Configuration-interaction time-dependent density functional theory for nuclear dynamics

Pengwei Zhao 赵鹏巍

School of Physics, Peking University

Outline

From **Mean-Field** to **Configuration-Interaction** Dynamics in DFT

- Motivation: limitations of mean-field approaches
- Pairing Correlations in Relativistic DFT: SLAP
- Beyond Mean Field: Relativistic CI-DFT (ReCD)
- Nuclear Dynamics: CI-TDDFT
- Summary

Density functional theory

The many-body problem is mapped onto a one-body problem

Hohenberg-Kohn Theorem

The exact ground-state energy of a quantum mechanical many-body system is a universal functional of the local density.

$$E[\rho] = T[\rho] + U[\rho] + \int V(\mathbf{r})\rho(\mathbf{r})\, \mathrm{d}^3\mathbf{r}$$

Kohn-Sham DFT

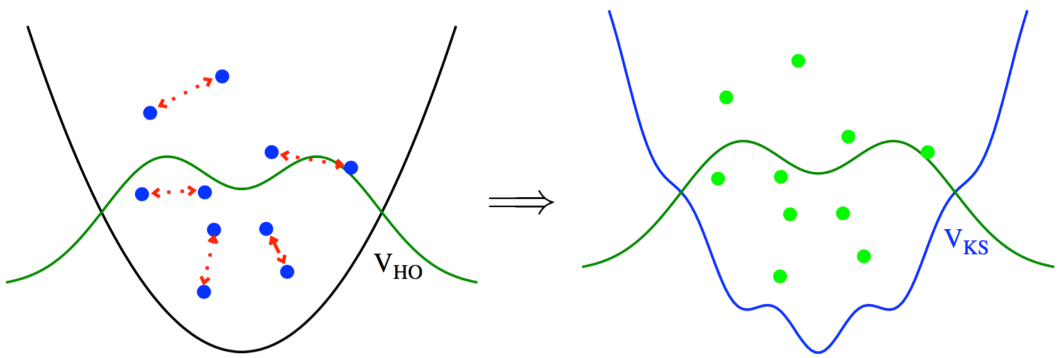


Figure from Drut PPNP 2010

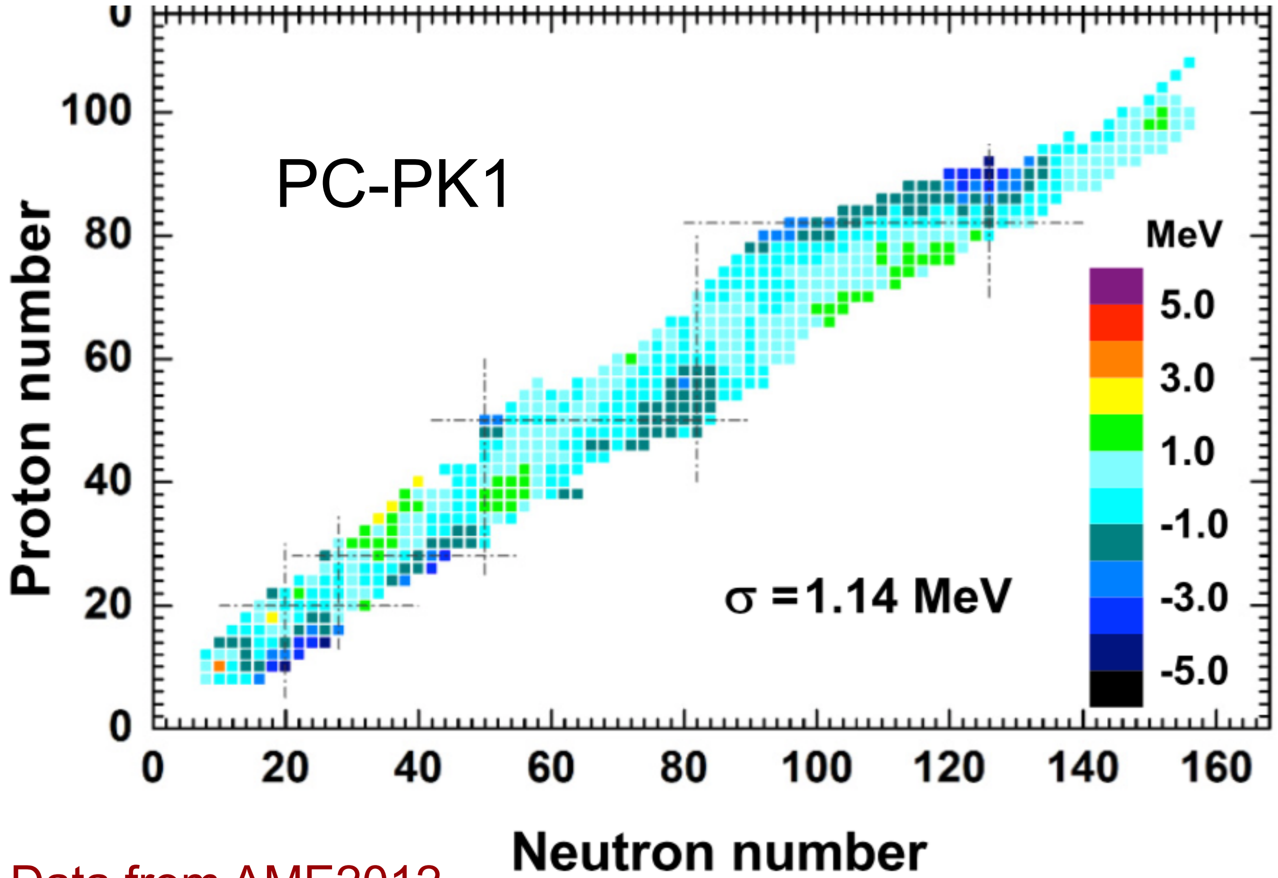
$$T[\rho] \doteq \sum_{i=1}^{N} \left\langle \varphi_i \left| -\frac{\hbar^2}{2m}\nabla^2 \right| \varphi_i \right\rangle$$

$$E[\rho] \Rightarrow \boxed{\hat{h} = \frac{\delta E}{\delta \rho}} \Rightarrow \boxed{\hat{h}\varphi_i = \varepsilon_i \varphi_i} \Rightarrow \boxed{\rho = \sum_{i=1}^{A} |\varphi_i|^2}$$

The practical usefulness of the Kohn-Sham theory depends entirely on whether an **Accurate Energy Density Functional** can be found!

Covariant density functional：PC-PK1

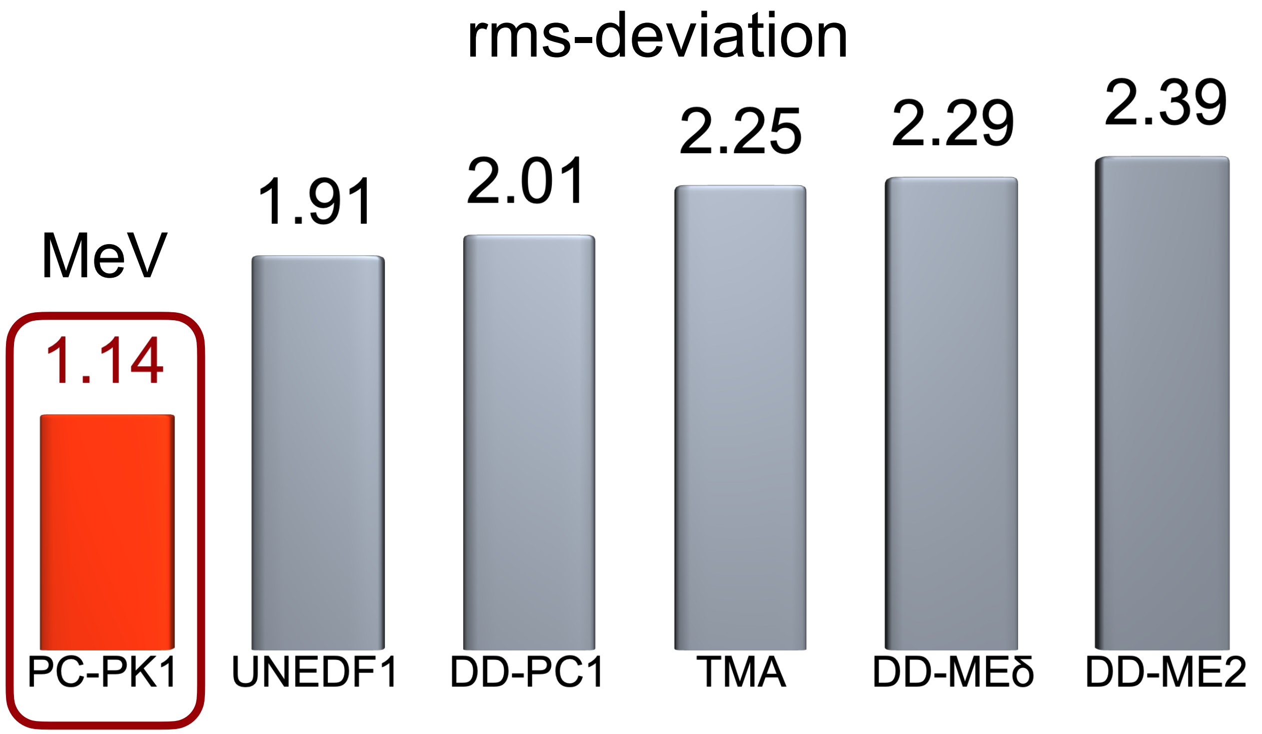
Mass Differences: M_{cal} - M_{exp}



Data from AME2012

PWZ, Li, Yao, Meng, PRC 82, 054319 (2010)

Lu, Li, Li, Yao, Meng, PRC 91, 027304 (2015)



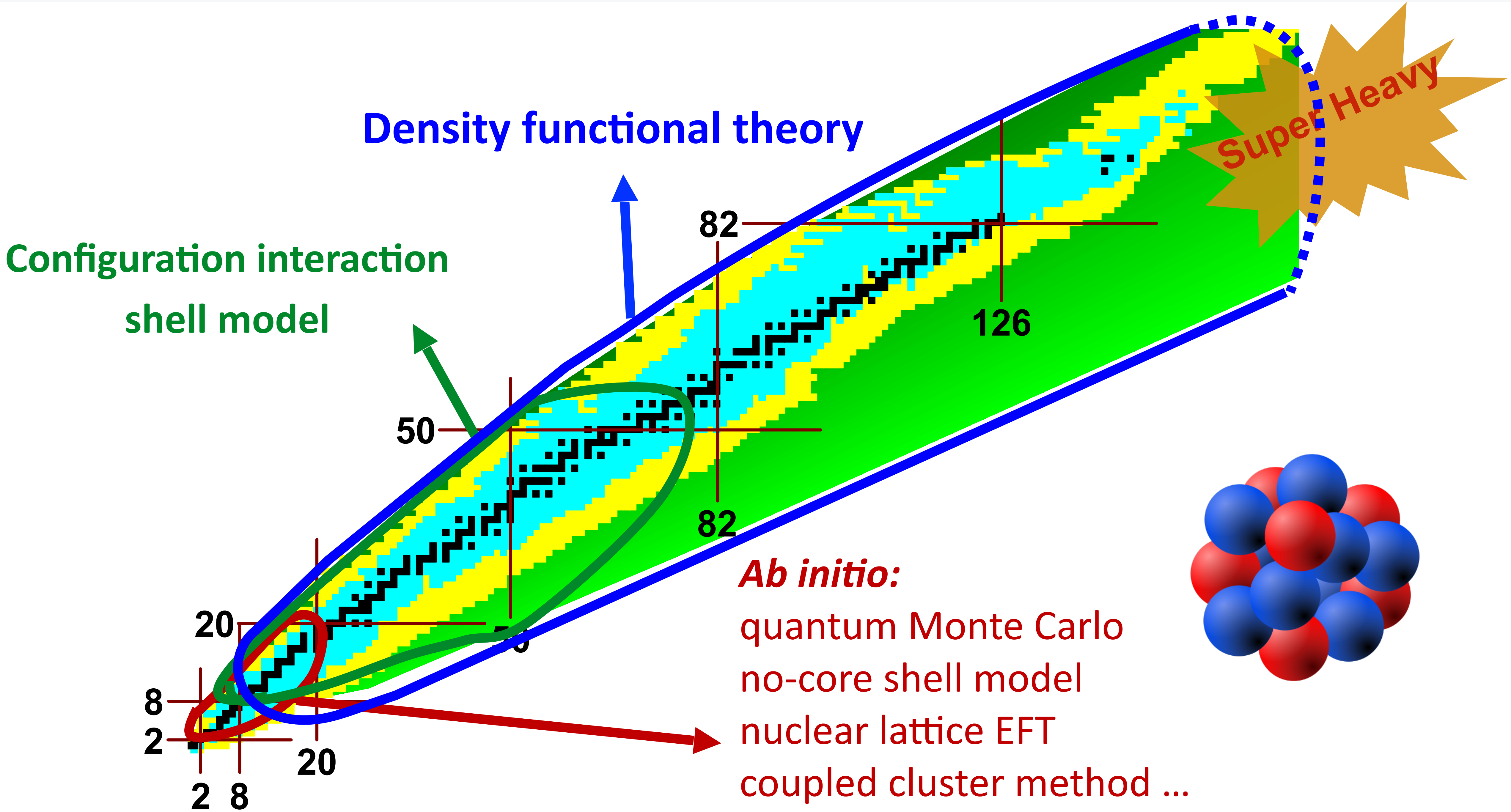
http://nuclearmap.jcnp.org

Yang, Wang, PWZ, Li, PRC 104, 054312 (2021)

Yang, PWZ, Li, PRC 107, 024308 (2023)

Among the best density-functional description for nuclear masses!

State-of-the-art theories for nuclei



It would be interesting to investigate the intersections between different theories for a unified and comprehensive description of nuclei.

DFT and Shell Model

DFT

- ☑ Universal density functionals
  - Symmetry breaking
  - Full model space
  - Single config. fruitful physics
  - No Configuration mixing
- ☑ Applicable for almost all nuclei
- ☐ No spectroscopic properties

Shell Model

- ☐ Non-universal effective interactions
  - No symmetry breaking
  - Limited model space
  - Single config. little physics
  - Configuration mixing
- ☐ Intractable for deformed heavy nuclei
- ☑ Spectroscopy from multi config.

a theory combining the advantages from both approaches

Outline

From **Mean-Field** to **Configuration-Interaction** Dynamics in DFT

- Motivation: limitations of mean-field approaches
- Pairing Correlations in Relativistic DFT: SLAP
- Beyond Mean Field: Relativistic CI-DFT (ReCD)
- Nuclear Dynamics: CI-TDDFT
- Summary

Pairing correlations

- Pairing correlations are widely observed in atomic nuclei
- BCS/Bogoliubov method: variational quasiparticle vacuum, **particle number violation**
- Shell-model like approach (SLAP): configuration mixing, **particle number conservation**

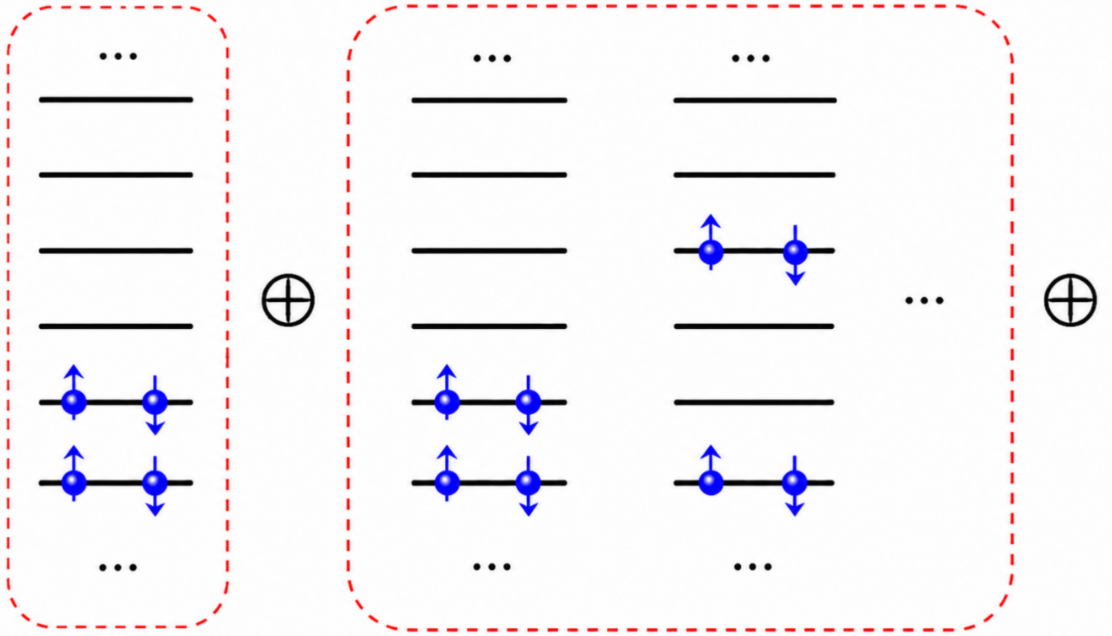
Yang, Zeng, Acta Physica Sinica 20, 846 (1964); Zeng, Cheng, NPA 405, 1 (1983)

Meng, Guo, Liu, Zhang, Front. Phys. China 1, 38 (2006)

Treat Pairing correlations exactly by diagonalizing the pairing Hamiltonian in a many-particle configuration (MPC) space with good particle number

Advantages

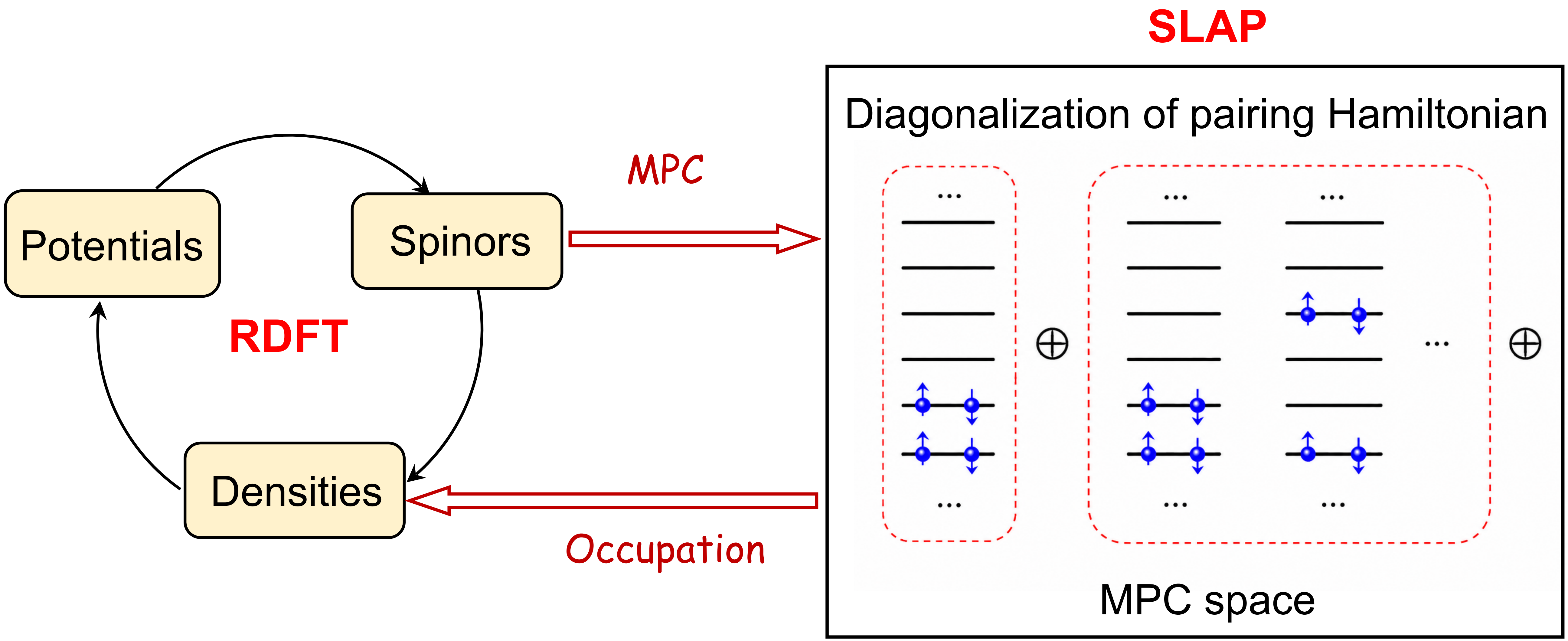
✓ particle number conservation
✓ treat the blocking effects exactly
✓ no pairing collapse
✓ …



MPC space

RDFT + SLAP

Relativistic density functional theory (RDFT) + Shell-model-like approach (SLAP)

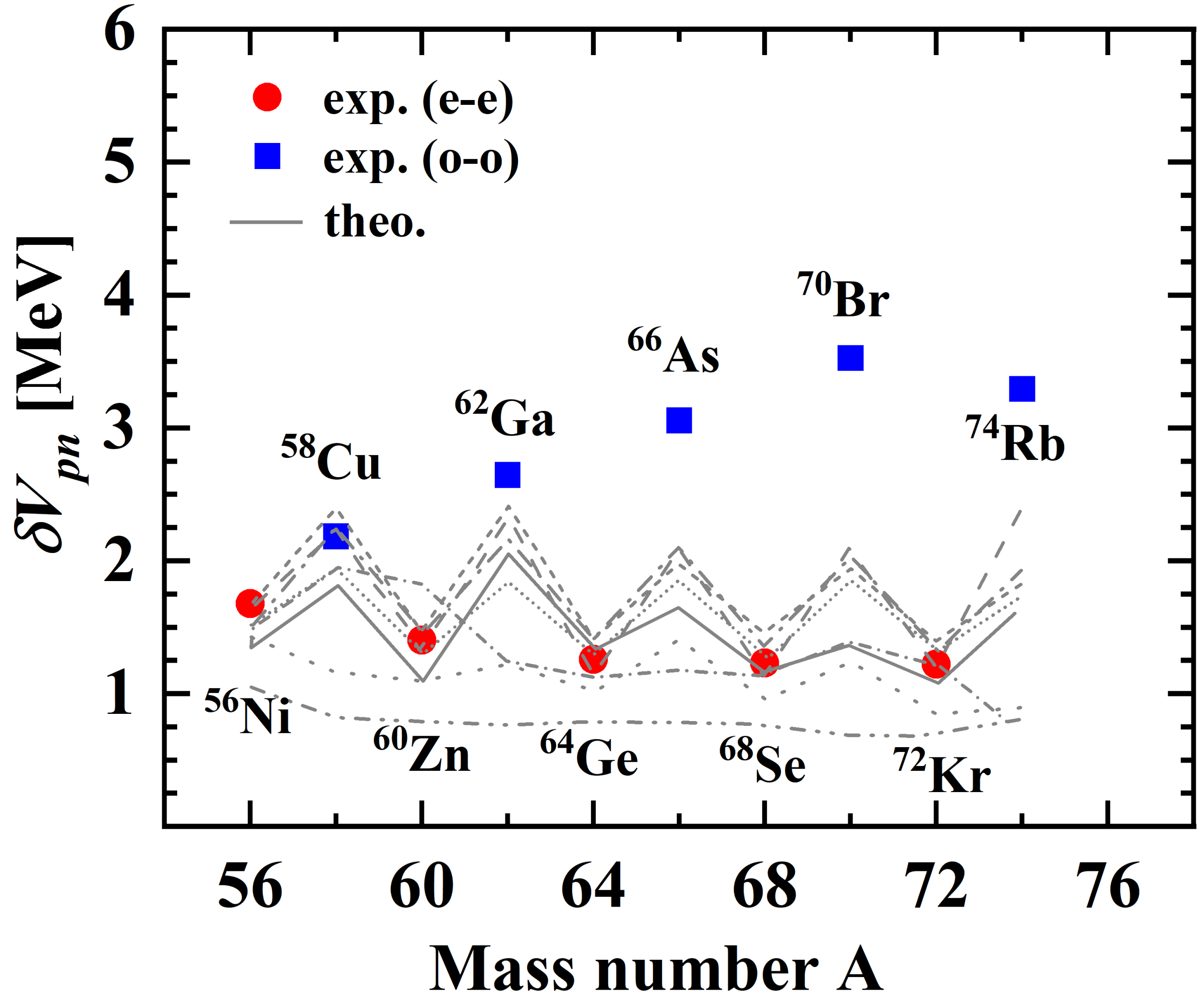


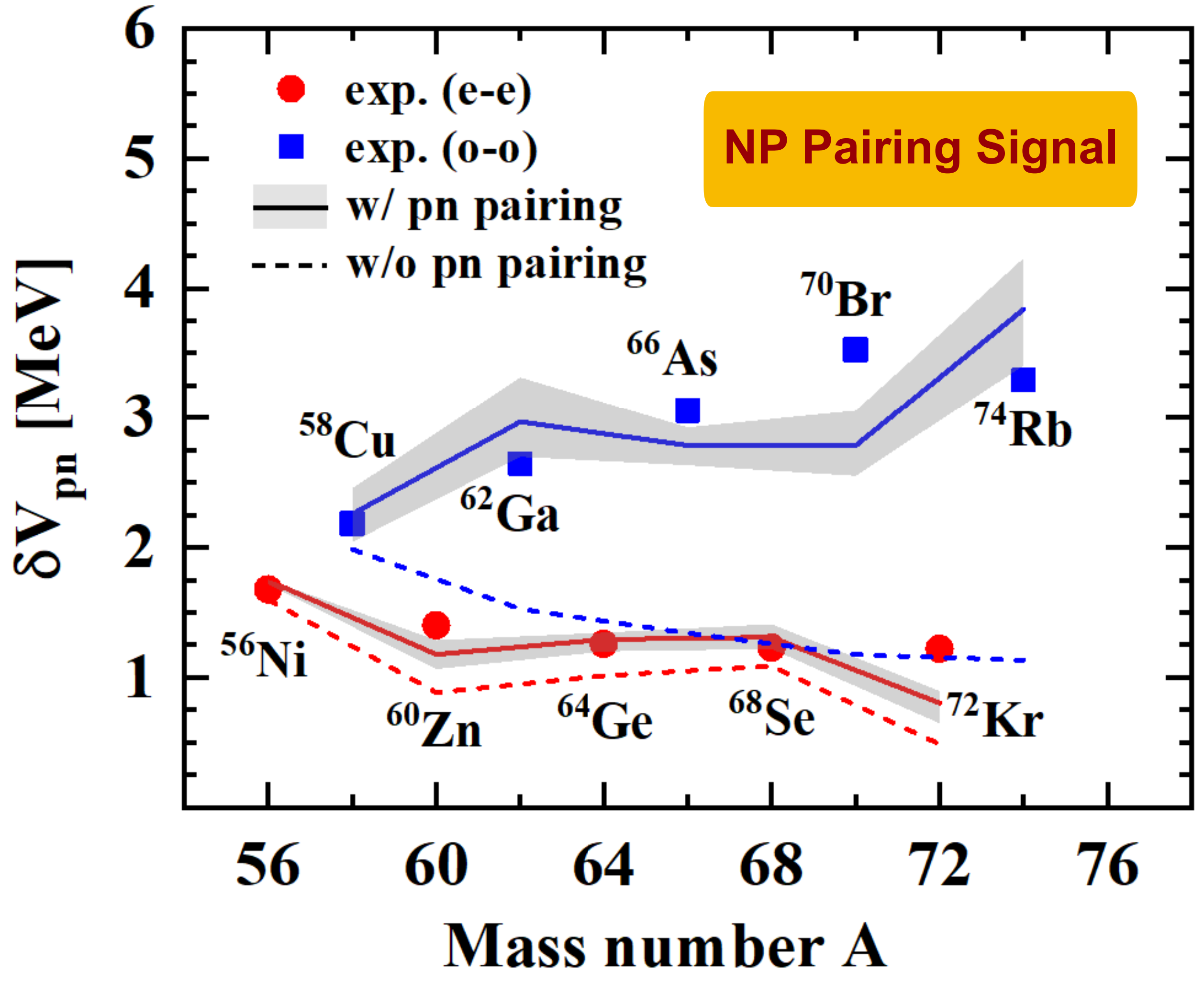
RDFT+SLAP: NN, PP, and NP pairing are treated simultaneously, microscopically, and self-consistently.

Wang, Wang, Xu, **PWZ**, Meng, PRL 132, 232501 (2024)

New mass measurement of upper fp-shell nuclei

This bifurcation in the double binding energy differences δV_{pn} cannot be reproduced by existing mass models.



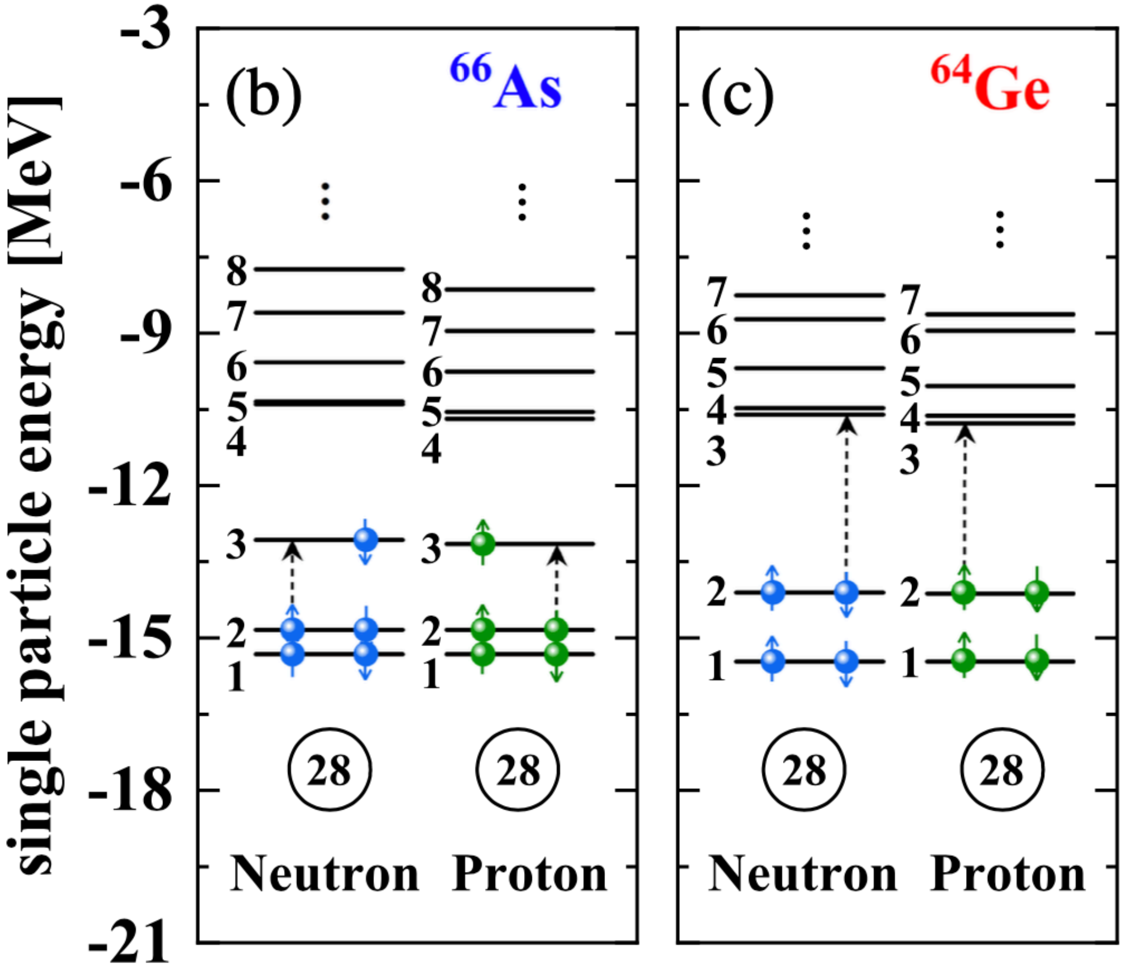


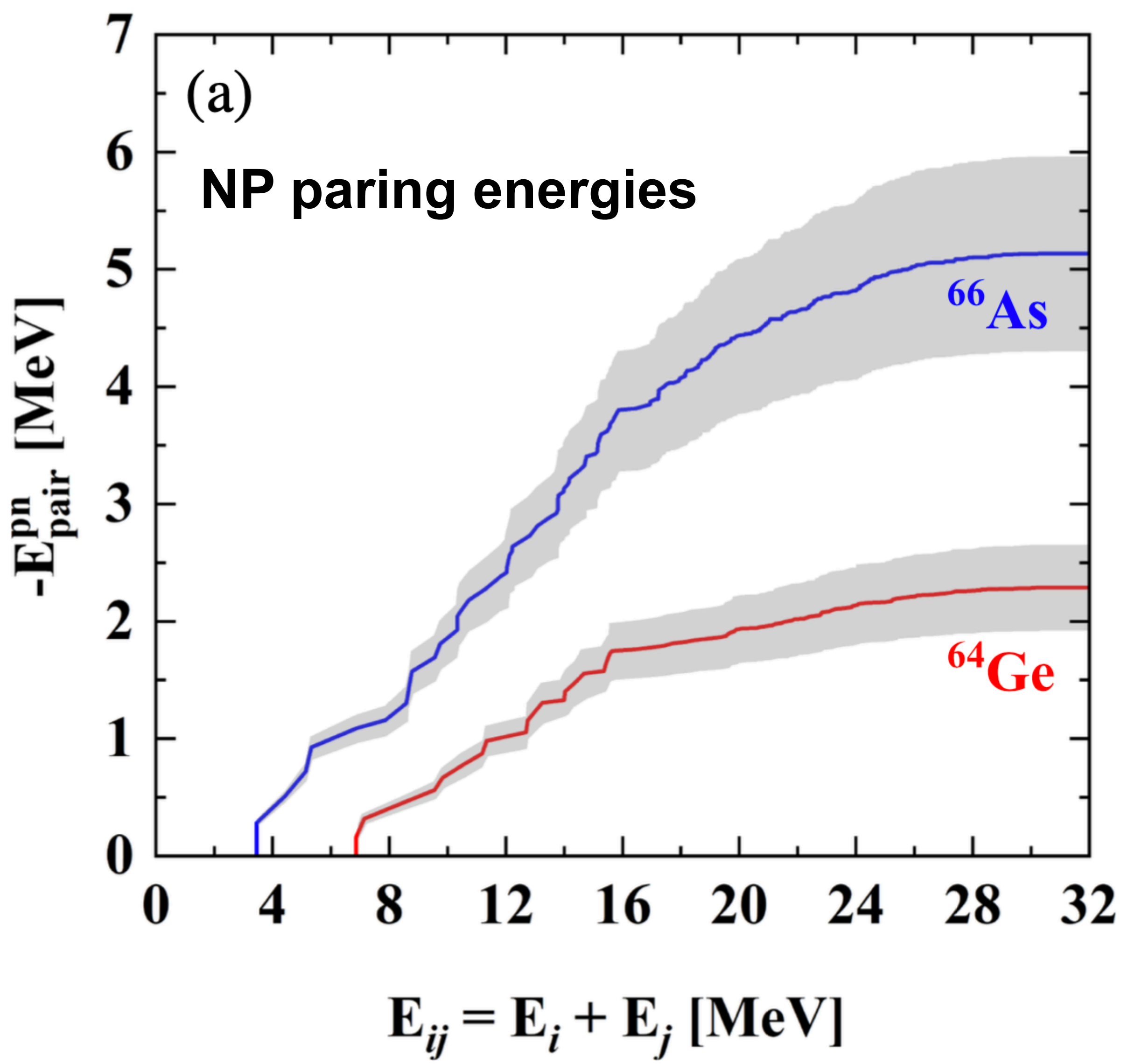
Exp: M. Wang et al., PRL 130, 192501 (2023)

Wang, Wang, Xu, **PWZ**, Meng, PRL 132, 232501 (2024)

NP pairing: odd-odd vs even-even

NP pairing is stronger in odd-odd nuclei than in the even-even ones.





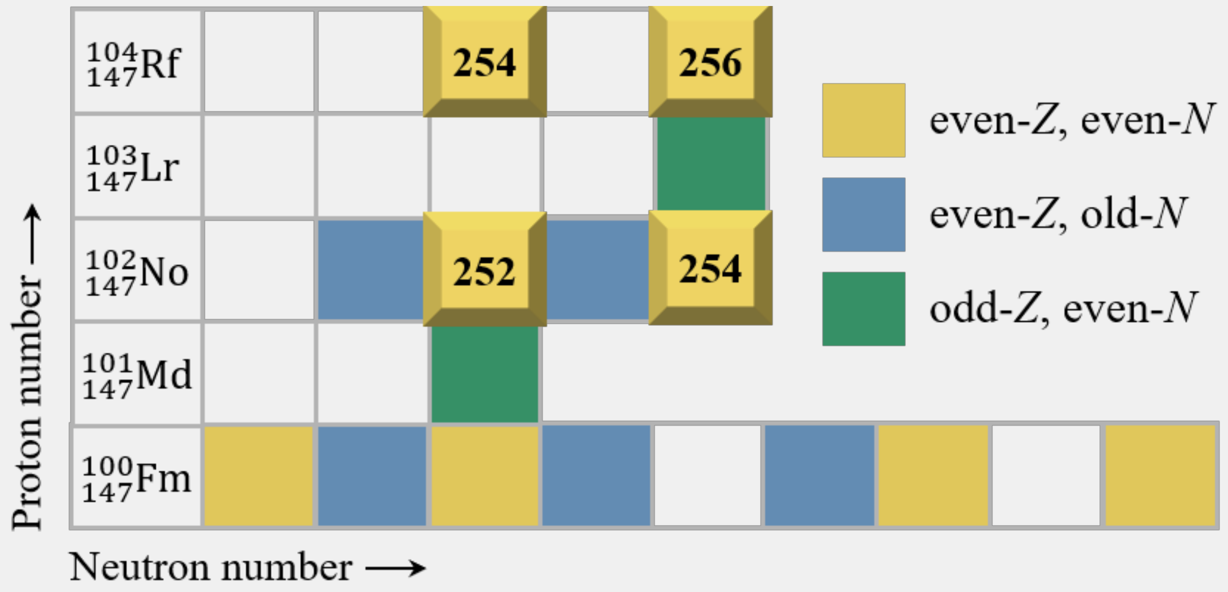
Wang, Wang, Xu, **PWZ**, Meng, PRL 132, 232501 (2024)

Transfermium nuclei

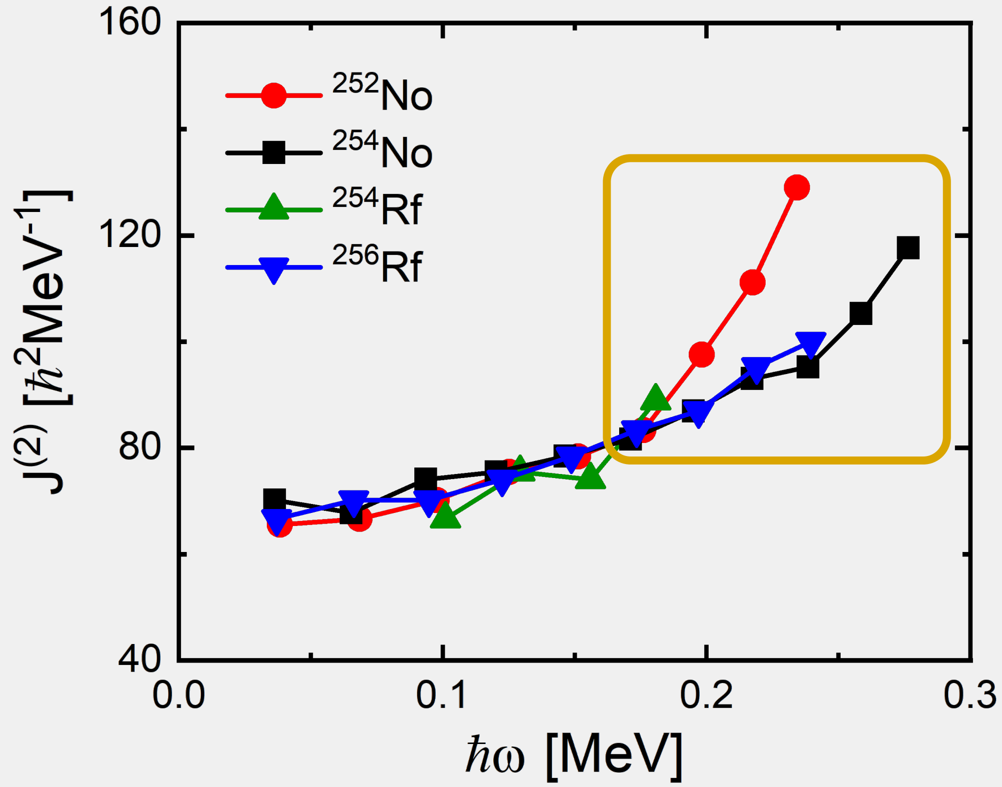
- **Transfermium nuclei** are the heaviest ones, whose rotational spectra have been measured experimentally; important for the location of the **"island of stability"**.

Herzberg, Greenlees, Prog. Part. Nucl. Phys. 61, 674 (2008); Ackermann, Theisen, Phys. Scr. 92, 083002 (2017)

ANL、FLNR、GANIL、GSI、JAEA、JYFL ...



PRL 82, 509 (1999) PRL 85, 1198 (2000) PRL 89, 202501 (2002)
PRL 95, 102502 (2005) PRL 95, 032501 (2005)
PRL 97, 082502 (2006) PRL 98, 132503 (2007)
PRL 102, 212501 (2009) PRL 109, 102501 (2012)
...



PRL 82, 509 (1999) PRL 109, 102501 (2012)
PRC 65, 014303 (2001) PRC 107, L061302 (2023)

The physical mechanism of the abnormal behavior in ^{252}No and ^{254}No?

Dynamic moments of inertia

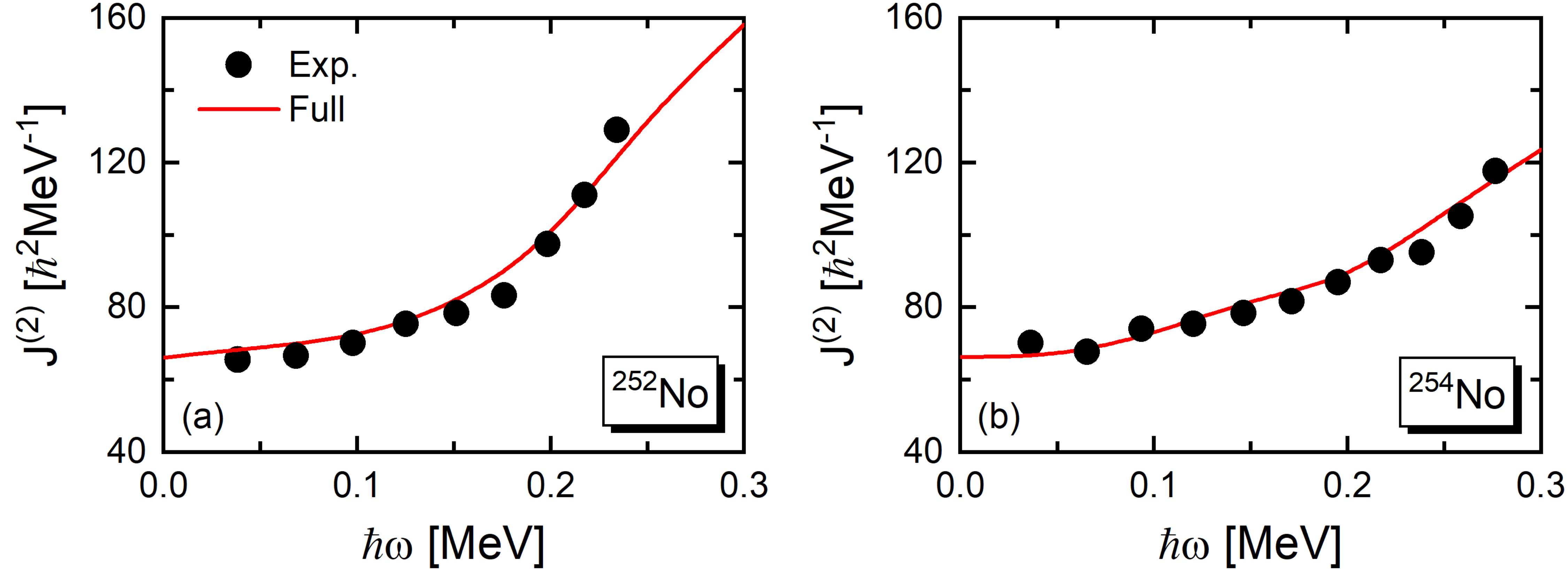
Cranking RDFT in 3D lattice with a shell-model-like approach (SLAP):

✓ self-consistent and microscopic description

✓ no adjustable parameter beyond a well-determined functional

✓ no spatial symmetry restriction

✓ pairing correlations is treated with particle number conservation



Xu, Wang, Wang, Ring, **PWZ**, PRL 133, 022501 (2024)

The experimental moments of inertia are well reproduced.

Outline

From **Mean-Field** to **Configuration-Interaction** Dynamics in DFT

- Motivation: limitations of mean-field approaches
- Pairing Correlations in Relativistic DFT: SLAP
- Beyond Mean Field: Relativistic CI-DFT (ReCD)
- Nuclear Dynamics: CI-TDDFT
- Summary

The ReCD Method

Relativistic **C**onfiguration-interaction **D**ensity functional theory (ReCD)

a theory combining the advantages from both Shell model and DFT

1. **Covariant Density Functional Theory**
   a minimum of the energy surface
2. **Configuration space**
   multi-quasiparticle states
3. **Angular momentum projection**
   rotational symmetry restoration
4. **Shell model calculation**
   configuration mixing / interaction from CDFT

Energy Density Functional

good angular momentum;
from low- to high- spin;

Nuclear Spectroscopy

PWZ, Ring, Meng, PRC 94 (2016) 041301(R)

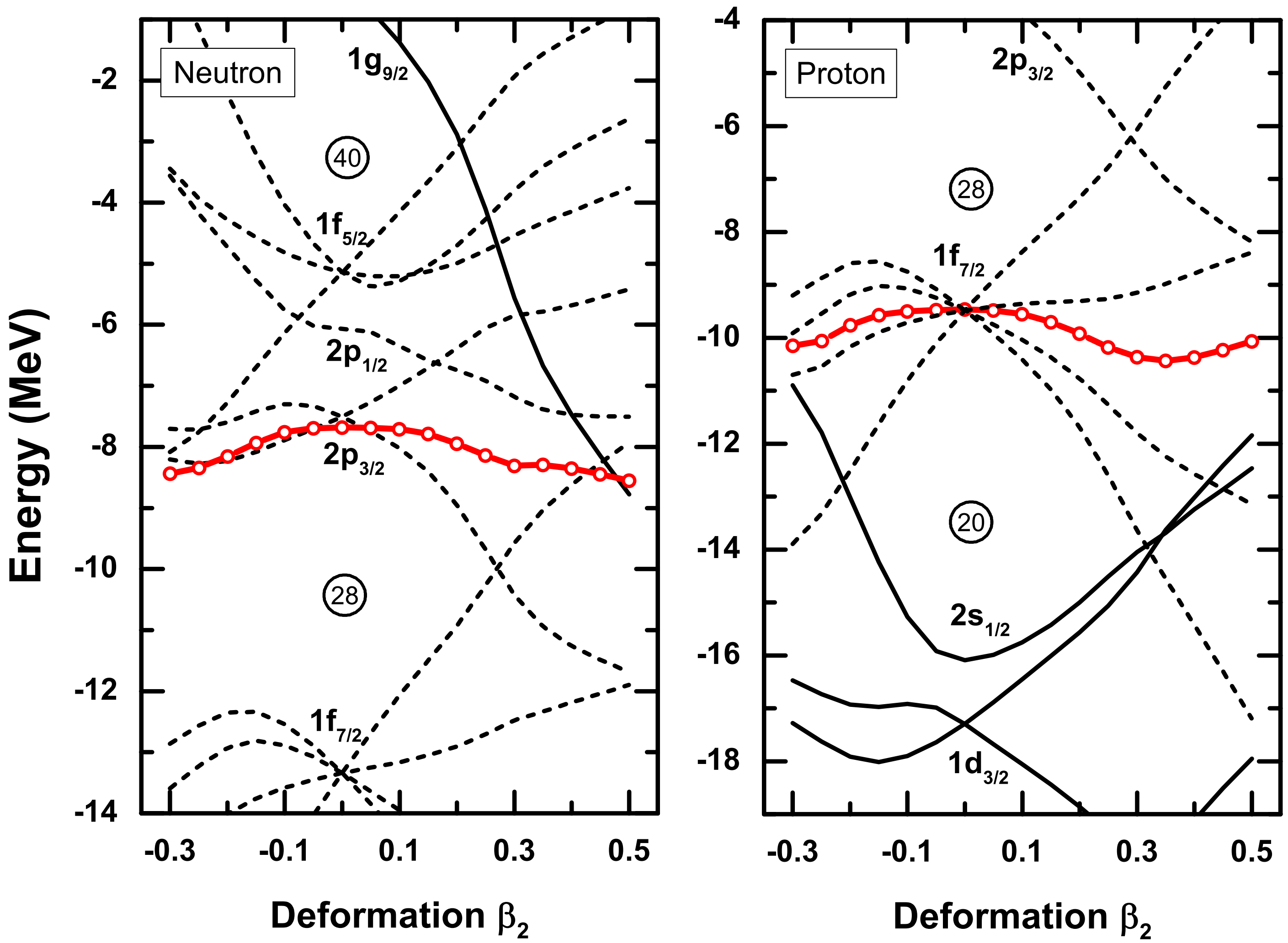
to provide a global study of nuclear structure and decay properties with no parameters beyond a well-established density functional.

First application for ^{54}Cr

PWZ, Ring, Meng, 94 (2016) 041301(R)

- Axial symmetry assumed
- Density functional:
  PC-PK1+ δ-force BCS
- Configuration space
  0-qp and 2-qp excitations &
  E < 6.5 MeV

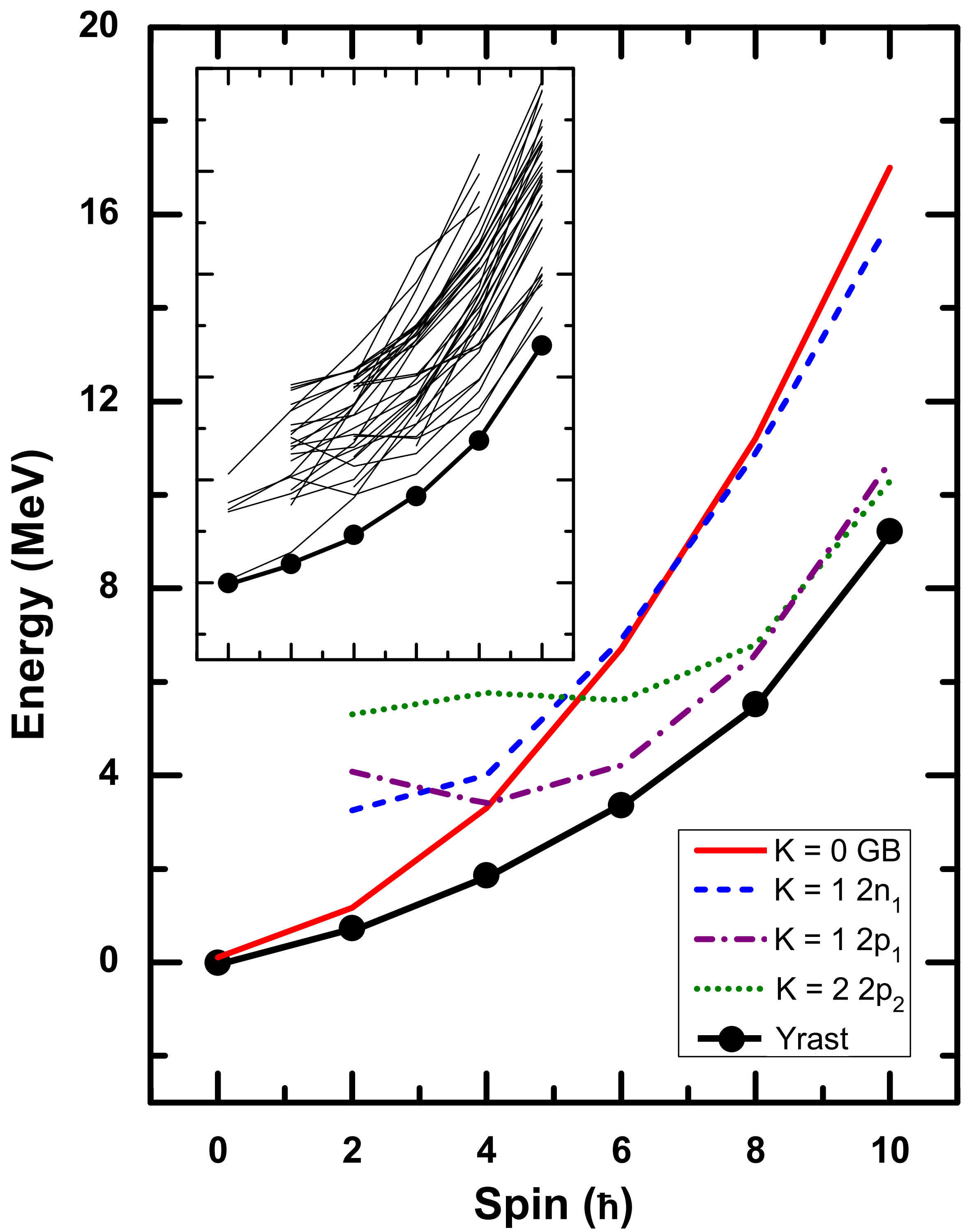
$$|0\rangle, \quad \alpha^\dagger_\nu \alpha^\dagger_{\nu'}|0\rangle, \quad \alpha^\dagger_\pi \alpha^\dagger_{\pi'}|0\rangle$$



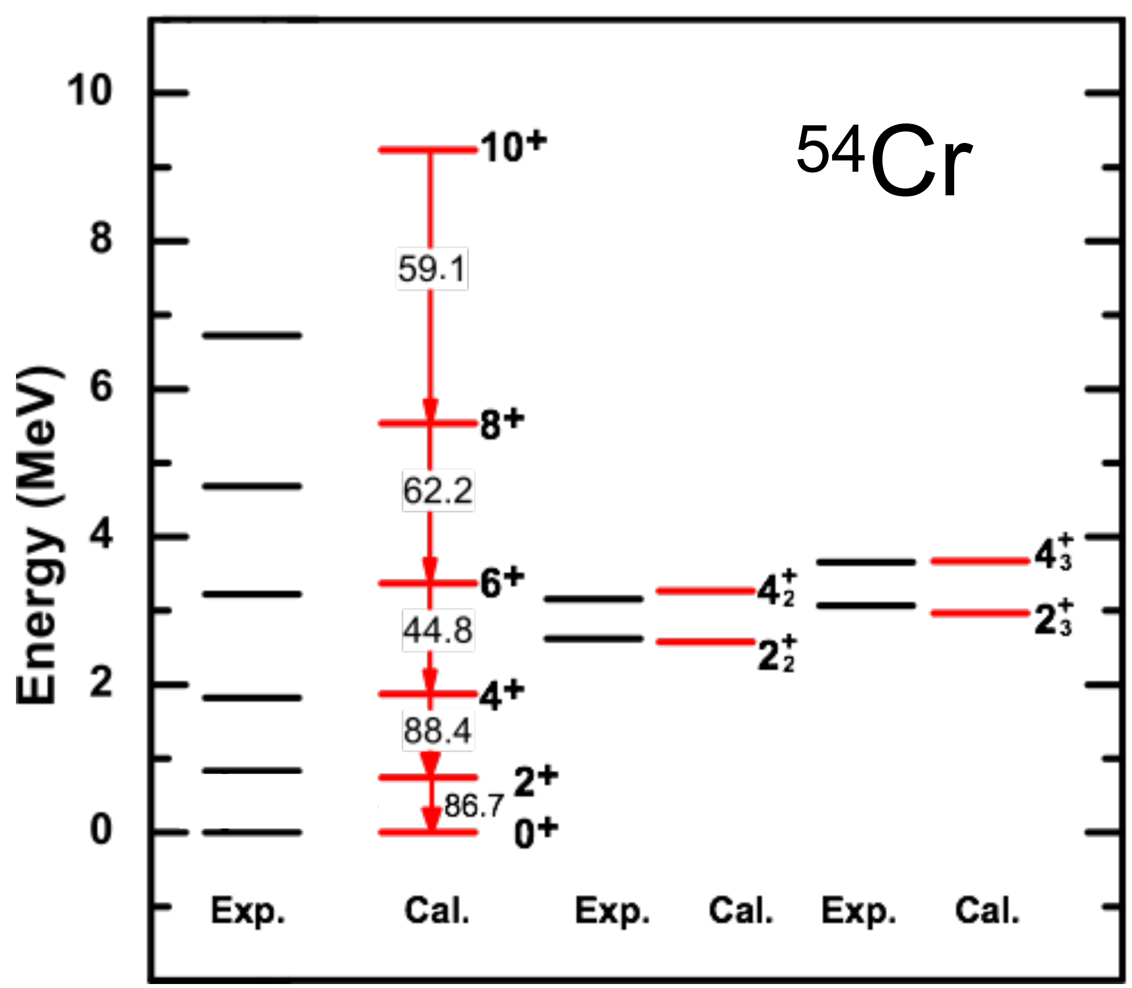
The configuration space consists of 37 states including 18 two-quasi-neutron, 18 two-quasi-proton excited states, and the quasi-particle vacuum $|0\rangle$.

First application: ^{54}Cr

PWZ, Ring, Meng, PRC 94 (2016) 041301(R)

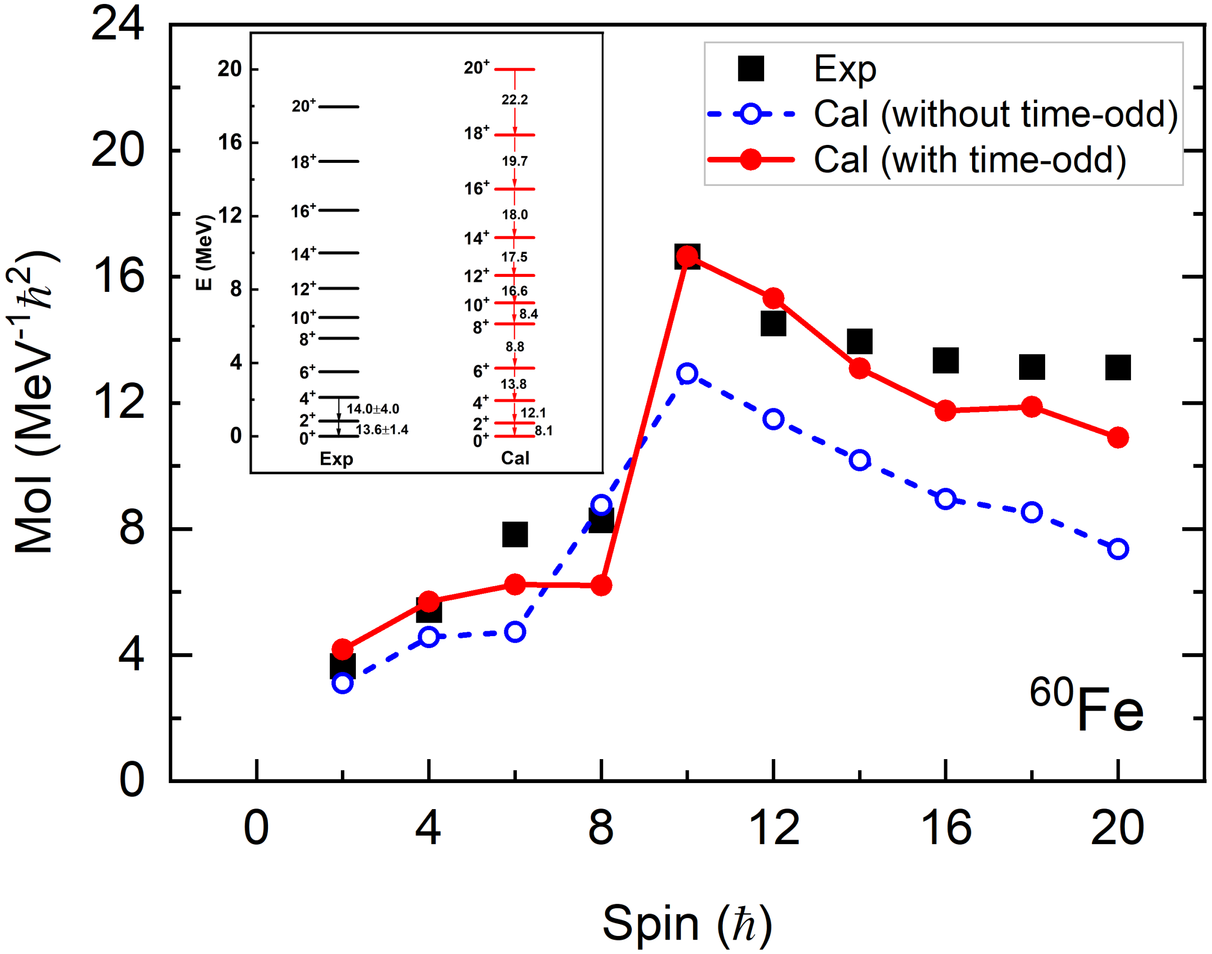


time-odd interaction;
beyond 2-qp configurations;



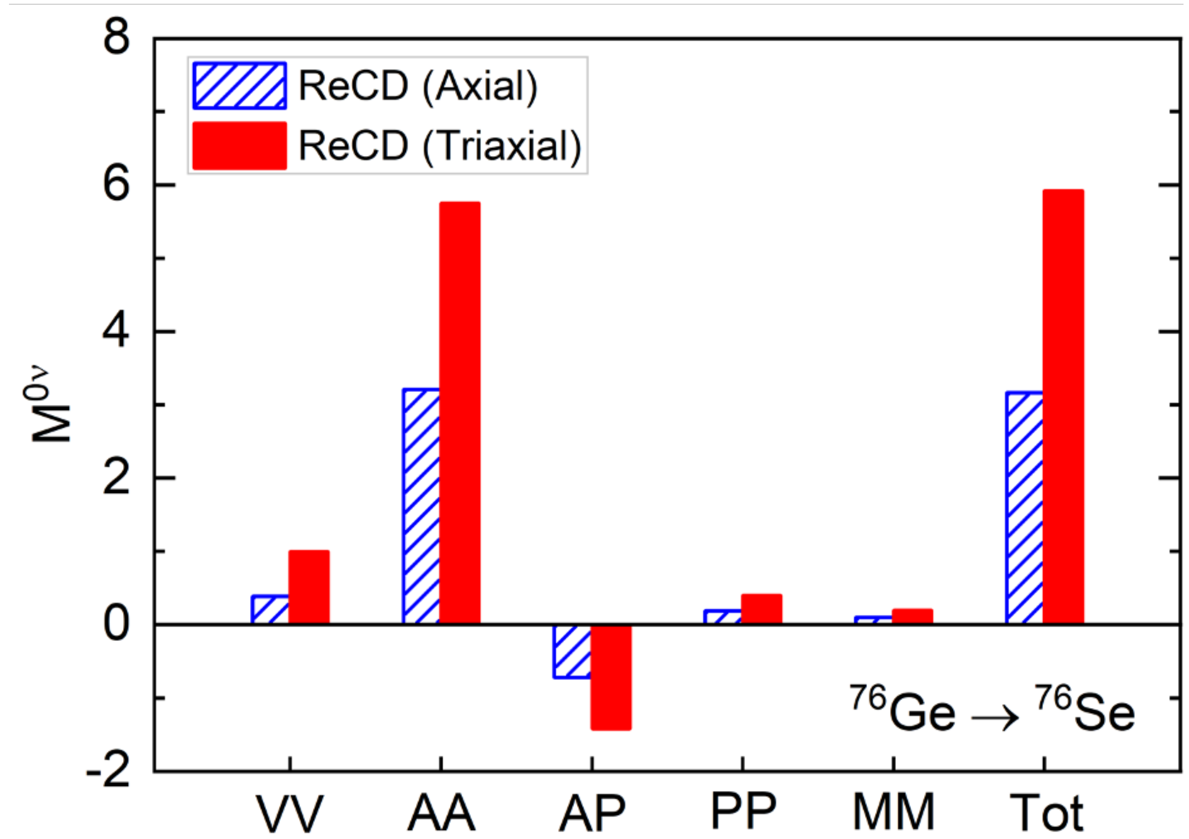
Applications of the ReCD method

Kinetic moment of inertia



Wang, PWZ, Meng, PRC 105 (2022) 054311

Neutrinoless double beta-decay



Wang, PWZ, Meng, Science Bulletin 59 (2024) 2017-2020

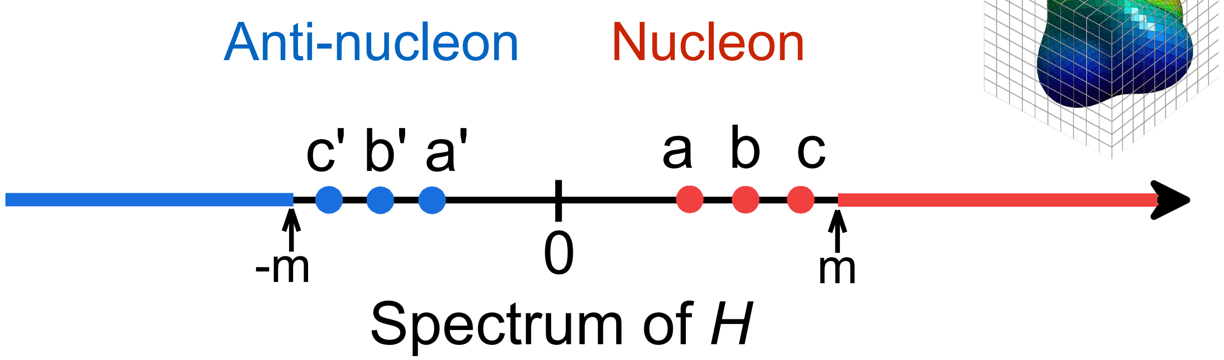
Outline

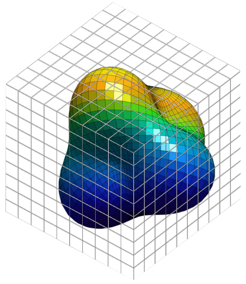
From **Mean-Field** to **Configuration-Interaction** Dynamics in DFT

- Motivation: limitations of mean-field approaches
- Pairing Correlations in Relativistic DFT: SLAP
- Beyond Mean Field: Relativistic CI-DFT (ReCD)
- Nuclear Dynamics: CI-TDDFT
- Summary

Lattice RDFT

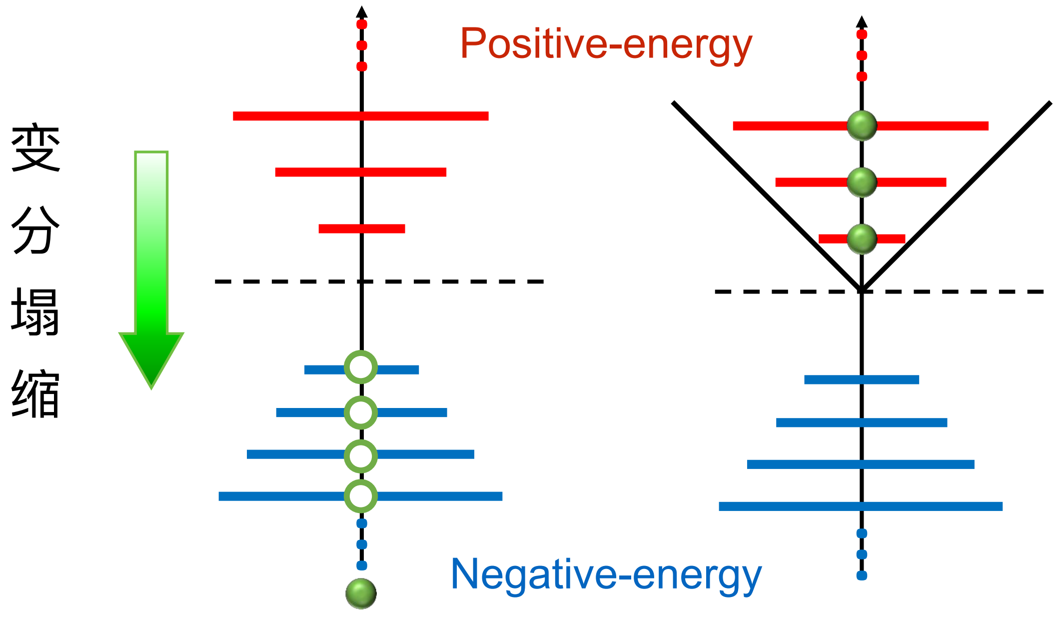
- ✓ No spatial symmetry restriction
- ✓ A long-term challenge due to
  - a) variational collapse problem
  - b) fermion doubling problem





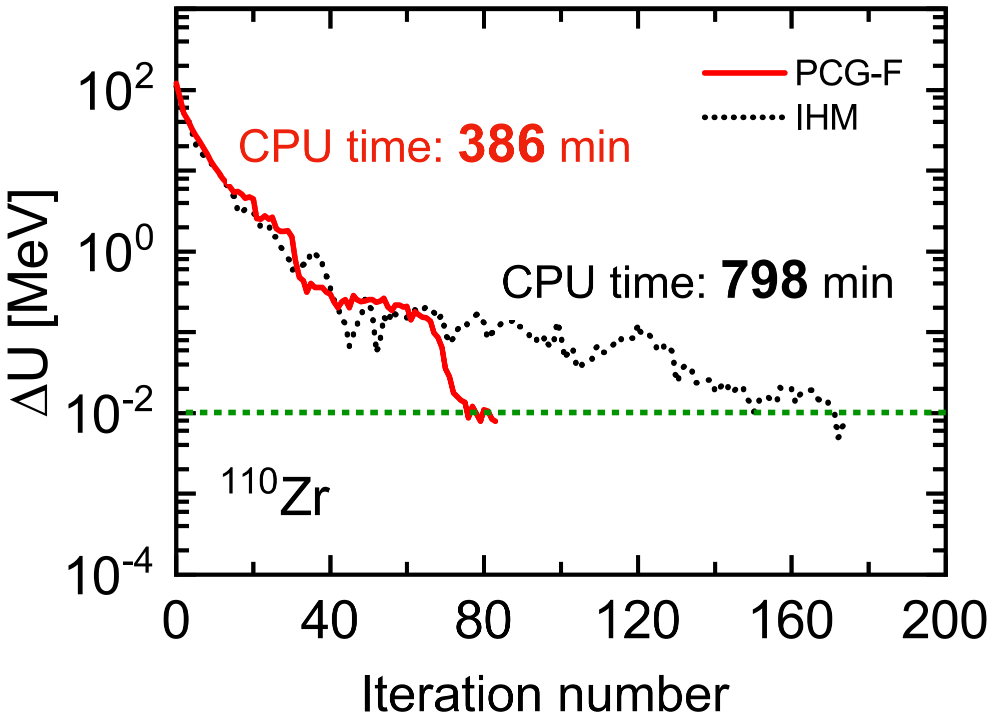
Hagino and Tanimura, PRC 82, 057301 (2010)

PCG-F Method



Li, Ren, **PWZ**, PRC 102, 044307 (2020)

PCG-F saves **~52%** of the CPU time



Xu, Li, Ren, **PWZ**, PRC 109, 014311 (2024)

Time-dependent RDFT

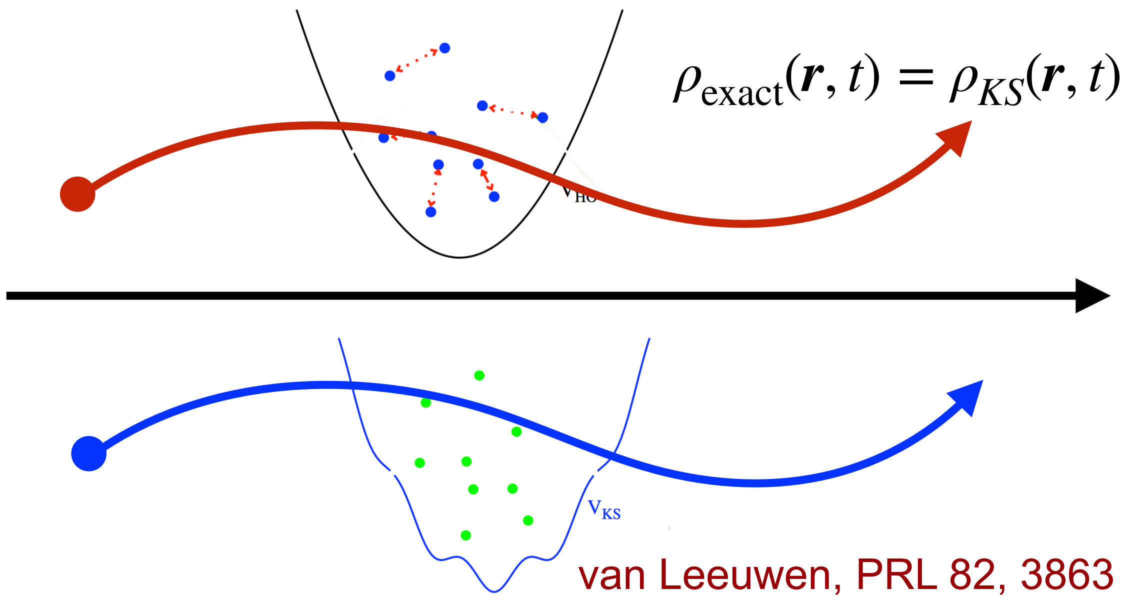
The many-body problem is mapped onto a one-body problem!

Runge-Gross Theorem

There is a unique mapping between the time dependent external potential and the density, for many body systems evolving from a given initial state.

Runge and Gross, PRL 52, 997 (1984)

Time-dependent Kohn-Sham DFT



van Leeuwen, PRL 82, 3863 (1999)

Ren, **PWZ**, Meng, PLB 801,135194 (2020)

$$i\partial_t \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} m + V + S & \boldsymbol{\sigma}\cdot\boldsymbol{p} - \boldsymbol{\sigma}\cdot\boldsymbol{V} \\ \boldsymbol{\sigma}\cdot\boldsymbol{p} - \boldsymbol{\sigma}\cdot\boldsymbol{V} & -m + V - S \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix}$$

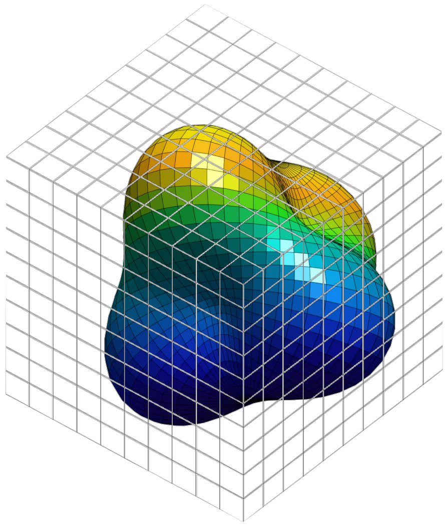
$$\rho(\boldsymbol{r},t) = \sum_i^N f_i^2 + g_i^2$$

$$V[\rho](\boldsymbol{r},t)$$

No memory effects !

Applications of the TD-RDFT

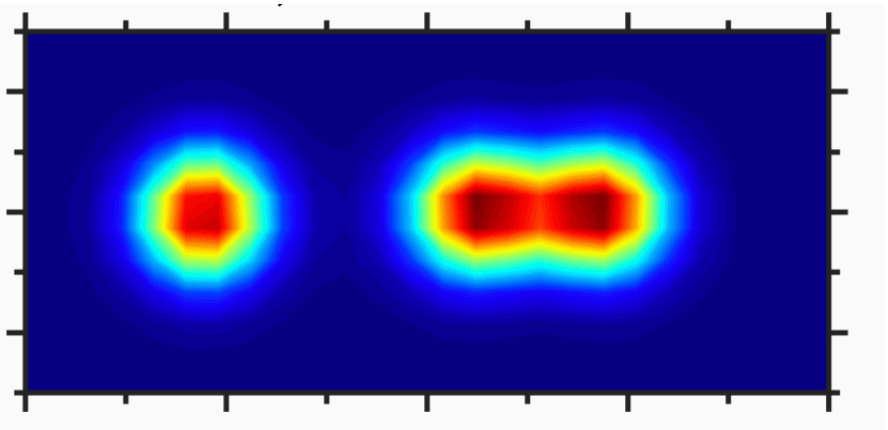
<u>3D Lattice: no spatial symmetry restriction</u>

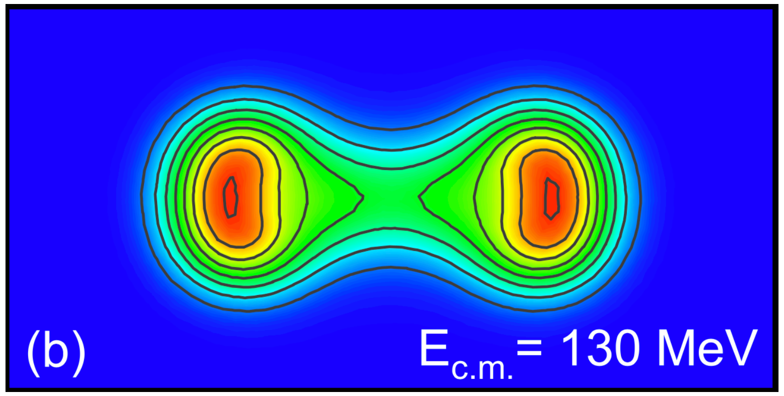


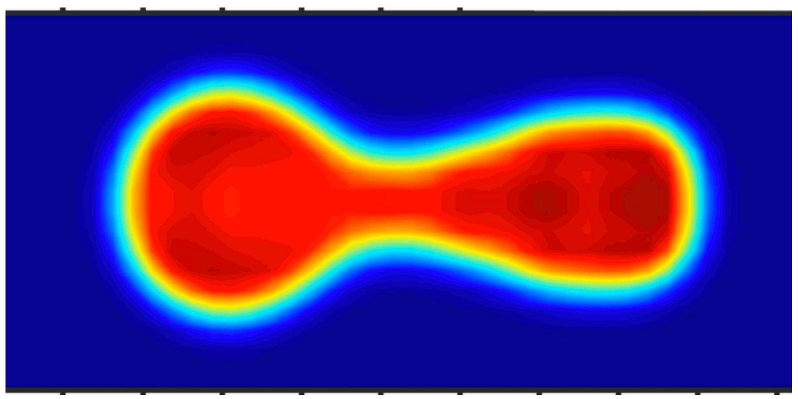
✓ Applications include:

Linear alpha-chain	PRL 115, 022501 (2015)	PLB 801,135194 (2020)	
Nuclear fission	PRL 128, 172501 (2022)	PRC 111, L051302 (2025) …	
Chiral dynamics	PRC 105, L011301 (2022)	PLB 856, 138877 (2024)	
Nuclear reaction	PRC 102, 044603 (2020)	PRC 109, 024614 (2024)	PRC 109, 024316 (2024) Editors' Suggestion

…

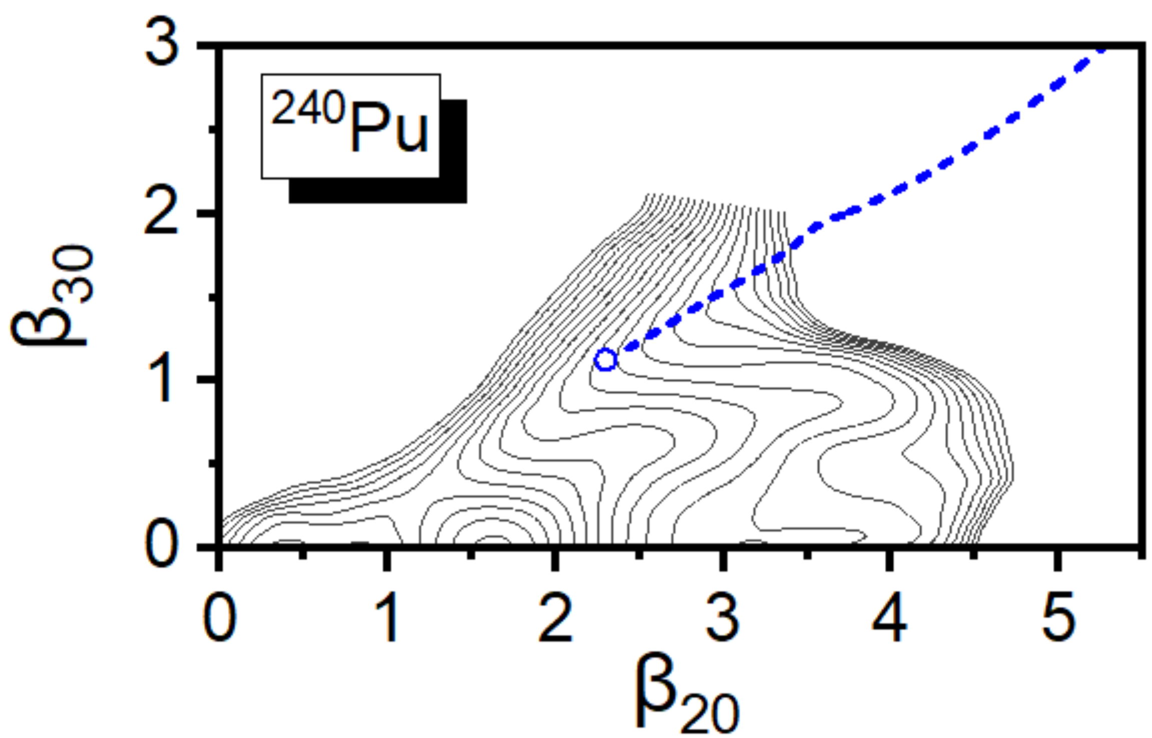


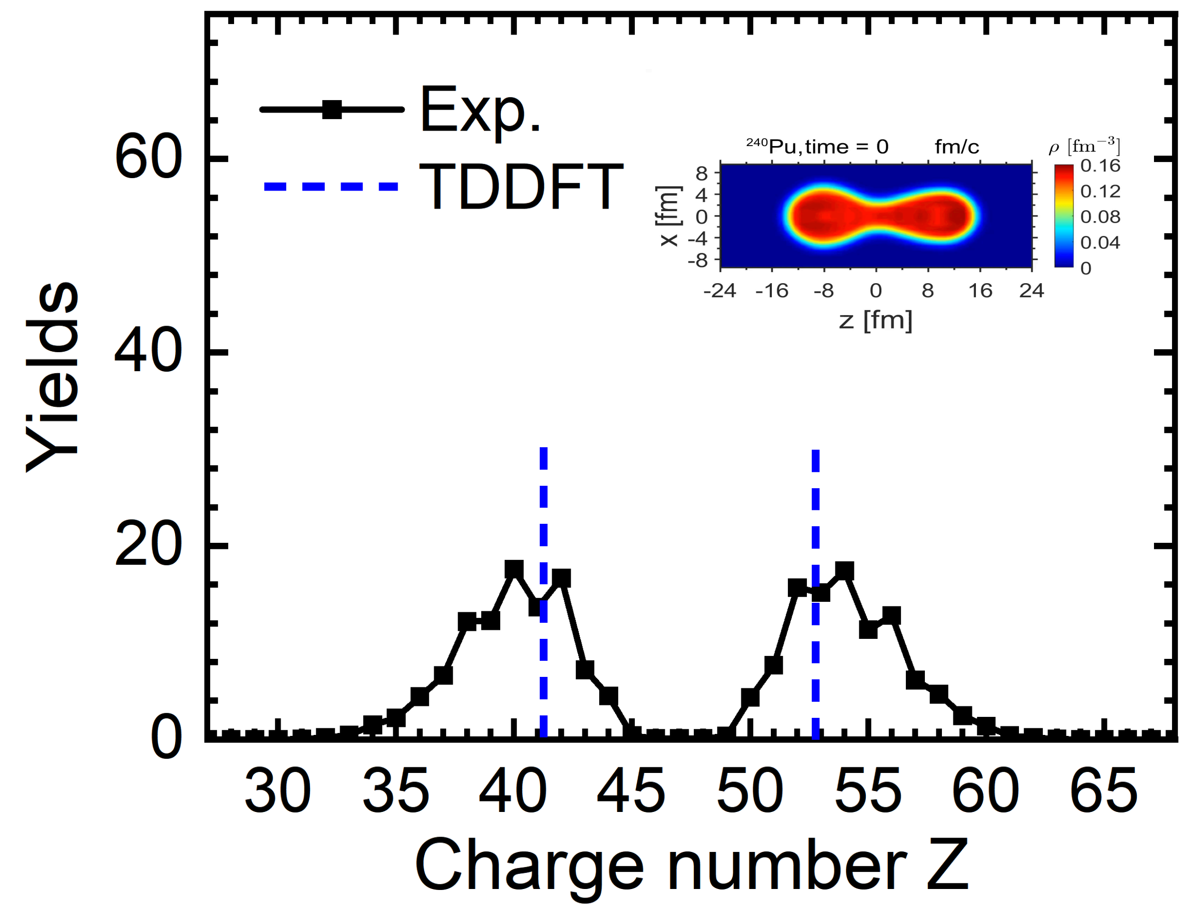




Limitations of TDDFT

- Due to its mean-field character, TDDFT has certain limitations:
  - ✓ For large-amplitude processes, TDDFT describes the classical evolution of independent nucleons; it lacks quantum fluctuations in collective space.





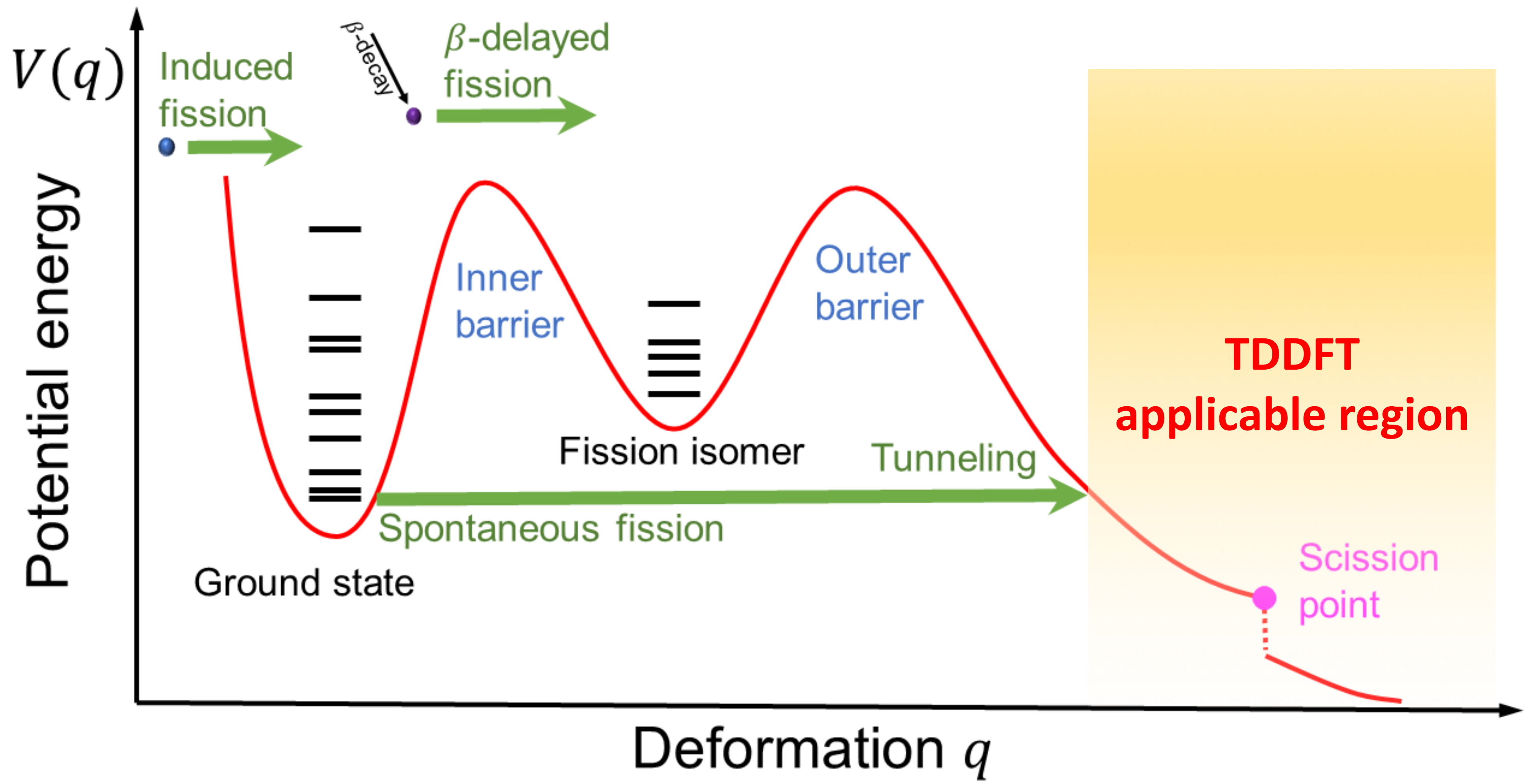
Z. X. Ren et al., PRC 105, 044313 (2022)

TDDFT cannot reproduce the widths of charge or mass distributions.

Limitations of TDDFT

- Due to its mean-field character, TDDFT has certain limitations:

  ✓ TDDFT does not consider quantum tunneling effects.



Schunck and Robledo, Prog. Part. Nucl. Phys. 79, 116301 (2016)

TDDFT cannot be applied in the classically forbidden region.

Beyond TDDFT methods

✓ Time-dependent density matrix (TDDM) theory and its extensions

Assié and Lacroix, PRL102, 202501 (2009)
Wen, Barton, Rios, Stevenson, PRC 98, 014603 (2018); Tohyama, FP 8, 67 (2020)

✓ Time-dependent random-phase approximation (TDRPA) method

Balian and Vénéroni, PRL 47, 1353 (1981)
Simenel, PRL 106, 112502 (2011); Williams et al. PRL 120, 022501 (2018)
Simenel, Godbey, and Umar, PRL 124, 212504 (2020)

✓ Stochastic time-dependent Hartree-Fock method

Ayik, PLB 658, 174 (2008); Lacroix and Ayik, EPJA 50, 95 (2014)
Tanimura, Lacroix, and Ayik, PRL 118, 152501 (2017)

✓ **Generalized time-dependent generator-coordinate method**

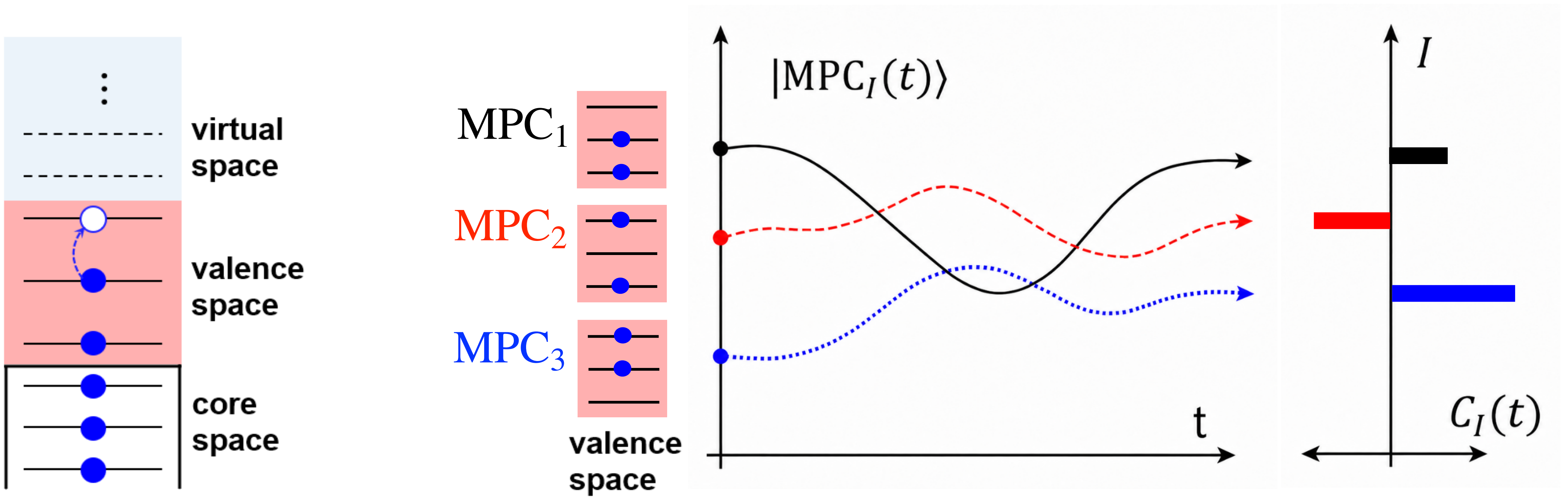
the wave function is expanded in terms of the **time-dependent generator states** initialized from deformation-constrained mean-field calculations

Li, Vretenar, Nikšić, **PWZ**, and Meng, PRC 108, 014321 (2023)
Li, Vretenar, Nikšić, Zhao, **PWZ**, Meng, FP 19, 44201 (2024) ; Li, Vretenar, Nikšić, **PWZ**, Meng, PRC 111, L051302 (2025)
Marević, Regnier, Lacroix, PRC 108, 014620 (2023); Marević, Regnier, Lacroix, EPJA 60, 10 (2024)

Configuration-interaction TDDFT

Wave function

$$|\Psi(t)\rangle = \sum_I C_I(t)|\mathrm{MPC}_I(t)\rangle$$



- ✓ a quantum framework to include beyond-mean-field correlations
- ✓ systematically improvable by increasing the number of MPCs
- ✓ strictly following the variational principle
- ✓ energy and particle-number conservation

Wang et al., in preparation

Equations of motion in CI-TDDFT

- Correlated wave function: $|\Psi(t)\rangle = \sum_I C_I(t)|\mathrm{MPC}_I(t)\rangle$
- Hamiltonian: $\hat{H} = \hat{H}_{\mathrm{DFT}} + \hat{H}_{\mathrm{pair}}$
- Action functional:

$$S\left[\{C_I\},\{\phi_{i,\tau}\},\{\mu_{ij}^{\tau}\}\right] = \int_{t=t_0}^{t_1} dt \left[\left\langle \Psi \middle| \left(\hat{H} - i\hbar\partial_t\right) \middle| \Psi \right\rangle - \sum_{\tau}\sum_{ij} \mu_{ij}^{\tau}\left(\langle\phi_{i,\tau}|\phi_{j,\tau}\rangle - \delta_{ij}\right)\right]$$

- Equations of motion in CI-TDDFT:

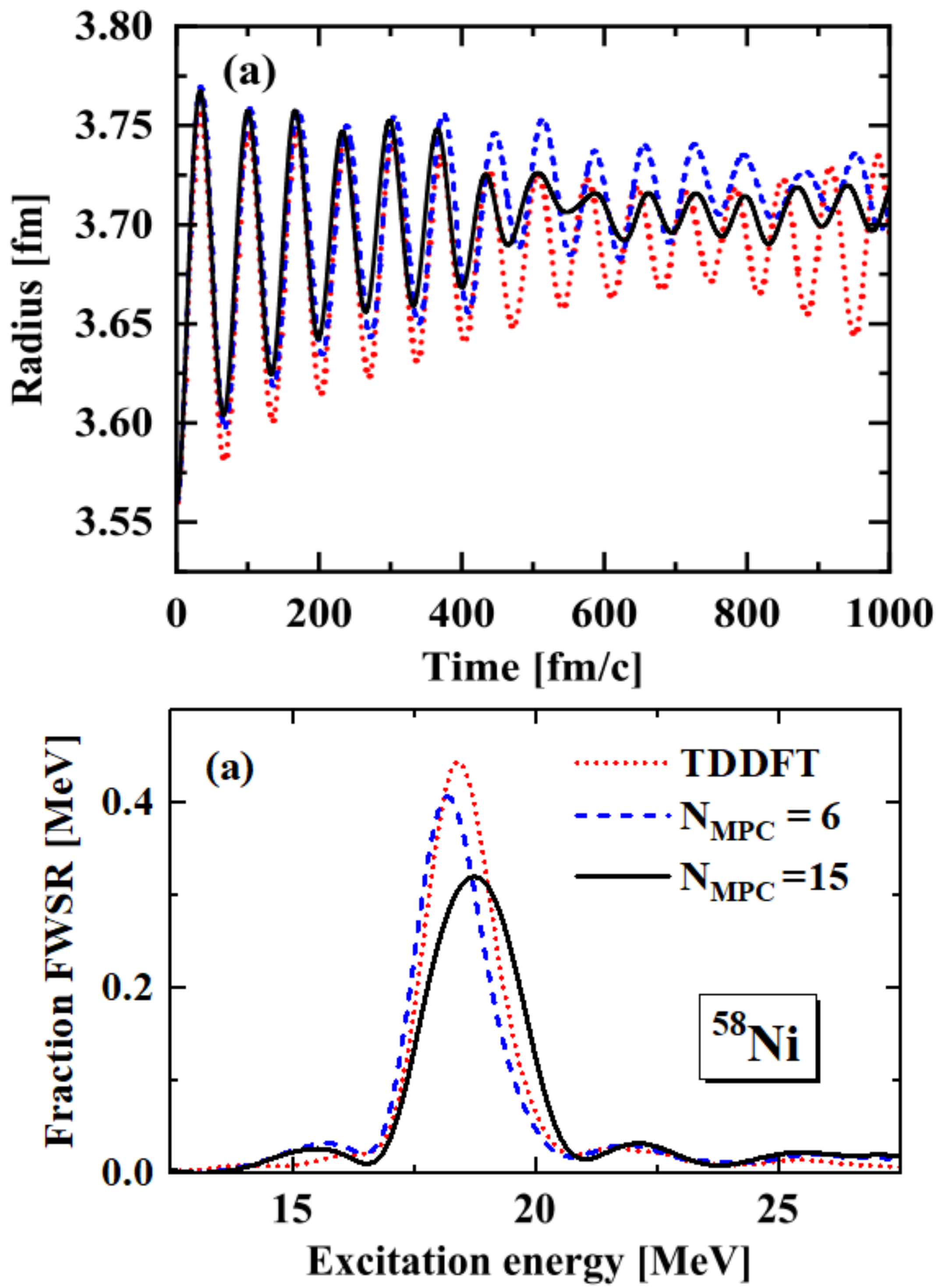
$$\frac{\delta S}{\delta C_J^*} = 0 \quad \Rightarrow \quad \mathrm{i}\hbar\dot{C}_J = \sum_I (\mathcal{H}_{JI} - \mathcal{H}_{JI}^{\mathrm{MF}}) C_I$$

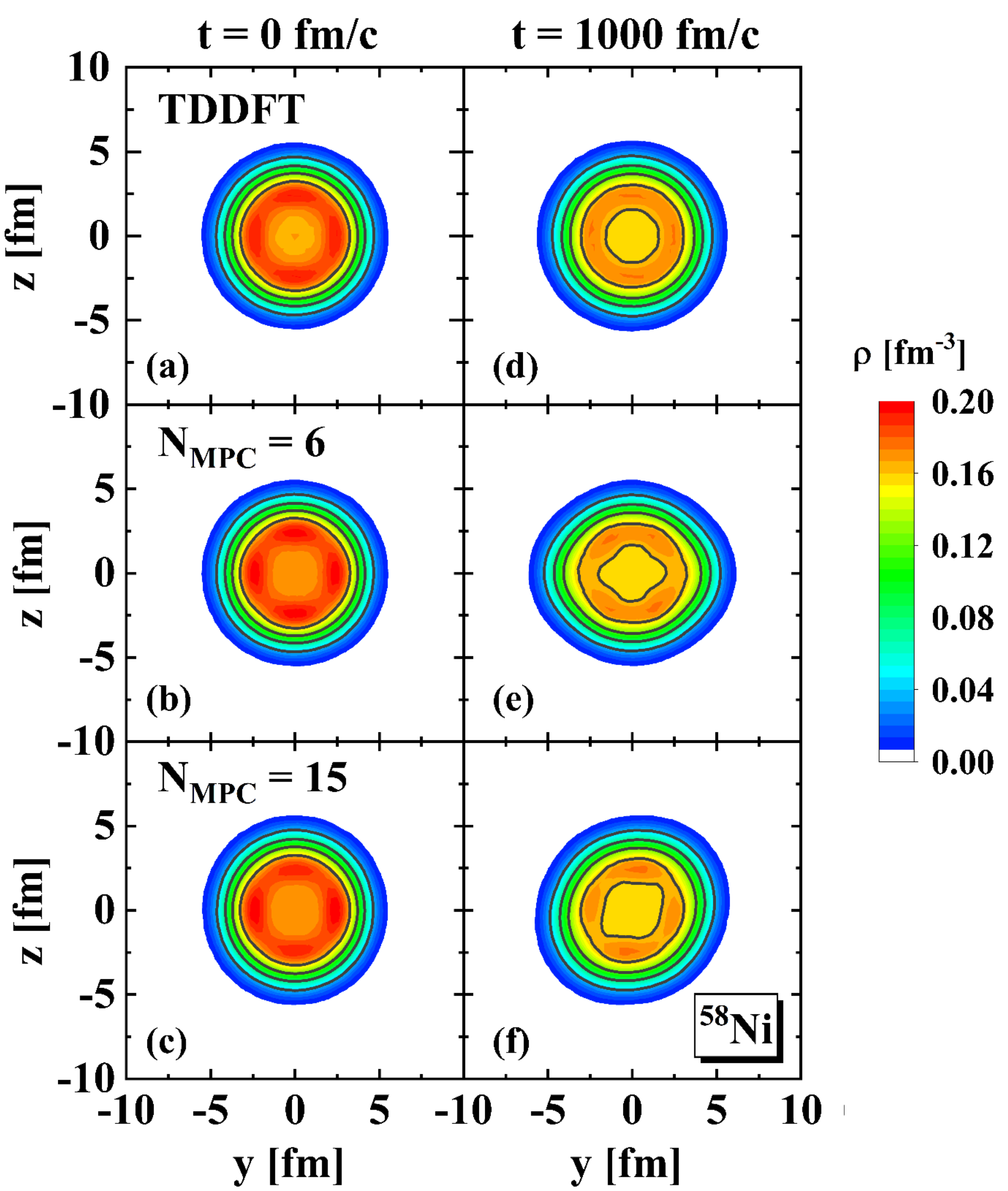
$$\frac{\delta S}{\langle\delta\phi_{i,\tau}|} = 0 \quad \Rightarrow$$

$$\mathrm{i}\hbar|\dot{\phi}_{p,\tau}\rangle = \hat{P}_\tau \left\{ \left(\hat{h} + \hat{W}_0\right)|\phi_{p,\tau}\rangle + \sum_{ijkl} (\rho_{pi}^{\tau})^{-1} \left[\sum_{\tau'} \rho_{ijkl}^{\tau\tau'} \hat{W}_{kl}^{\tau\tau'} |\phi_{j,\tau}\rangle + \kappa_{ijkl}^{\tau}\langle\phi_{j,\tau}|\tilde{Q}_{kl}^{\tau}\right]\right\}$$

Wang et al., in preparation

ISGMR strength distributions

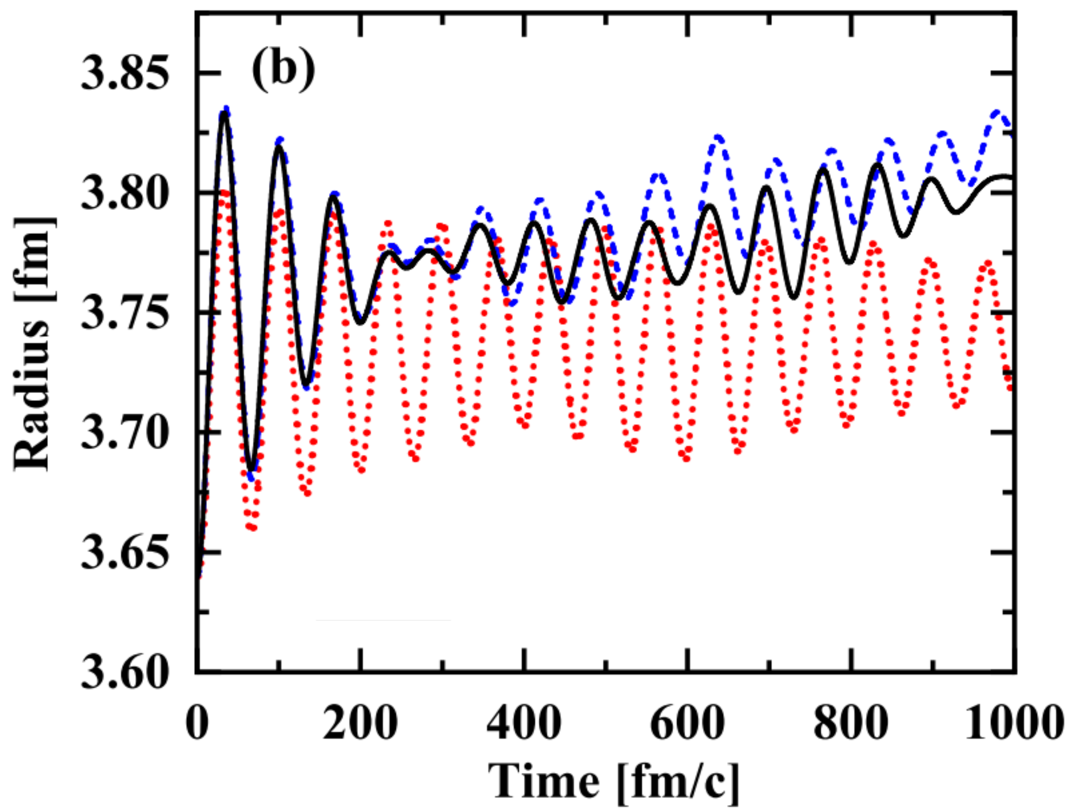


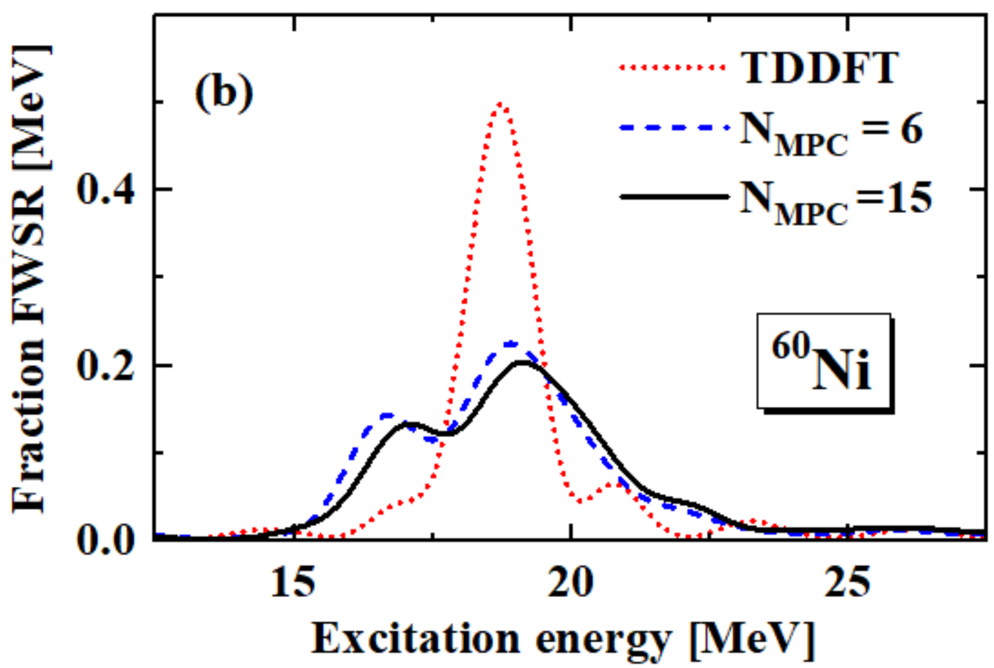


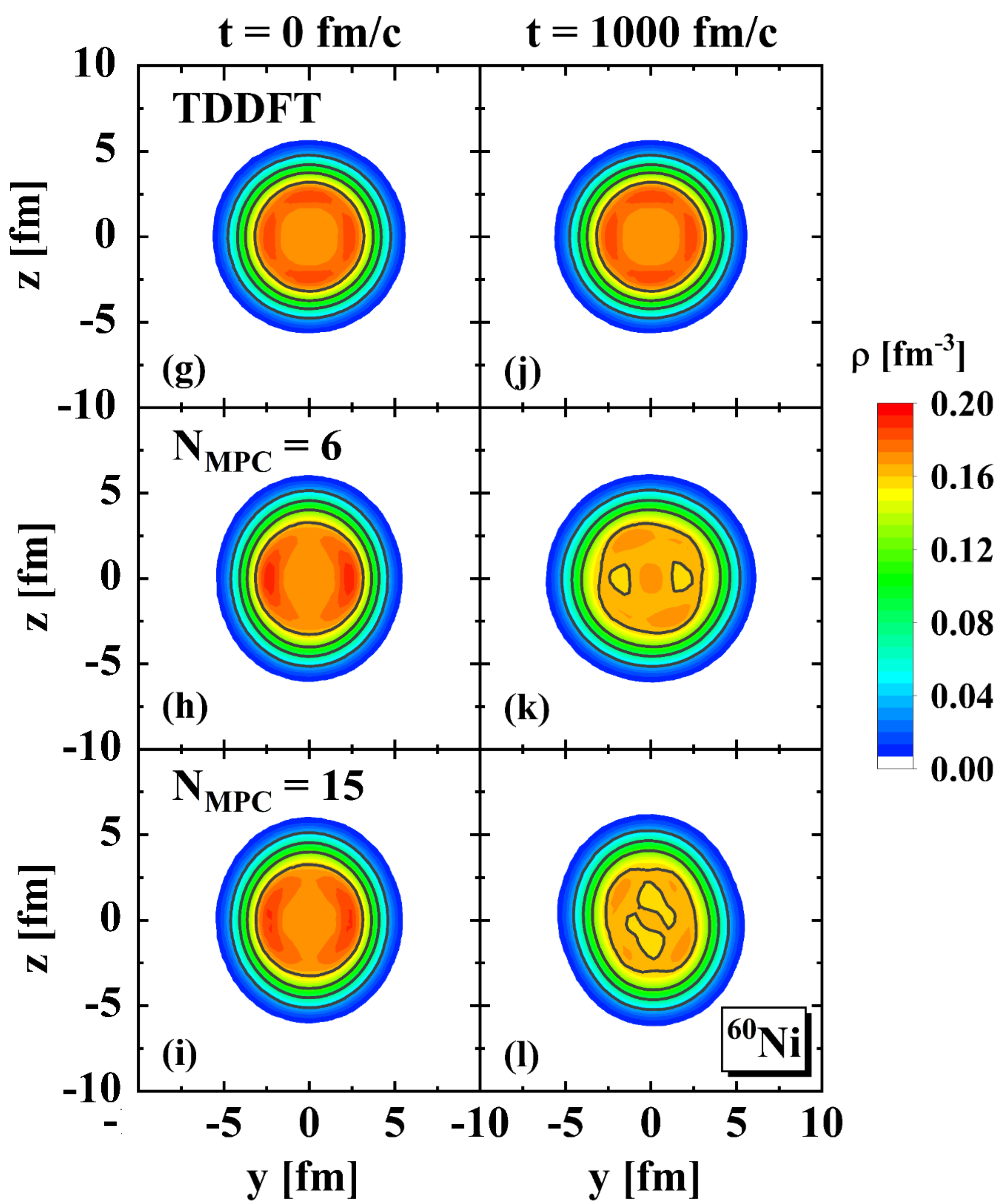
Wang et al., in preparation

CI-TDDFT produces broader strength distributions compared with TDDFT.

ISGMR strength distributions







Wang et al., in preparation

The effects of configuration mixing are more pronounced in ^{60}Ni.

Summary

CI-DFT models that combine **Configuration Interaction** with **Density Functional Theory** have been quite successful from nuclear structure to dynamics.

- Pairing correlations: RDFT+SLAP

  exact particle number conservation

  signal of proton-neutron pairing

  rotating transfermium nuclei

- Beyond the mean field: Relativistic CI-DFT (ReCD)

  merits of DFT and Shell Model preserved

  good performance for nuclear spectroscopic properties

- Nuclear dynamics: CI-TDDFT

  a quantum framework strictly following the variational principle

  broader strength distributions compared with TDDFT

- Future

  fission, fusion, multinucleon transfer process …


Thank you.