Towards the self-consistent and relativistic study of spin-isospin excitations in deformed nuclei

Haozhao LIANG（梁豪兆）

RIKEN Nishina Center, Japan

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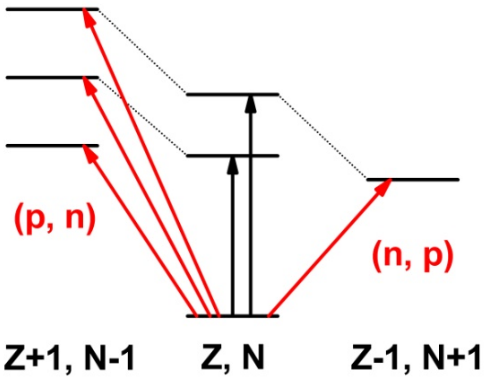
Contents

- Introduction
- Theoretical framework
- Spin-isospin resonances in spherical nuclei
- **Covariant DFT on 3D mesh**
  - ground-states calculations *with inverse Hamiltonian method*
  - excited-states calculations *with finite amplitude method*
- Summary and Perspectives

Nuclear spin-isospin physics

Nuclear spin-isospin excitations

- β-decays in nature
- charge-exchange reactions in lab



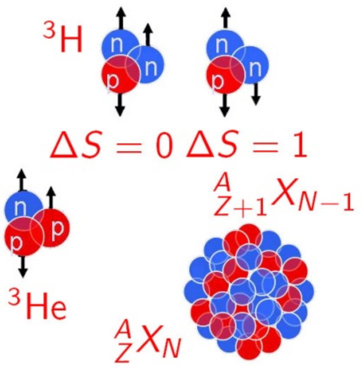
These excitations are important to understand

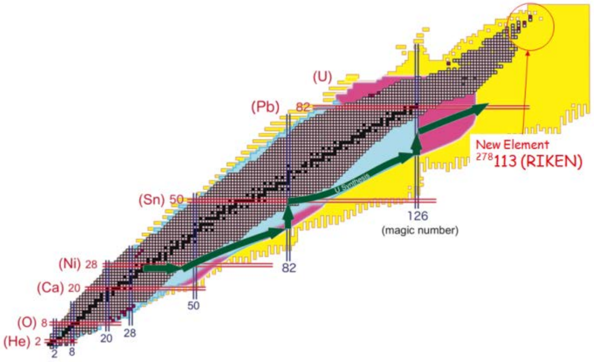
"What are the spin and isospin properties of nuclear force and nuclei?" *(nuclear physics)*

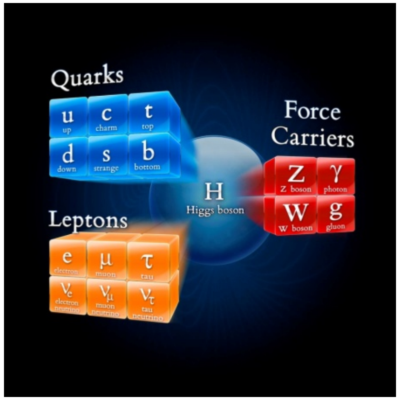
"Where and how does the rapid neutron-capture process (*r*-process) happen?" *(astrophysics)*

"Are there only three families of quarks in nature?" *(particle physics)*

Key exp. @
RIKEN
RCNP
CERN
GSI
MSU
TRIUMF
……



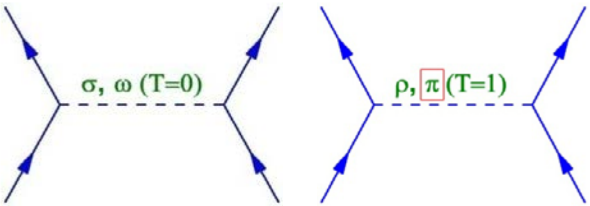




Covariant density functional theory

- Fundamental: **Kohn-Sham** Density Functional Theory
- Scheme: **Yukawa** meson-exchange nuclear interactions   talks by Khan, Meng, ...

$$\mathscr{L} = \bar{\psi}\left[i\gamma^{\mu}\partial_{\mu} - M - g_{\sigma}\sigma - \gamma^{\mu}\left(g_{\omega}\omega_{\mu} + g_{\rho}\vec{\tau}\cdot\vec{\rho}_{\mu} + e\frac{1-\tau_3}{2}A_{\mu}\right) - \frac{f_{\pi}}{m_{\pi}}\gamma_5\gamma^{\mu}\partial_{\mu}\vec{\pi}\cdot\vec{\tau}\right]\psi$$
$$+\frac{1}{2}\partial^{\mu}\sigma\partial_{\mu}\sigma - \frac{1}{2}m_{\sigma}^2\sigma^2 - \frac{1}{4}\Omega^{\mu\nu}\Omega_{\mu\nu} + \frac{1}{2}m_{\omega}^2\omega_{\mu}\omega^{\mu} - \frac{1}{4}\vec{R}_{\mu\nu}\cdot\vec{R}^{\mu\nu} + \frac{1}{2}m_{\rho}^2\vec{\rho}^{\mu}\cdot\vec{\rho}_{\mu}$$
$$+\frac{1}{2}\partial_{\mu}\vec{\pi}\cdot\partial^{\mu}\vec{\pi} - \frac{1}{2}m_{\pi}^2\vec{\pi}\cdot\vec{\pi} - \frac{1}{4}F^{\mu\nu}F_{\mu\nu}$$



Comparing to traditional non-relativistic DFT

- Effective Lagrangian
  connections to underlying theories, QCD at low energy
- Dirac equation   HZL, Meng, Zhou, *Phys. Rep.* **570**, 1-84 (2015)
  consistent treatment of **spin** d.o.f. & nuclear saturation properties (**3-body effect**)
- Lorentz covariant symmetry
  unification of time-even and **time-odd** components

Dirac and RPA equations

- **Energy functional** of the system (**Hartree** or **Hartree-Fock**)

$$E[\rho] = \langle \Phi_0 | \mathcal{H} | \Phi_0 \rangle = E_k + E_\sigma^D + E_\omega^D + E_\rho^D + E_A^D + E_\sigma^E + E_\omega^E + E_\rho^E + E_\pi^E + E_A^E$$

- **Dirac equations** for the ground-state properties

$$\int d\boldsymbol{r}' h(\boldsymbol{r}, \boldsymbol{r}') \psi(\boldsymbol{r}') = \varepsilon \psi(\boldsymbol{r}), \quad \text{with} \quad \begin{aligned} h^{\text{kin}}(\boldsymbol{r}, \boldsymbol{r}') &= [\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta M]\, \delta(\boldsymbol{r} - \boldsymbol{r}'), \\ h^{\text{D}}(\boldsymbol{r}, \boldsymbol{r}') &= [\Sigma_T(\boldsymbol{r})\gamma_5 + \Sigma_0(\boldsymbol{r}) + \beta \Sigma_S(\boldsymbol{r})]\, \delta(\boldsymbol{r} - \boldsymbol{r}'), \\ h^{\text{E}}(\boldsymbol{r}, \boldsymbol{r}') &= \begin{pmatrix} Y_G(\boldsymbol{r}, \boldsymbol{r}') & Y_F(\boldsymbol{r}, \boldsymbol{r}') \\ X_G(\boldsymbol{r}, \boldsymbol{r}') & X_F(\boldsymbol{r}, \boldsymbol{r}') \end{pmatrix}. \end{aligned}$$

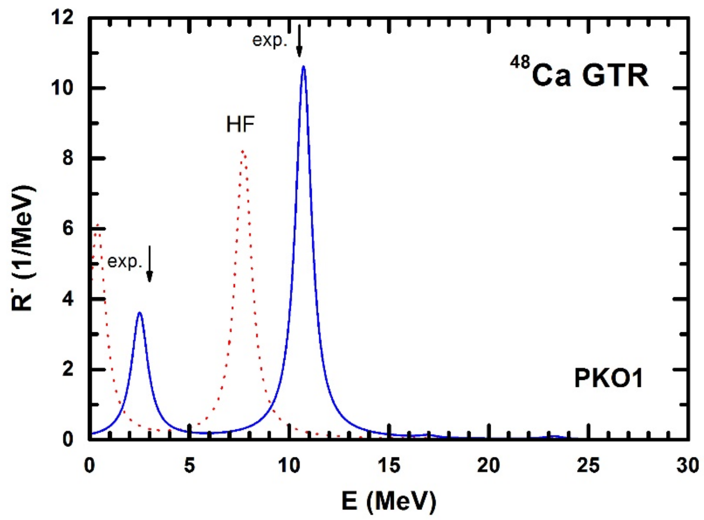
- **RPA equations** for the vibrational excitation properties

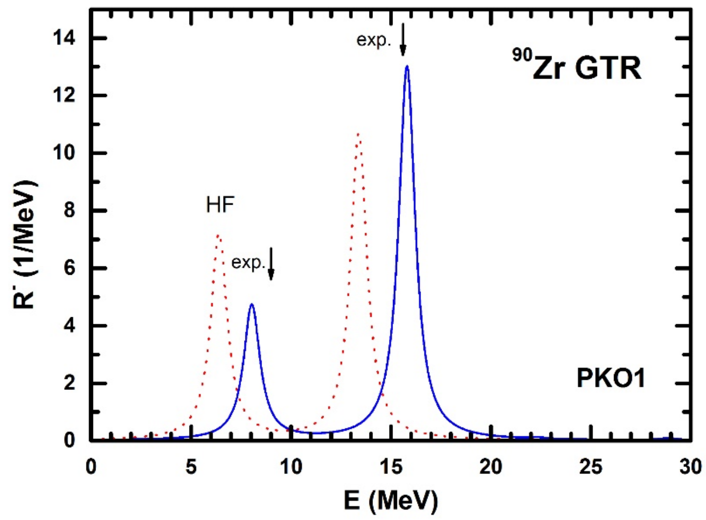
$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B} & -\mathcal{A} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega_\nu \begin{pmatrix} X \\ Y \end{pmatrix}$$

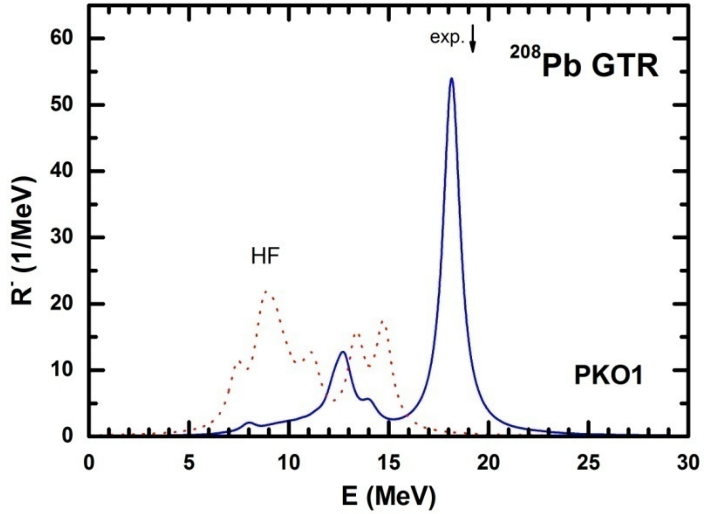
- ***δE/δρ*** → equation of motion for nucleons: Dirac (-Bogoliubov) equations
- ***δ²E/δρ²*** → linear response equation: (Q)RPA equations

Gamow-Teller resonances

CDFT+RPA for Gamow-Teller resonances (with both Hartree & Fock terms)





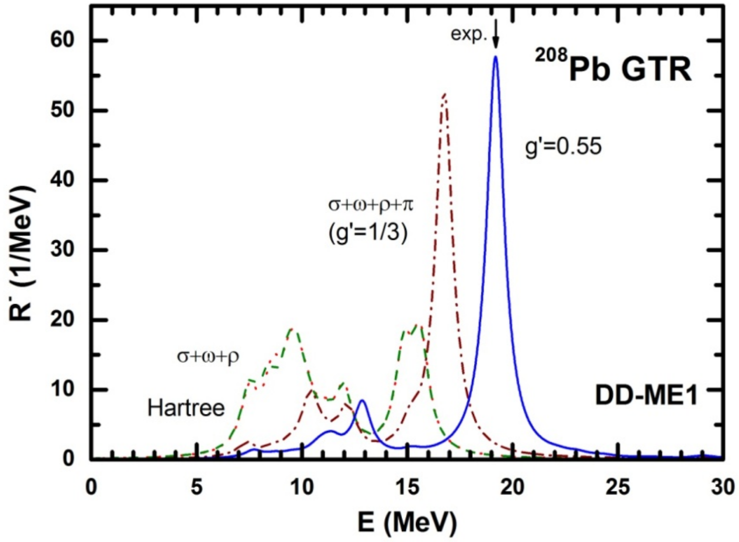


cf. Skyrme interaction **SAMi**
by Roca-Maza, Colo, Sagawa

- ✓ GTR excitation energies can be reproduced in a fully self-consistent way.

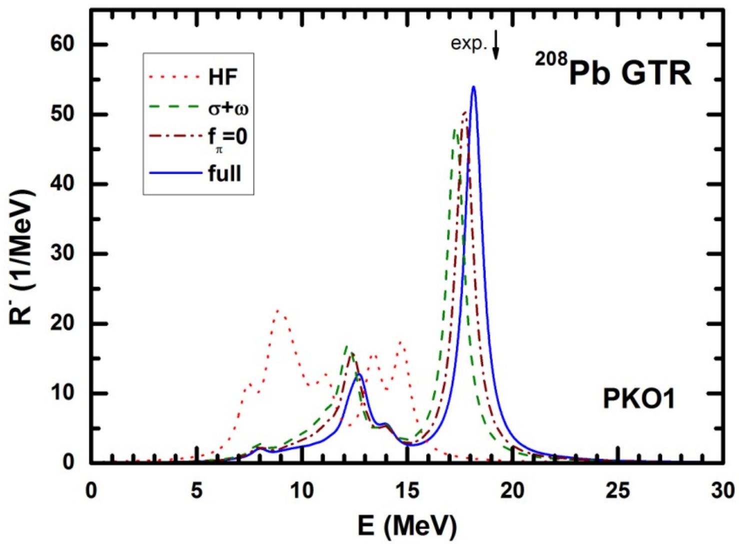
HZL, Giai, Meng, *Phys. Rev. Lett.* **101**, 122502 (2008)

Physical mechanisms of GTR



With only Hartree terms

- No contribution from isoscalar σ and ω mesons, because exchange terms are missing.
- π-meson is dominant in this resonance.
- g' has to be retted to reproduce the experimental data.



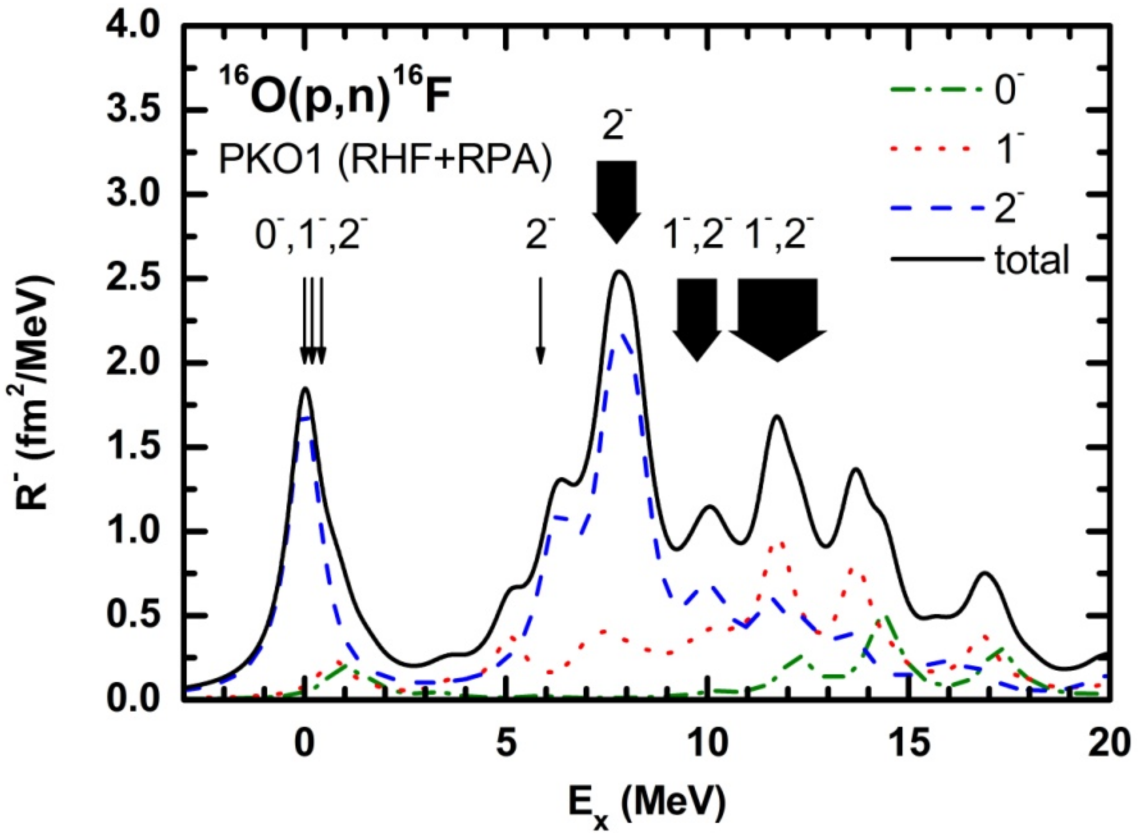
With both Hartree & Fock terms

- Isoscalar σ and ω mesons play an essential role via the exchange terms.
- π-meson plays a minor role.
- $g' = 1/3$ is kept for self-consistency.

HZL, Giai, Meng, *Phys. Rev. Lett.* **101**, 122502 (2008)
HZL, Zhao, Ring, Roca-Maza, Meng, *Phys. Rev. C* **86**, 021302(R) (2012)

Spin-dipole resonances

CDFT+RPA for Spin-dipole resonances ($\Delta S = 1$, $\Delta L = 1$, $J^{\pi} = 0^-, 1^-, 2^-$)



$E_x(0^-) \sim$ **15 MeV**
with Fock term

$E_x(0^-) \sim$ **11 MeV**
w/o Fock term

(Exp.) Wakasa *et al.*, PRC 84, 014614 (2011); (Theory) HZL, Zhao, Meng, *Phys. Rev. C* **85**, 064302 (2012)

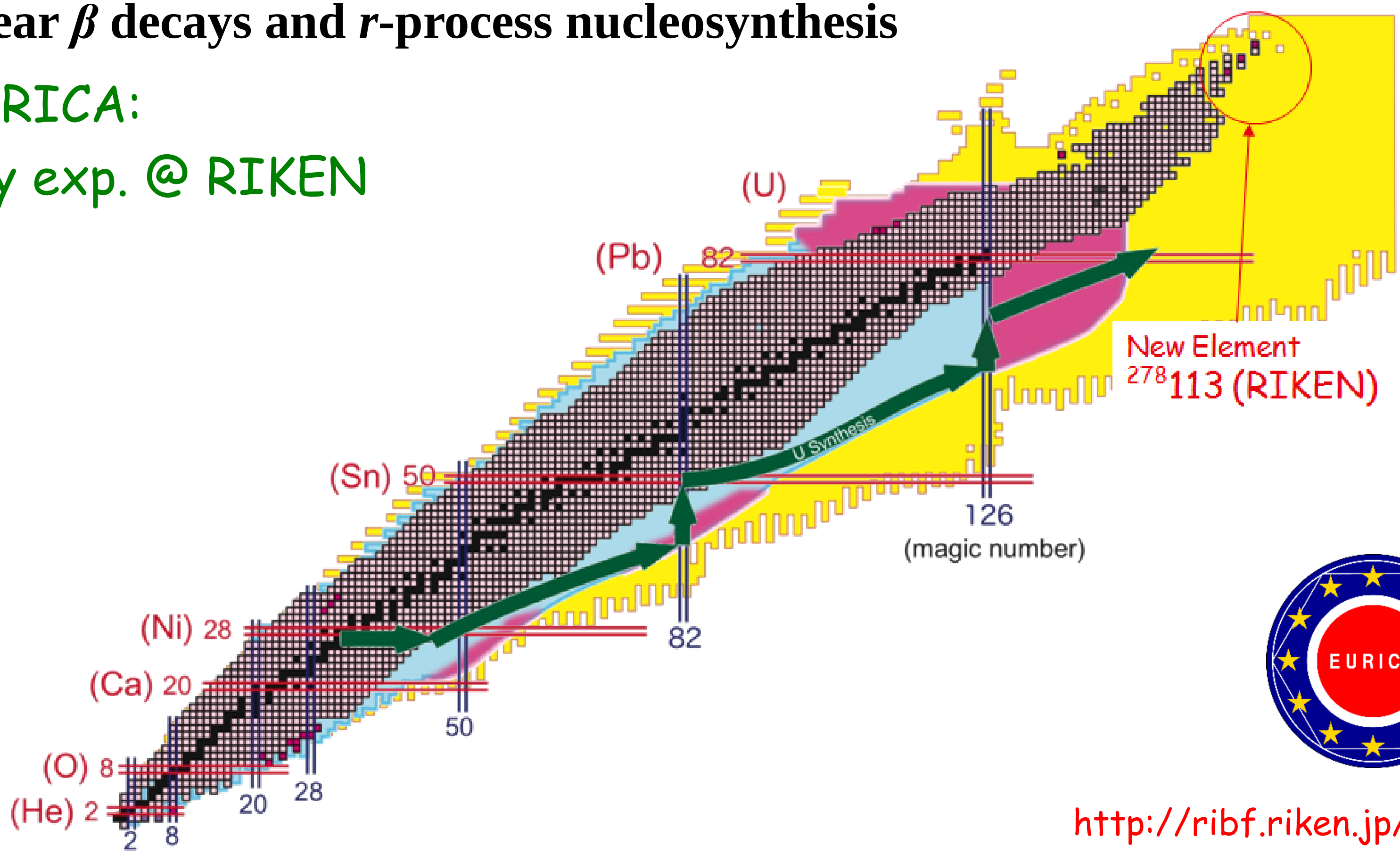
- a crucial test for the theoretical predictive power cf. Dozono's talk

β decays and r-process

Nuclear β decays and r-process nucleosynthesis

EURICA:

Key exp. @ RIKEN

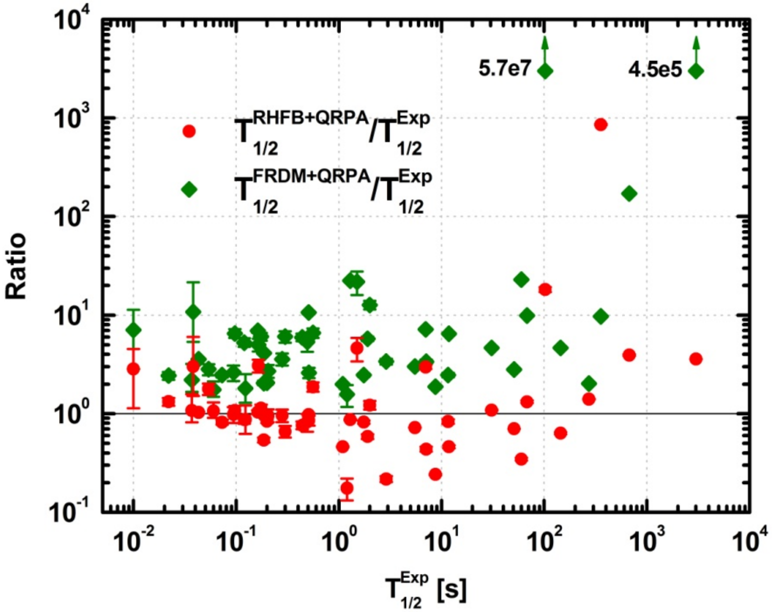


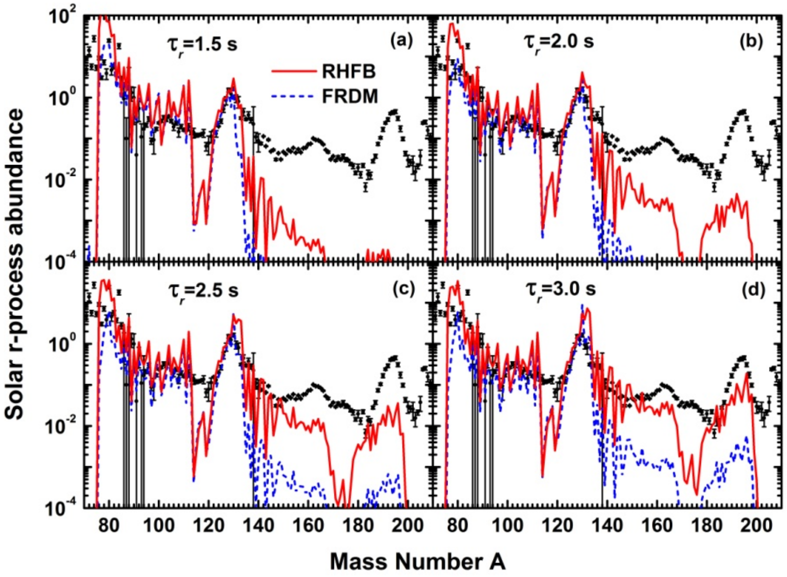
http://ribf.riken.jp/EURICA/

- EURICA project is providing lots of new β-decay data towards r-process path.

β decays and r-process

Nuclear β-decay rates and r-process flow (**Z = 20 ~ 50** region)





FRDM+QRPA: widely used nuclear input

RHFB+QRPA: our results

Niu, Niu, HZL, Long, Niksic, Vretenar, Meng,
Phys. Lett. B **723**, 172 (2013)

✓ Classical r-process calculation shows a faster r-matter flow at the **N = 82** region and higher r-process abundances of elements with **A ~ 140**.

From spherical to deformed

Our goals: To study the physics in exotic deformed nuclei

- correct asymptotic behavior
- to break all geometric symmetries
- exotic shapes / exotic excitation modes
- reasonable computational time

To develop CDFT on 3D mesh:
ground states & excitations

PRL **112,** 142501 (2014) PHYSICAL REVIEW LETTERS

Deformation-Driven *p*-Wave Halos at the Drip Line: ^{31}Ne

PRL **112,** 242501 (2014) PHYSICAL REVIEW LETTERS

Observation of a *p*-Wave One-Neutron Halo Configuration in ^{37}Mg

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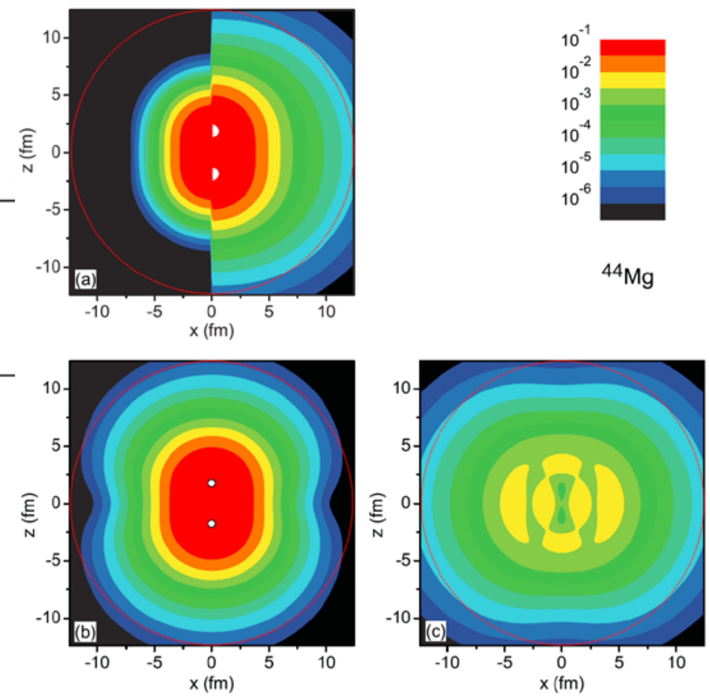


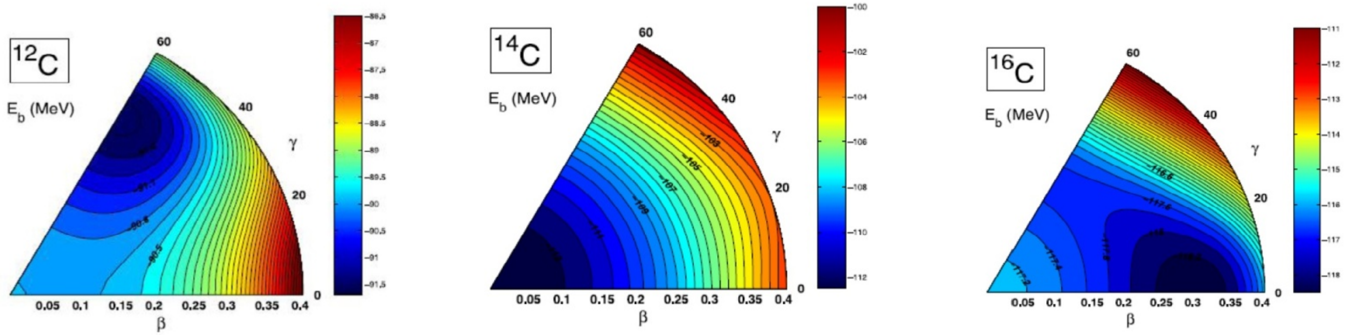
Zhou, Meng, Ring, Zhao,
Phys. Rev. C **82**, 011301(R) (2010)

Imaginary time step method

Imaginary time step (ITS) method

$$\lim_{\tau\to\infty} e^{-h\tau}\left|\psi^{(0)}\right\rangle = \lim_{\tau\to\infty}\sum_i c_i e^{-\epsilon_i\tau}\left|\phi_i\right\rangle \propto \left|\phi_1\right\rangle$$

- ITS has been realized for Skyrme Hartree-Fock calculations on 3D Cartesian mesh. Davies, Flocard, Krieger, Weiss, *Nucl. Phys. A* **342**, 111 (1980)
  - Schrödinger equations



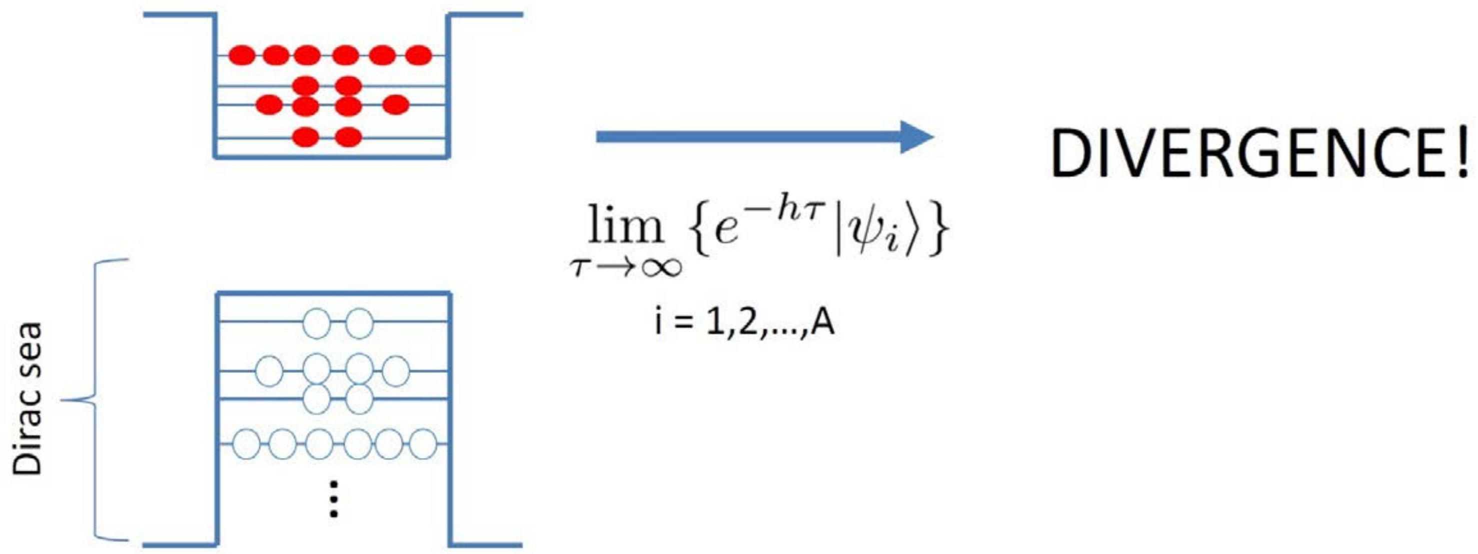
see, e.g., Zhang, Sagawa, Yoshino, Hagino, Meng, *Prog. Theor. Phys.* **120**, 129 (2008)

- To solve Dirac equations in 3D space
  - Challenge I: ***Variational collapse***
  - Challenge II: ***Fermion doubling***

ITS for Dirac equations

- ITS for Dirac equations

$$\{\boldsymbol{\alpha}\cdot\mathbf{p}+\beta[M+S(\mathbf{r})]+V(\mathbf{r})\}\phi(\mathbf{r})=\epsilon\phi(\mathbf{r})$$

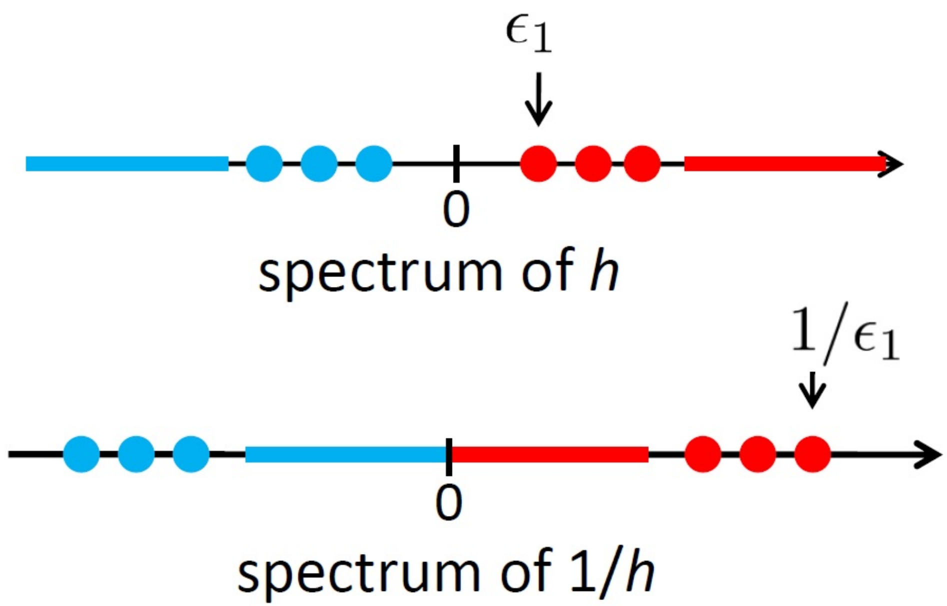


- ITS evolution leads to contamination of single-paticle states by the Dirac sea.
Variational collapse Stanton & Havriliak, *J. Chem. Phys.* **81**, 1910 (1984)

To avoid variational collapse

- To avoid variational collapse: maximizing **□*1/h*□** instead of minimizing **□*h*□**
  Hill & Krauthauser, *Phys. Rev. Lett.* **72**, 2151 (1994)

$$\frac{\langle\psi|\, h^{-1}\, |\psi\rangle}{\langle\psi|\psi\rangle} \leq \frac{1}{\epsilon_1}$$



- ***h*** is unbounded, but ***1/h*** is bounded.

Inverse Hamiltonian method

- Inverse Hamiltonian method

$$\lim_{\tau\to\infty} e^{\tau/(h-w)} \left|\psi^{(0)}\right\rangle = \lim_{\tau\to\infty}\sum_i c_i e^{\tau/(\epsilon_i - w)} \left|\phi_i\right\rangle \propto \left|\phi_1\right\rangle$$

- For a small step □□ Hagino & Tanimura, *Phys. Rev. C* **82**, 057301 (2010)

$$\left|\psi^{(n+1)}\right\rangle = e^{\Delta\tau/(h^{(n)}-w)} \left|\psi^{(n)}\right\rangle \simeq \left(1 + \frac{\Delta\tau}{h^{(n)} - w}\right)\left|\psi^{(n)}\right\rangle = \left|\psi^{(n)}\right\rangle + \Delta\tau \left|\varphi^{(n)}\right\rangle$$

with

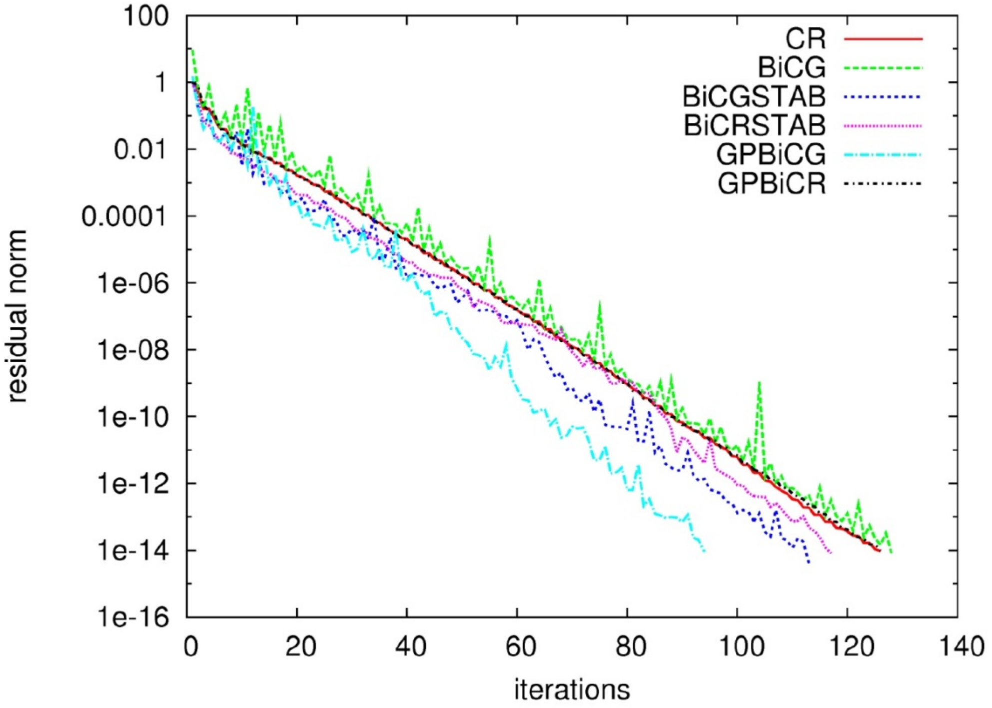
$$\boxed{\left(h^{(n)} - w\right)\left|\varphi^{(n)}\right\rangle = \left|\psi^{(n)}\right\rangle}$$

TO SOLVE KNOWN

Iterative methods

- Of the form $\boldsymbol{Ax = b}$ can be solved iteratively, e.g., Krylov subspace method
  Saad, Iterative Methods for Sparse Linear Systems (2003)
  - do not need the matrix element of $\boldsymbol{A}$
  - only need the result of $\boldsymbol{Ay}$ for any given $\boldsymbol{y}$

$$\boxed{\left(h^{(n)} - w\right)\left|\varphi^{(n)}\right\rangle = \left|\psi^{(n)}\right\rangle}$$



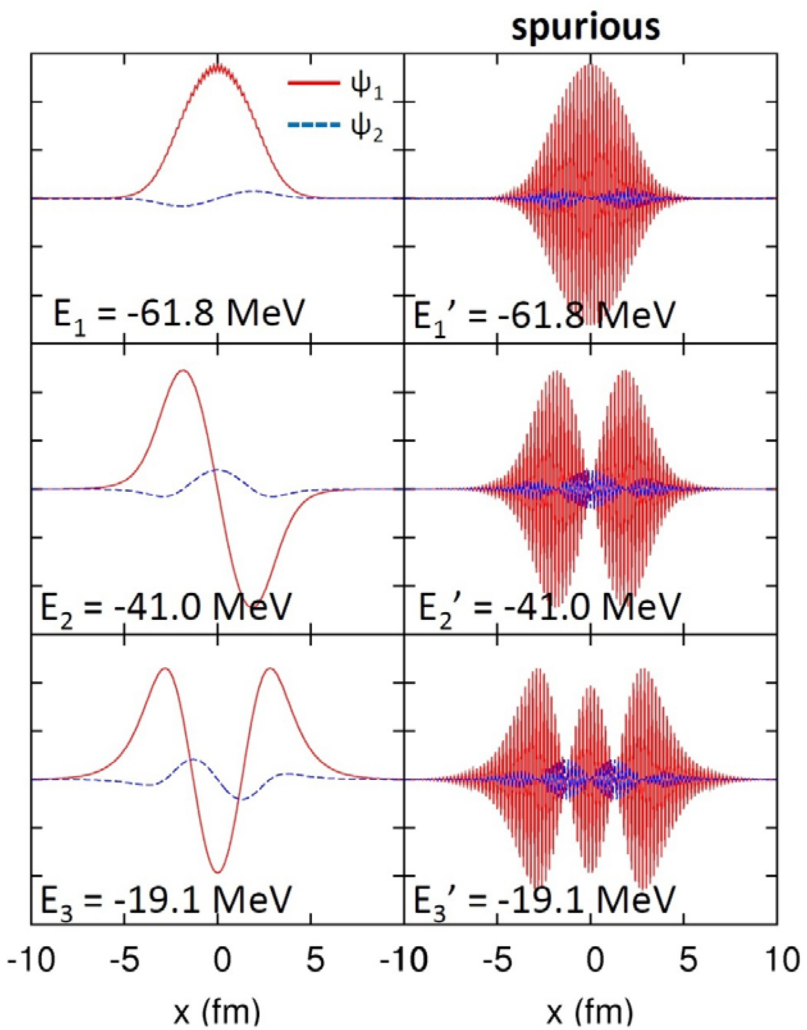
CR=Conjugate Residual, (Bi)CG=(Bi-)Conjugate Gradient, GP=Generalized Product

Fermion doubling (I)

- Dirac Fermion on lattice → spurious states with high momentum and low energy

  - Solutions of 1D Dirac equation

- Physical and spurious states have the same energy, and mix with each other.



Fermion doubling (II)

- Dirac Fermion on lattice → **spurious states** with high momentum and low energy

- 1D Dirac equation in coordinate space

$$(-i\alpha\partial_x + \beta M)\phi(x) = \epsilon\phi(x)$$

e.g.

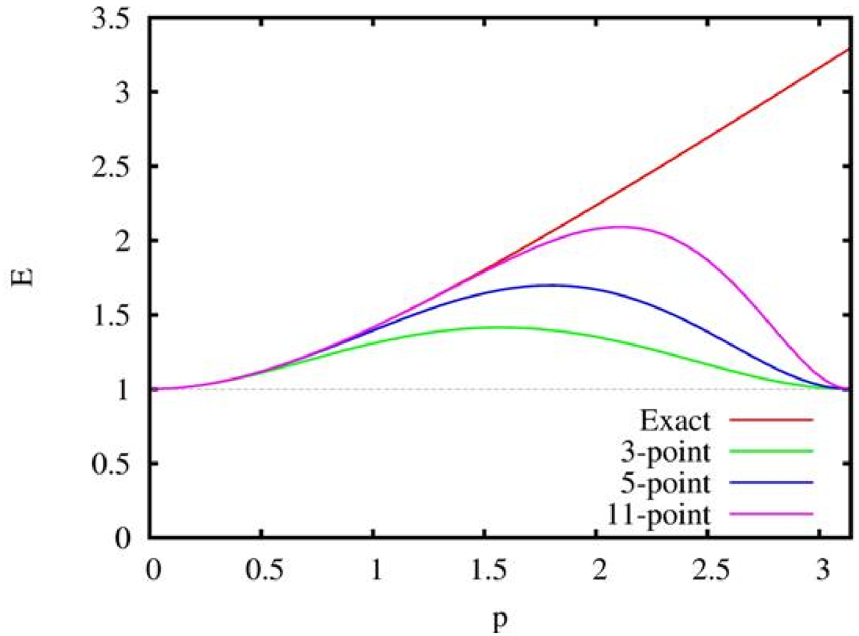
$$\partial_x\phi(x) \to \frac{\phi(i+1) - \phi(i-1)}{2a}$$

- 1D Dirac equation in momentum space

$$(\alpha\frac{1}{a}\sin(pa) + \beta M)\tilde{\phi}(p) = \epsilon\tilde{\phi}(p)$$

- Dispersion relation

$$\epsilon^2 = M^2 + p^2 \quad \to \quad \epsilon^2 = M^2 + \frac{\sin^2(pa)}{a^2}$$



Tanimura, Hagino, HZL,
Prog. Theor. Exp. Phys. **2015**, 073D01 (2015)

To eliminate fermion doubling

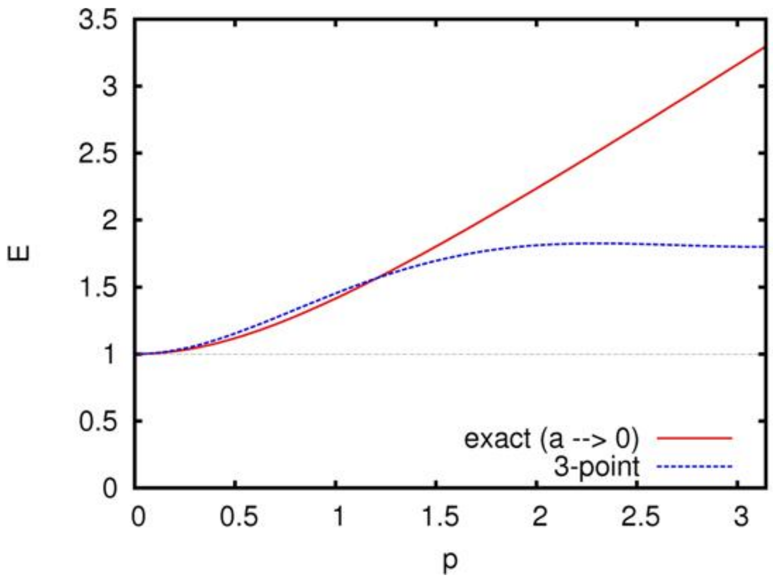
Wilson Fermion:

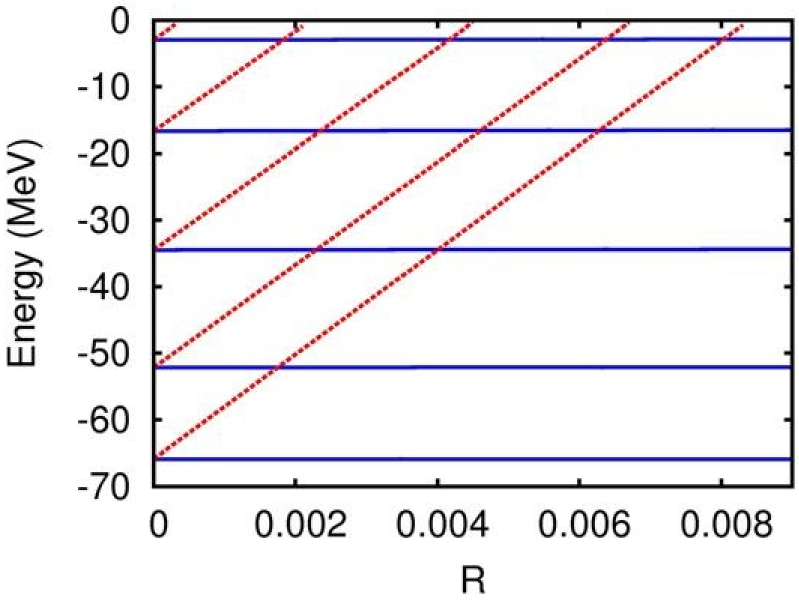
a famous problem in lattice QCD Wilson, *Phys. Rev. D* **10**, 2445 (1974)

$$H_W = -i\boldsymbol{\alpha}\cdot\nabla + \beta[M + S(\mathbf{r})] + V(\mathbf{r}) - aR\beta\triangle$$

- Dispersion relation (1D, no potential)

$$\epsilon^2 = \frac{\sin^2(pa)}{a^2} + \left[M + \frac{4R}{a}\sin^2(pa/2)\right]^2$$

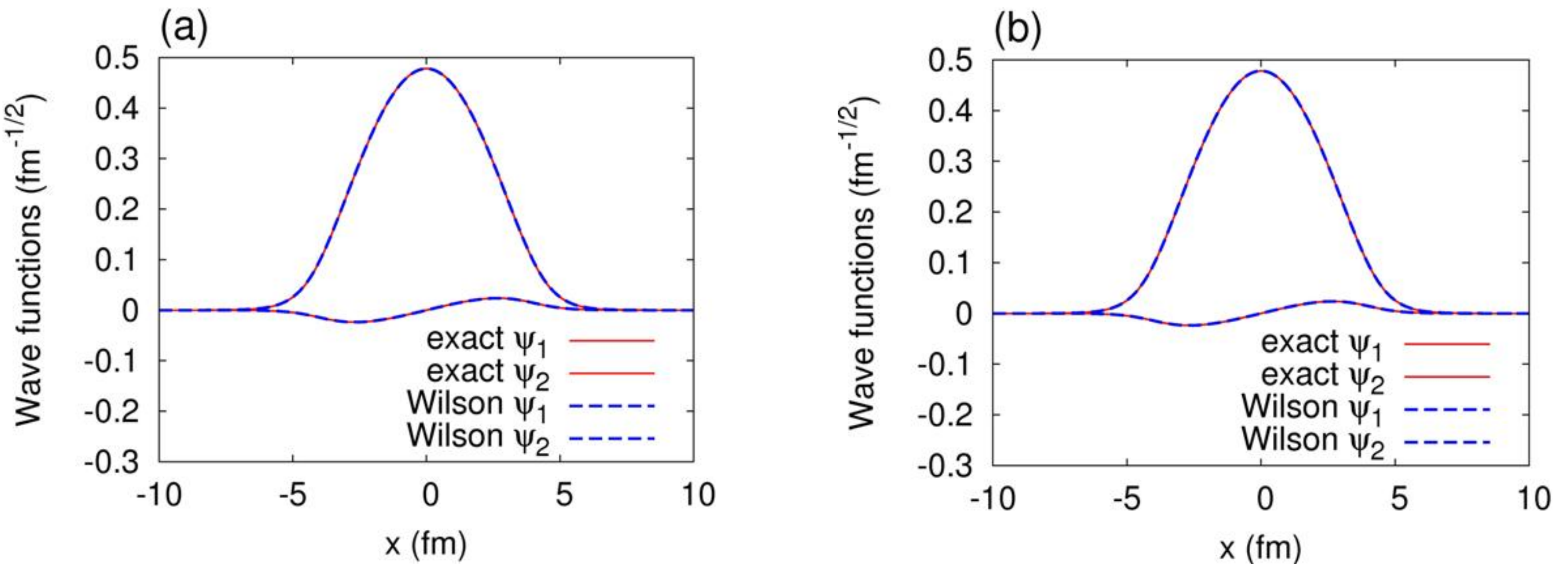




Single-particle energies and wave functions

- Single-particle energies and wave functions

	$m = 1$ $R = 0.01$	$m = 4$ $R = 0.00015$	Shooting
E (MeV)	-65.8726	-65.8918	-65.8918

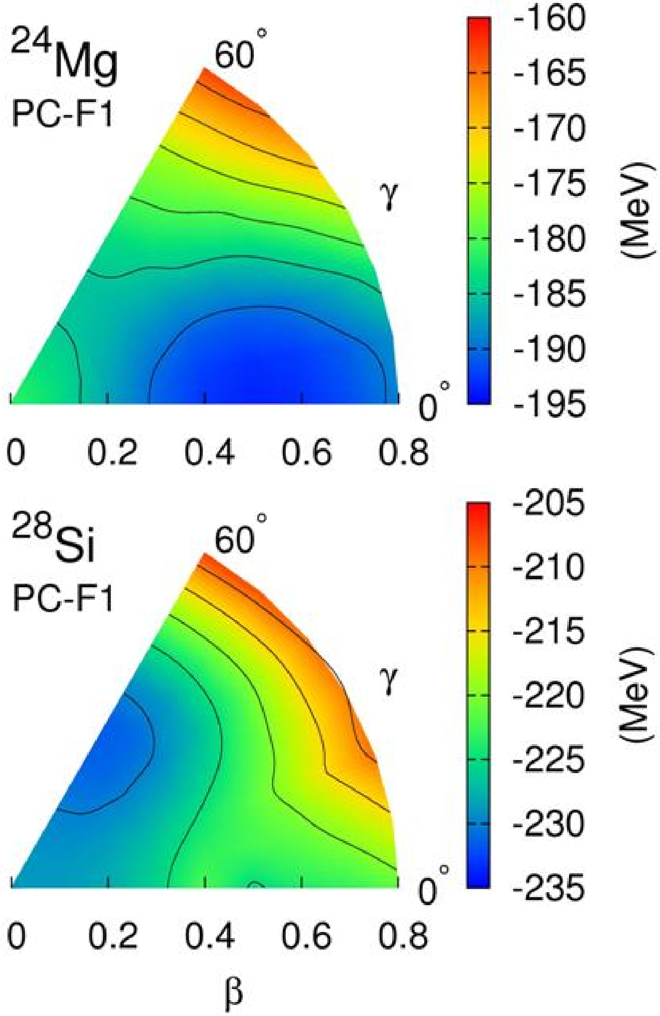


- Higher-order Wilson terms: less effect on physical states, stronger effect on spurious states.

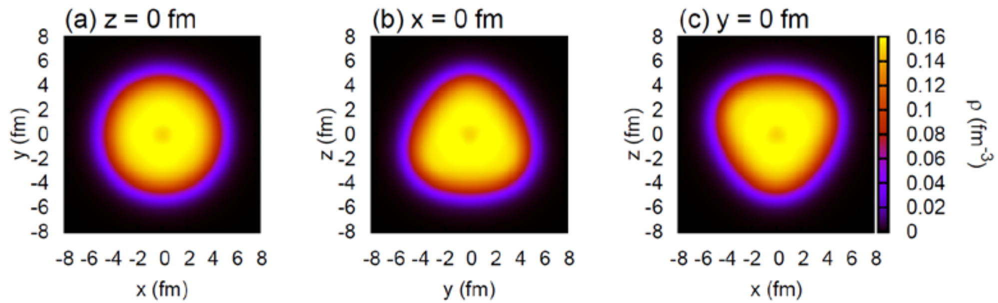
Tanimura, Hagino, HZL,
Prog. Theor. Exp. Phys. **2015**, 073D01 (2015)

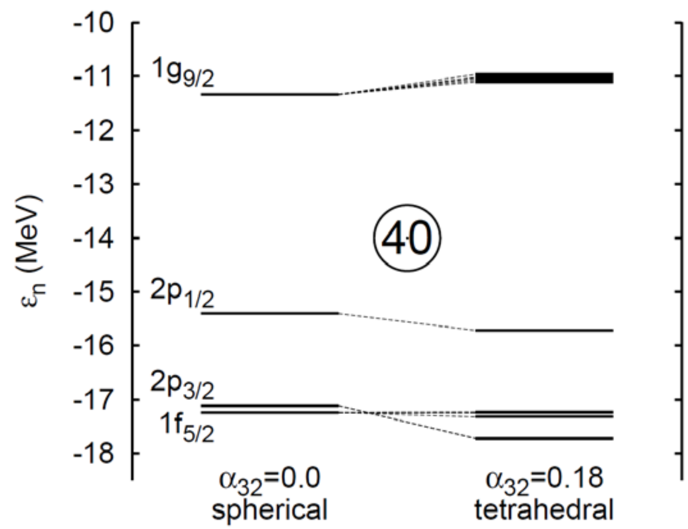
Application in self-consistent CDFT

- Potential energy surfaces (PES) of ^{24}Mg and ^{28}Si



- Tetrahedral (Y_{32}) solution in ^{80}Zr

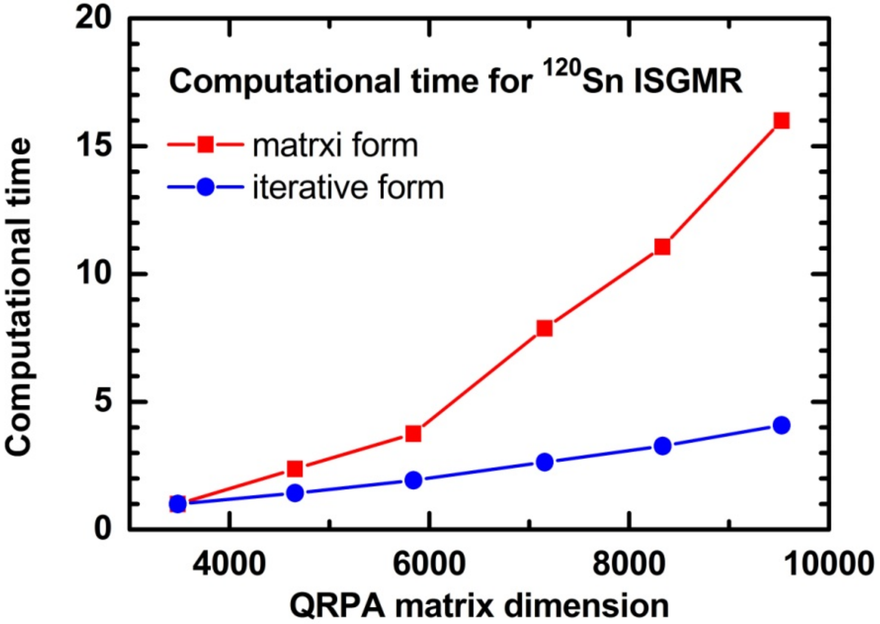




Tanimura, Hagino, HZL, in preparation

Excitations in 3D CDFT

Computational challenge for the excitations in deformed systems



A promising solution:

Finite amplitude method (FAM)

Nakatsukasa, Inakura, Yabana, *Phys. Rev. C* **76**, 024318 (2007)

review: Nakatsukasa, PTEP **2012**, 01A207 (2012)

data from *Avogadro & Nakatsukasa*, *Phys. Rev. C* **87**, 014331 (2013)

TDHF and linear response equation

- The static HF equation $[h[\rho], \rho] = 0$
  determines the ground-state density $\boldsymbol{\rho = \rho_0}$ $\boldsymbol{(\rho^2 = \rho)}$ and $\boldsymbol{h_0 = h[\rho_0]}$.

- With a time-dependent external perturbation,

$$i\frac{d}{dt}\delta\rho(t) = [h_0, \delta\rho(t)] + [\delta h(t) + V_{\mathrm{ext}}(t), \rho_0], \qquad \delta\rho(t) \equiv \rho(t) - \rho_0$$

  For given frequencies $\boldsymbol{\omega}$,

$$\omega\delta\rho(\omega) = [h_0, \delta\rho(\omega)] + [\delta h(\omega) + V_{\mathrm{ext}}(\omega), \rho_0]$$

- By introducing the single-particle (Kohn-Sham) orbitals

$$\rho_0 = \sum_{i=1}^{A} |\phi_i\rangle\langle\phi_i|, \qquad h_0|\phi_\mu\rangle = \epsilon_\mu|\phi_\mu\rangle$$

$$\rho(t) = \sum_{i=1}^{A} |\psi_i(t)\rangle\langle\psi_i(t)|, \qquad |\psi_i(t)\rangle = (|\phi_i\rangle + |\delta\psi_i(t)\rangle)e^{-i\epsilon_i t}$$

$$\delta\rho(t) = \sum_{i=1}^{A}\{|\delta\psi_i(t)\rangle\langle\phi_i| + |\phi_i\rangle\langle\delta\psi_i(t)|\}, \qquad \delta\rho(\omega) = \sum_{i=1}^{A}\{|X_i(\omega)\rangle\langle\phi_i| + |\phi_i\rangle\langle Y_i(\omega)|\}$$

Conventional RPA

- Expanding $|X_i(\omega)\rangle = \sum_{m>A} |\phi_m\rangle X_{mi}(\omega)$ and $|Y_i(\omega)\rangle = \sum_{m>A} |\phi_m\rangle Y^*_{mi}(\omega)$
- RPA equations

$$\left\{ \begin{pmatrix} \mathcal{A}_{mi,nj} & \mathcal{B}_{mi,nj} \\ \mathcal{B}^*_{mi,nj} & \mathcal{A}^*_{mi,nj} \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \begin{pmatrix} X_{nj}(\omega) \\ Y_{nj}(\omega) \end{pmatrix} = - \begin{pmatrix} f_{mi}(\omega) \\ g_{mi}(\omega) \end{pmatrix}$$

where the matrix elements of particle-hole residual interactions

$$\mathcal{A}_{mi,nj} \equiv (\epsilon_m - \epsilon_i)\delta_{mn}\delta_{ij} + \left\langle \phi_m \left| \left. \frac{\partial h}{\partial \rho_{nj}} \right|_{\rho=\rho_0} \right| \phi_i \right\rangle = (\epsilon_m - \epsilon_i)\delta_{mn}\delta_{ij} + \langle \phi_m \phi_j | V_{ph} | \phi_n \phi_i \rangle$$

$$\mathcal{B}_{mi,nj} \equiv \left\langle \phi_m \left| \left. \frac{\partial h}{\partial \rho_{jn}} \right|_{\rho=\rho_0} \right| \phi_i \right\rangle = \langle \phi_m \phi_n | V_{ph} | \phi_j \phi_i \rangle$$

- Density-dependent couplings ➔ **rearrangement terms** in particle-hole residual interactions V_{ph}.
- In relativistic RPA, particle states ***m, n*** include unoccupied states in both Fermi and **Dirac sea**. Ring, Ma, Giai, Vretenar, Wandelt, Cao, *Nucl. Phys. A* **694**, 249 (2001)

Finite Amplitude Method

- Starting from

$$\omega\delta\rho(\omega) = [h_0, \delta\rho(\omega)] + [\delta h(\omega) + V_{\mathrm{ext}}(\omega), \rho_0], \qquad \delta\rho(\omega) = \sum_{i=1}^{A}\{|X_i(\omega)\rangle\langle\phi_i| + |\phi_i\rangle\langle Y_i(\omega)|\}$$

- Multiplying with ket $|\phi_i\rangle$ and bra $\langle\phi_i|$ of hole states, respectively

$$\omega|X_i(\omega)\rangle = (h_0 - \epsilon_i)|X_i(\omega)\rangle + \hat{Q}(V_{\mathrm{ext}}(\omega) + \delta h(\omega))|\phi_i\rangle$$

$$\omega\langle Y_i(\omega)| = -\langle Y_i(\omega)|(h_0 - \epsilon_i) - \langle\phi_i|(V_{\mathrm{ext}}(\omega) + \delta h(\omega))\hat{Q}$$

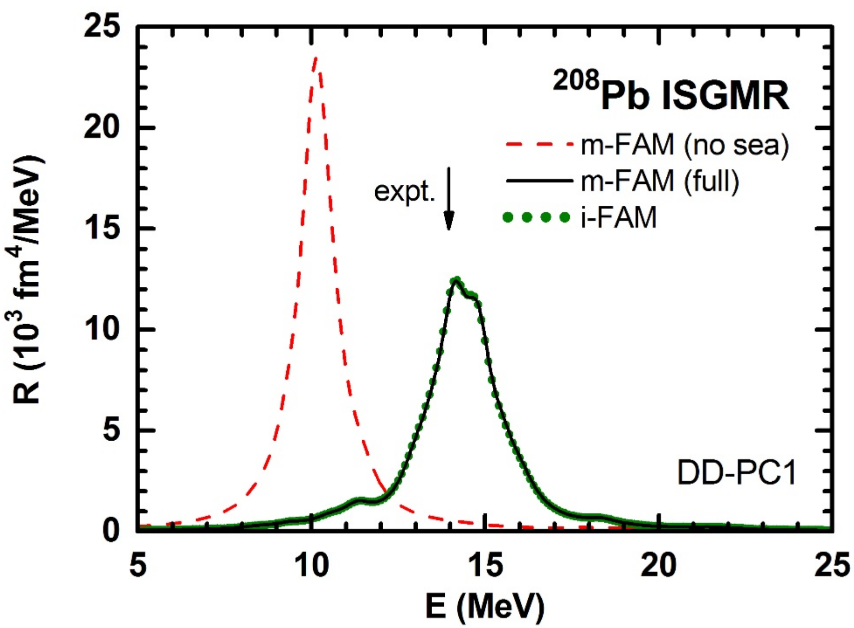
- FAM technique

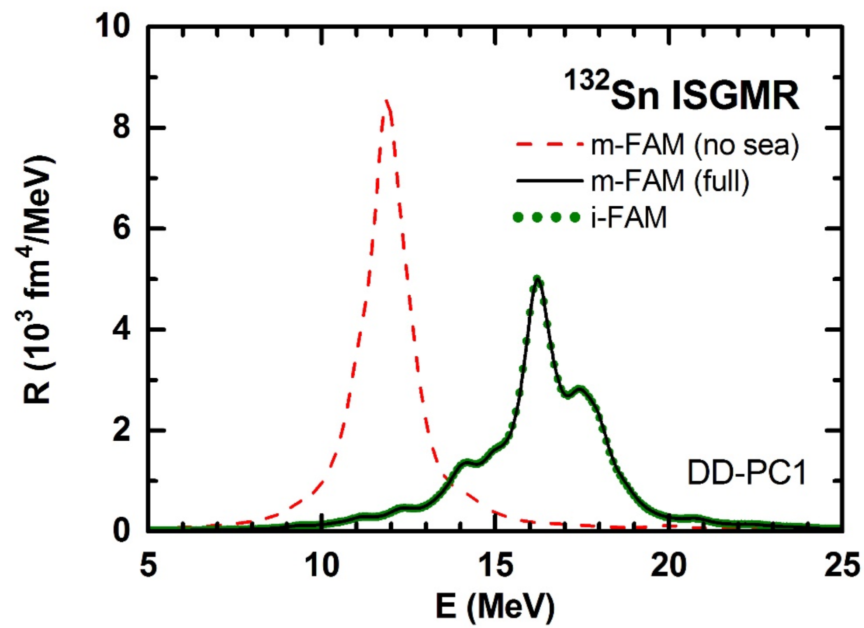
$$\delta h(\omega) = \frac{1}{\eta}(h[\langle\psi'|, |\psi\rangle] - h[\langle\phi|, |\phi\rangle]) \quad \text{with} \quad \langle\psi_i'| = \langle\phi_i| + \eta\langle Y_i(\omega)|, \quad |\psi_i\rangle = |\phi_i\rangle + \eta|X_i(\omega)\rangle$$

$$\delta h^\dagger(\omega) = \frac{1}{\eta}(h[\langle\psi'|, |\psi\rangle] - h[\langle\phi|, |\phi\rangle]) \quad \text{with} \quad \langle\psi_i'| = \langle\phi_i| + \eta\langle X_i(\omega)|, \quad |\psi_i\rangle = |\phi_i\rangle + \eta|Y_i(\omega)\rangle$$

- To solve these equations iteratively ***Ax = b***
- In ***h*[*ψ'*, *ψ*]**, bra and ket are independent ➔ **non-vanishing time-odd currents**
- **Rearrangement terms** ⬅ re-calculate coupling strengths with each new density

Effects of Dirac sea on ISGMR

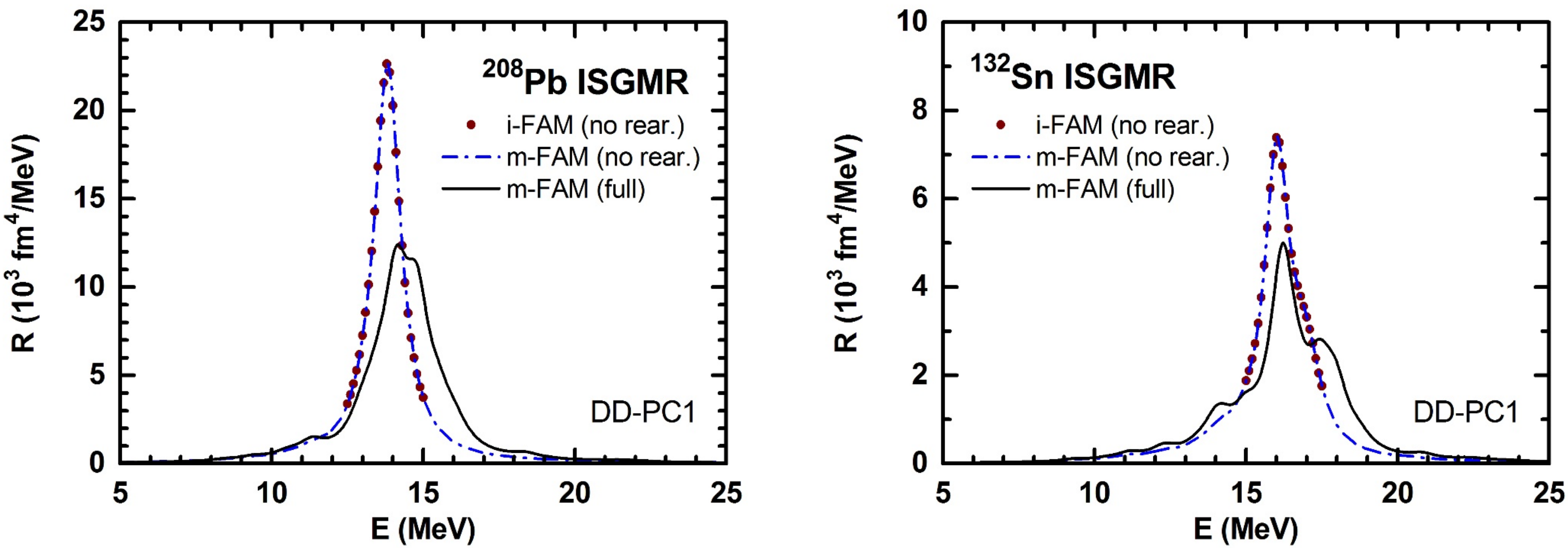




HZL, Nakatsukasa, Niu, Meng, *Phys. Rev. C* **87**, 054310 (2013); *Phys. Scr.* **89**, 054018 (2014)

- ✓ The existence of Dirac sea does not introduce extra difficulties for FAM.
- ✓ In r-space representation, the effects of Dirac sea can be included implicitly and automatically.
- ✓ This effect on m_1/m_0 of ISGMR: ^{208}Pb **4.00 MeV** & ^{132}Sn **4.26 MeV**

Effects of rearrangement terms on ISGMR



HZL, Nakatsukasa, Niu, Meng, *Phys. Rev. C* **87**, 054310 (2013); *Phys. Scr.* **89**, 054018 (2014)

- ✓ In FAM, **NO** extra computational costs due to the rearrangement terms.
- ✓ This effect on m_1/m_0 of ISGMR: ^{208}Pb **0.53 MeV** & ^{132}Sn **0.26 MeV**

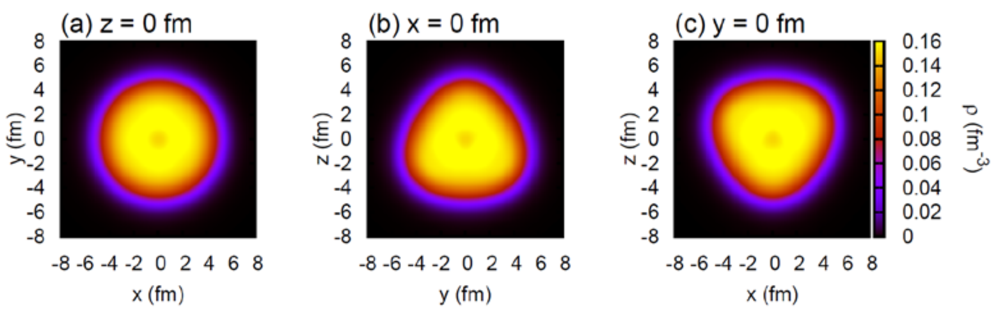
Summary and Perspectives

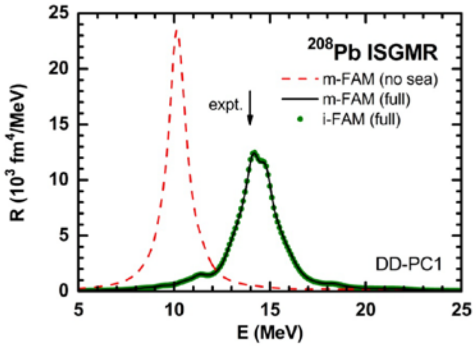
- The self-consistent and relativistic description of spin-isospin excitations in spherical nuclei.
- Towards the exotic deformed nuclei ➔ CDFT on 3D mesh

- **Ground-state calculations**
  - ✓ Challenge I: ***Variational collapse*** ← **inverse Hamiltonian method**
  - ✓ Challenge II: ***Fermion doubling*** ← **(higher-order) Wilson terms**

- **Excited-state calculations**
  - ✓ Computational challenge ← **finite amplitude method**

To study the spin-isospin physics in exotic deformed nuclei





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Thank you!

CDFT+RPA in charge-exchange channel

Particle-hole residual interactions *HZL, Giai, Meng, Phys. Rev. Lett.* **101**, 122502 (2008)

- σ-meson $$V_\sigma(1,2) = -[g_\sigma\gamma_0]_1[g_\sigma\gamma_0]_2 D_\sigma(1,2)$$
- ω-meson $$V_\omega(1,2) = [g_\omega\gamma_0\gamma^\mu]_1[g_\omega\gamma_0\gamma_\mu]_2 D_\omega(1,2)$$
- ρ-meson $$V_\rho(1,2) = [g_\rho\gamma_0\gamma^\mu\vec{\tau}]_1\cdot[g_\rho\gamma_0\gamma_\mu\vec{\tau}]_2 D_\rho(1,2)$$
- pseudovector π-N coupling
$$V_\pi(1,2) = -[\frac{f_\pi}{m_\pi}\vec{\tau}\gamma_0\gamma_5\gamma^k\partial_k]_1\cdot[\frac{f_\pi}{m_\pi}\vec{\tau}\gamma_0\gamma_5\gamma^l\partial_l]_2 D_\pi(1,2)$$
- zero-range counter-term of π-meson
$$V_{\pi\delta}(1,2) = g'[\frac{f_\pi}{m_\pi}\vec{\tau}\gamma_0\gamma_5\boldsymbol{\gamma}]_1\cdot[\frac{f_\pi}{m_\pi}\vec{\tau}\gamma_0\gamma_5\boldsymbol{\gamma}]_2\delta(\mathbf{r}_1-\mathbf{r}_2), \quad g'=1/3$$

- For the correct asymptotic behavior, ***g'*** is not a parameter, but must be **1/3**.