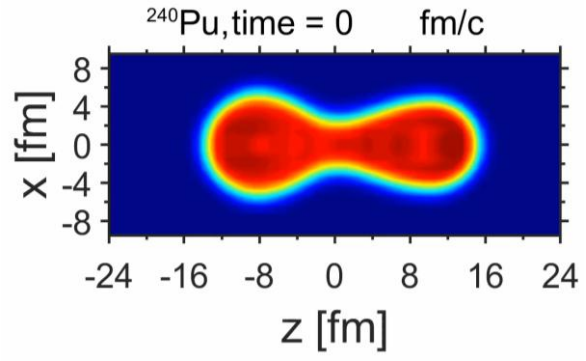
- Introduction
- Theoretical Framework
- Results and Discussions
- Summary and Outlook

Nuclear dynamics

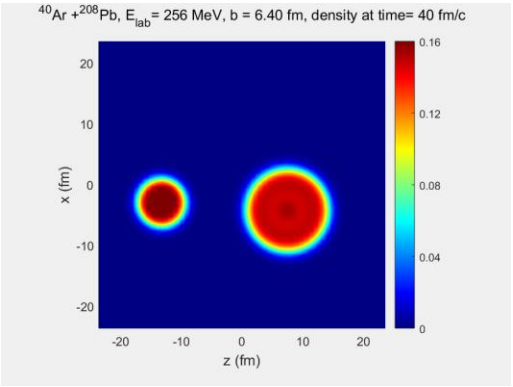
- The atomic nucleus is a complex quantum many-body system, which exhibits many interesting dynamical processes.



Collective vibration



Fission



Heavy-ion reaction

- The study of nuclear dynamical processes is important for the understanding of nuclear structure, the synthesis of superheavy elements, and the production of exotic nuclei far from stability, etc.

P. Ring, P, Schuck, *The Nuclear Many-body Problem* (1980)

- Finding a unified way to describe nuclear dynamics and understanding its mechanism are longstanding and challenging problems in nuclear physics.

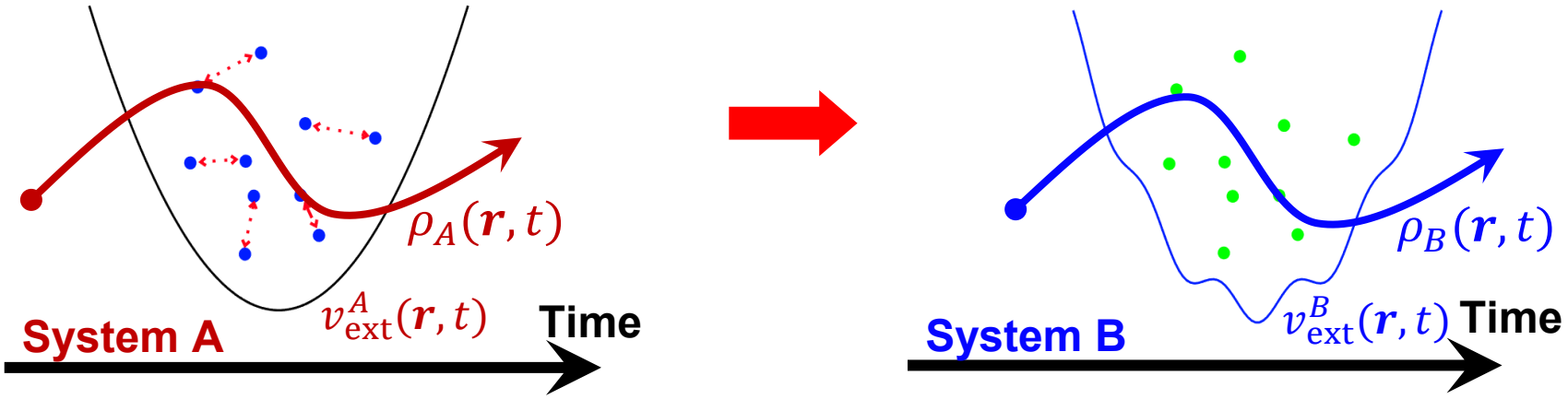
Time-dependent density functional theory

- Density functional theory (DFT) is currently the only microscopic theory that can be used to describe almost all nuclei in the nuclear chart.

Bender, Heenen, Reinhard, RMP 75, 121 (2003)

Relativistic Density Functional for Nuclear Structure, edited by J. Meng, 2016

- Its time-depedent version (time-dependent DFT, TDDFT) is an important tool which provides a unified description of nuclear dynamical processes.
- TDDFT models a complex many-body system in terms of a product-type wave function (Slater determinant), which describes the time evolution of independent nucleons in a self-consistent mean field.



E. Runge, E. K. U. Gross, PRL 52 (1984) 997; R. van Leeuwen, PRL 82 (1999) 3863

Application of TDDFT

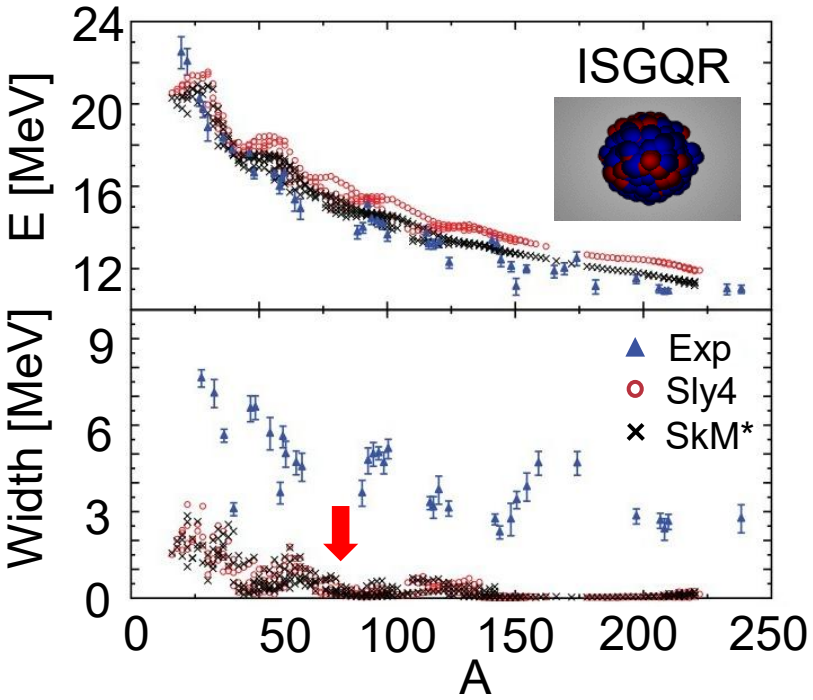
- TDDFT has been applied to a variety of nuclear dynamical processes:

  - Collective vibration — D. Vretenar, H. Berghammer, P. Ring, NPA 581 (1995) 679; P. -G. Reinhard, L. Guo, J. A. Maruhn, EPJA 32 (2007) 19
  - Dynamics of α-chain structure — A. S. Umar *et al.*, PRL 104 (2010) 212503; Z. X. Ren, P. W. Zhao, J. Meng, PLB 801 (2020) 135194
  - Fission — A. Bulgac *et al.*, PRL 116 (2016) 122504; Z. X. Ren et al., PRL 128 (2022) 172501
  - Multinucleon transfer reaction — C. Simenel, PRL 105 (2010) 192701; Z. J. Wu, L. Guo, PRC 100 (2019) 014612; D. D. Zhang et al., PRC 109 (2024) 024614
  - Chiral vibration — Z. X. Ren, P. W. Zhao, J. Meng, PRC 105 (2022) L011301; B. Li, P. W. Zhao, J. Meng, PLB 856 (2024) 138877
  - …

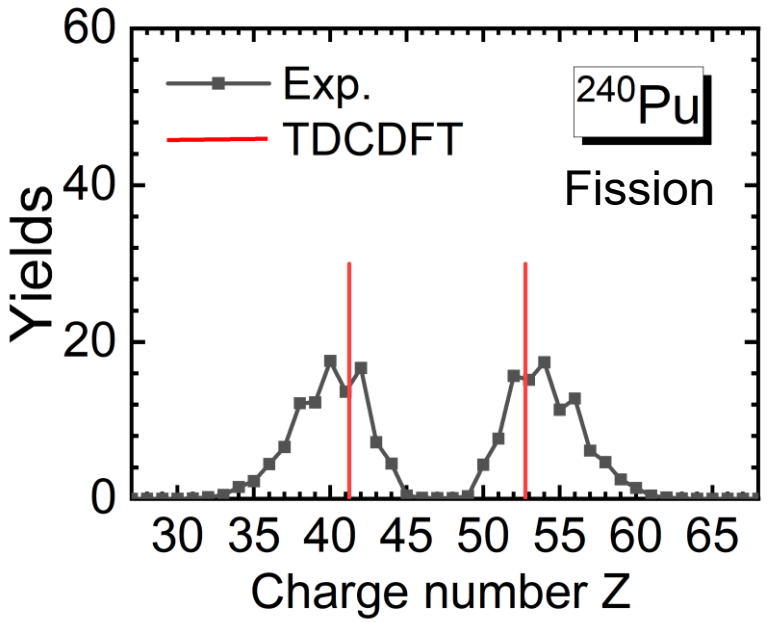
Limitation of TDDFT

- Due to the mean-field approximation, TDDFT has some limitations:
  - not consider 2p-2h, 3p-3h, … excitations
  - not take into account quantum fluctuations in collective space

➡ cannot reproduce spreading widths of one-body observables



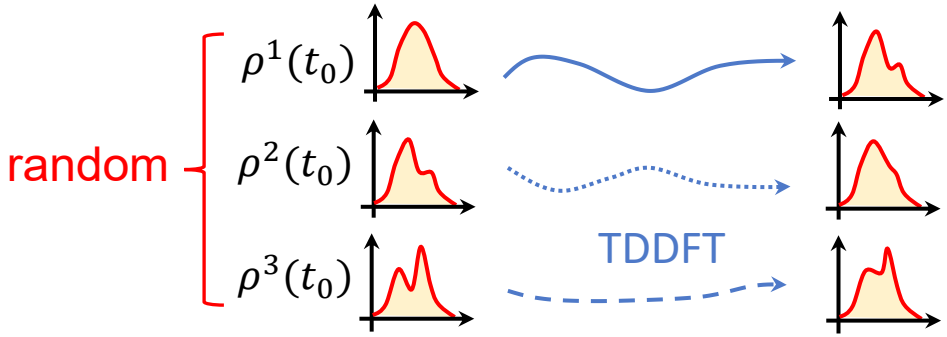
G. Scamps, D. Lacroix, PRC 88 (2013) 044310



Z. X. Ren *et al.*, PRC 105 (2022) 044313

Beyond TDDFT methods

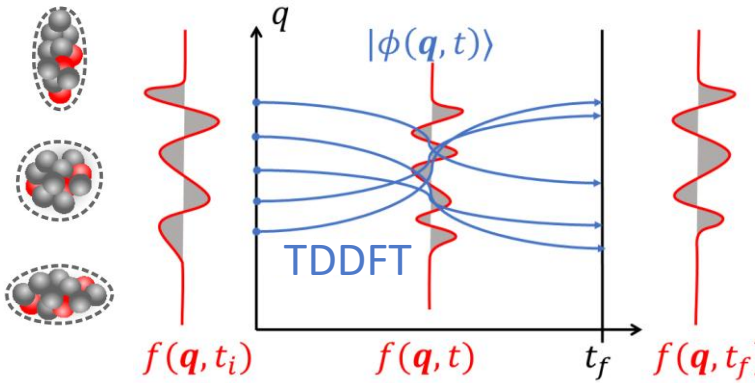
- Beyond TDDFT methods are developed to overcome the limitations:
  - Stochastic time-dependent Hartree-Fock method



$$i\hbar\frac{\partial}{\partial t}\rho^{\lambda}(t) = [h(\rho^{\lambda}), \rho^{\lambda}]$$

S. Ayik, PLB 658 (2008) 174
D. Lacroix, S. Ayik, EPJA 50 (2014) 95
Y. Tanimura *et al.*, PRL 118 (2017) 152501

  - Generalized time-dependent generator-coordinate method



$$|\Psi(t)\rangle = \int d\boldsymbol{q}\, f(\boldsymbol{q},t)|\phi(\boldsymbol{q},t)\rangle$$

B. Li *et al.*, PRC 108 (2023) 014321
P. Marević *et al.*, PRC 108 (2023) 014620

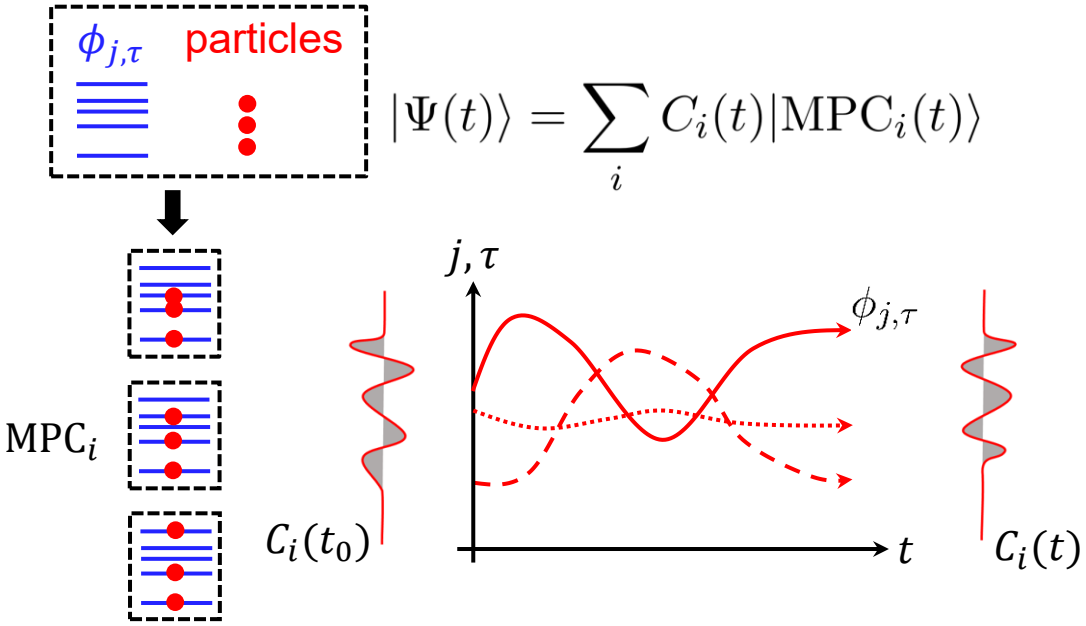
- A common approximation in these methods is that each trajectory follows the TDDFT evolution. This treatment violates the time-dependent variational principle and can lead to non-conservation of the total energy.

P. Marević *et al.*, EPJA 60 (2024) 10

This work

- In chemistry, there is a method named multiconfiguration time-dependent Hartree (MCTDH) which follows exactly the time-dependent variational principle.

M. H. Beck, H. -D. Meyer, ZPD 42 (1997) 113



Advantages

1. total energy conservation
2. include 2p-2h excitations…
3. include pairing correlations without particle number conservation broken

- In this work, we introduce the **configuration-interaction time-dependent density functional theory (CI-TDDFT)** for nuclear systems, inspired by the MCTDH method, and presents its first application.

Nuclear wave function

- In CI-TDDFT, the nuclear wave function is a superposition of Slater determinants (many-particle configurations, MPCs):

$$|\Psi(t)\rangle = \sum_i \underset{①}{C_i(t)} \underset{②}{|\mathrm{MPC}_i(t)\rangle}, \qquad |\mathrm{MPC}_i(t)\rangle = \prod_{k,\tau} a^\dagger_{k,\tau}|-\rangle$$

where $C_i(t)$ are the expansion coefficients and $a^\dagger_{k,\tau}$ is the creation operator for the single-particle state $\phi_{k,\tau}$.

- To determine the nuclear wave function, the action functional is defined:

$$S\left[\{C_i(t)\}, \{\phi_{k,\tau}(\boldsymbol{r},t)\}\right] = \int dt \left\{ \langle\Psi(t)|\hat{H} - i\hbar\partial_t|\Psi(t)\rangle - \sum_\tau \sum_{kq=1}^{M} \mu^\tau_{kq}(t)\left[\langle\phi_{k,\tau}|\phi_{q,\tau}\rangle - \delta_{kq}\right] \right\}$$

The Lagrange multipliers $\mu^\tau_{kq}(t)$ are introduced to ensure the orthonormality of single-particle states during the time evolution.

According to the time-dependent variational principle,

① $\dfrac{\delta S}{\delta C_i^*} = 0$ ② $\dfrac{\delta S}{\delta \phi^\dagger_{k,\tau}} = 0$

Time evolution of nuclear wave function

- Time evolution of expansion coefficients:

$$\frac{\delta S}{\delta C_i^*} = 0 \quad \Rightarrow \quad i\hbar\partial_t C_j(t) = \sum_i \left\{\mathcal{H}_{ji}(t) - \mathcal{H}_{ji}^{\mathrm{MF}}(t)\right\} C_i(t)$$

Energy kernel: $\mathcal{H}_{ji}(t) = \langle \mathrm{MPC}_j(t)|\hat{H}|\mathrm{MPC}_i(t)\rangle,$

Mean-field kernel: $\mathcal{H}_{ji}^{\mathrm{MF}}(t) = \langle \mathrm{MPC}_j(t)|\mathrm{i}\hbar\partial_t|\mathrm{MPC}_i(t)\rangle.$

Complex coupled equations

- Time evolution of single-particle states:

$$\frac{\delta S}{\delta \phi_{k,\tau}^\dagger} = 0 \quad \Rightarrow \quad i\hbar\partial_t \phi_{j,\tau} = \hat{P}_\tau \left[\hat{h}\phi_{j,\tau} + \sum_{\tau'} \sum_{kqsl=1}^{M} (\rho_{jk}^\tau)^{-1} \rho_{kqsl}^{\tau\tau'} \hat{W}_{sl}^{\tau\tau'} \phi_{q,\tau}\right]$$

One-body density matrix: $\rho_{jk}^\tau = \langle \Psi(t)|a_{j,\tau}^\dagger a_{k,\tau}|\Psi(t)\rangle$

Two-body density matrix: $\rho_{kqsl}^{\tau\tau'} = \langle \Psi(t)|(a_{k,\tau}^\dagger a_{q,\tau})(a_{s,\tau'}^\dagger a_{l,\tau'})|\Psi(t)\rangle$

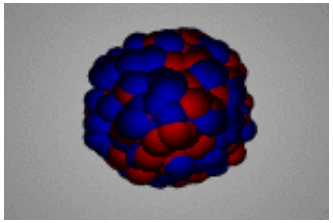
TDDFT

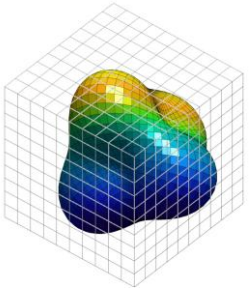
$i\hbar\partial_t \phi_{j,\tau} = \hat{h}\phi_{j,\tau}$

Here, the projection operator $\hat{P}_\tau = 1 - \sum_{q'=1}^{M} |\phi_{q',\tau}\rangle\langle\phi_{q',\tau}|$ is introduced to eliminate the Lagrange multiplier $\mu_{kq}^\tau(t)$.

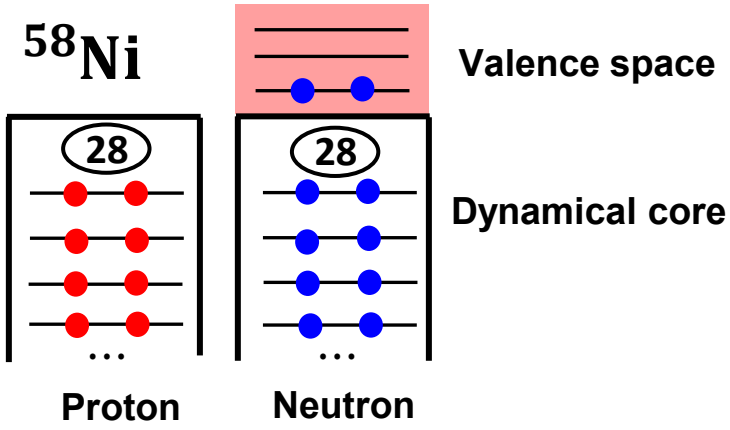
Numerical Details

- CI-TDDFT is firstly applied to study the isoscalar giant monopole resonance of ^{58}Ni:

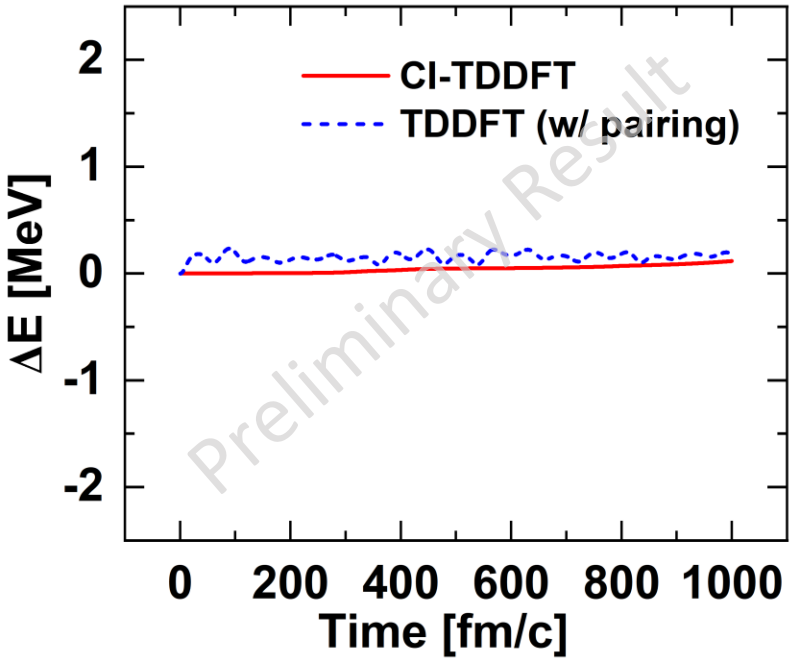


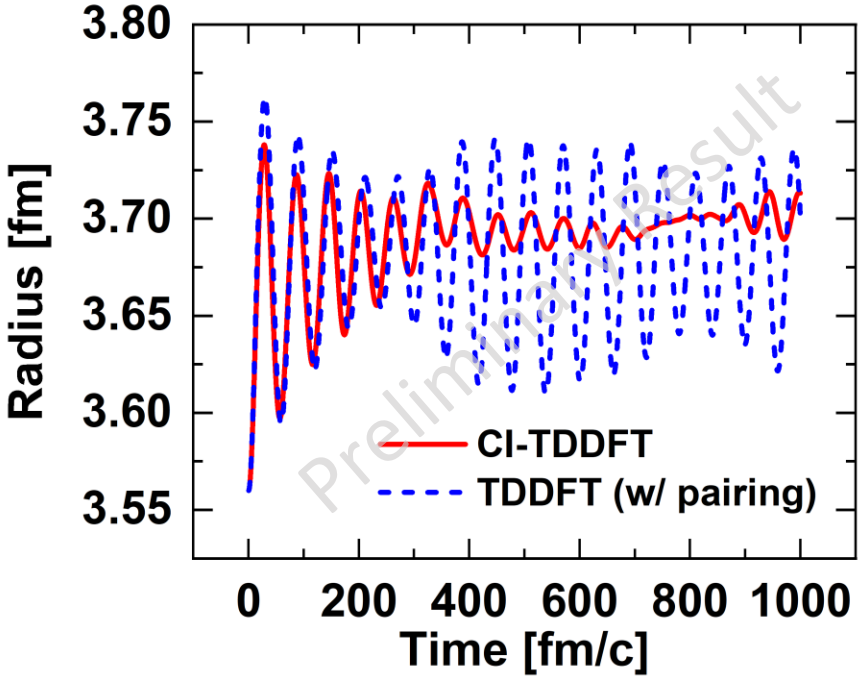


  - Relativistic density functional: PC−PK1
  - Mesh size: (dx, dy, dz) = (1.0, 1.0, 1.0) fm
  - Grid number: (nx, ny, nz) = (24, 24, 24)
  - Initial radius: $R_0 = 3.56$ fm $(R_{\text{g.s.}} = 3.66$ fm$)$
  - Configuration space: number of configurations: $C_6^2 = 15$



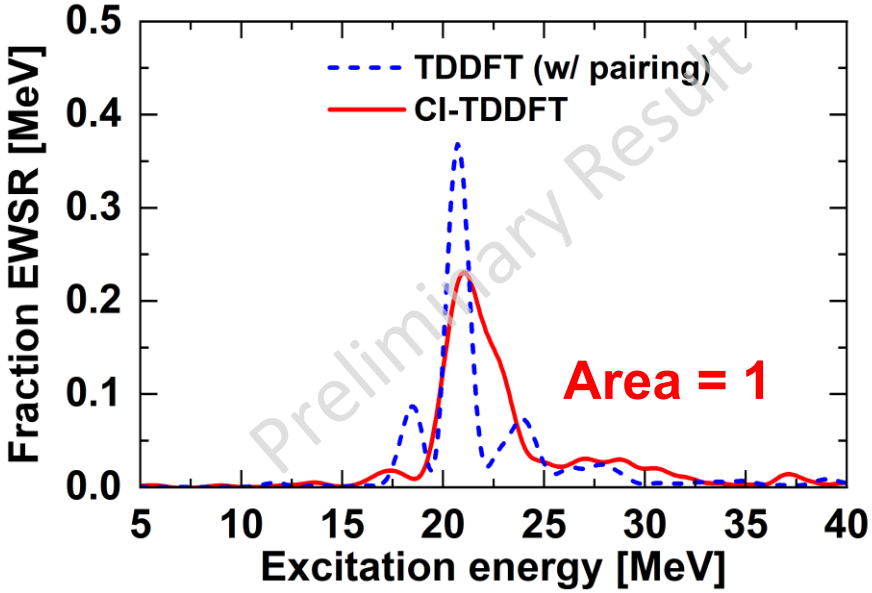
Time evolution of the total energy and radius

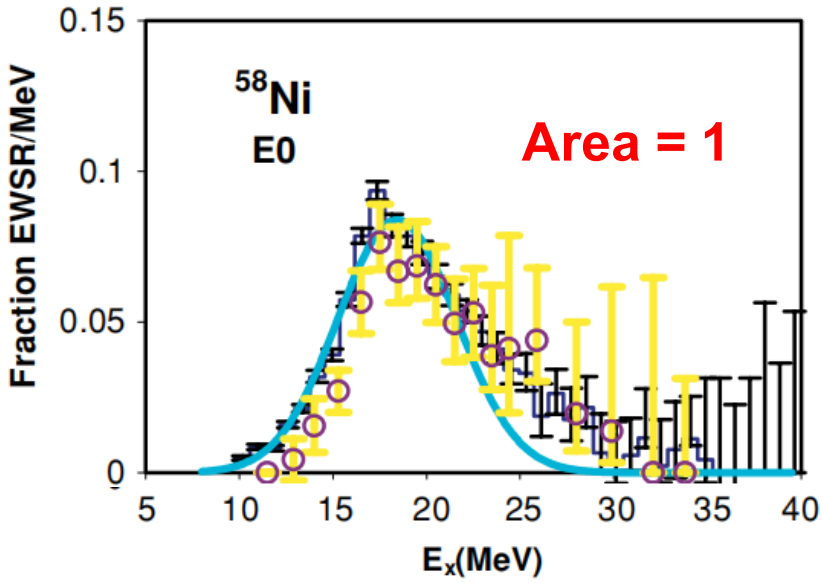




- The total energy is conserved in CI-TDDFT, while that of TDDFT with pairing has some small oscillations.
- The radius calculated by CI-TDDFT is more damped than TDDFT.

Strength distributions





Y. -W. Lui *et al.*, Phys. Rev. C 73 (2006) 014314

- CI-TDDFT produces a significant broadening of the resonance width compared to TDDFT.
- The experimental width is still underestimated. More configurations are required to reproduce it.

Summary and outlook

- Summary:
  - The configuration-interaction time-dependent density functional theory (CI-TDDFT) is established.
  - Apply to isoscalar giant monopole resonance of ^{58}Ni: CI-TDDFT yields a resonance width that is significantly broadened compared to standard TDDFT.
- Outlook:
  - Expand the configuration space to reproduce the resonance width of ^{58}Ni
  - Describe fission and heavy-ion reaction processes

Thank you for your attention!