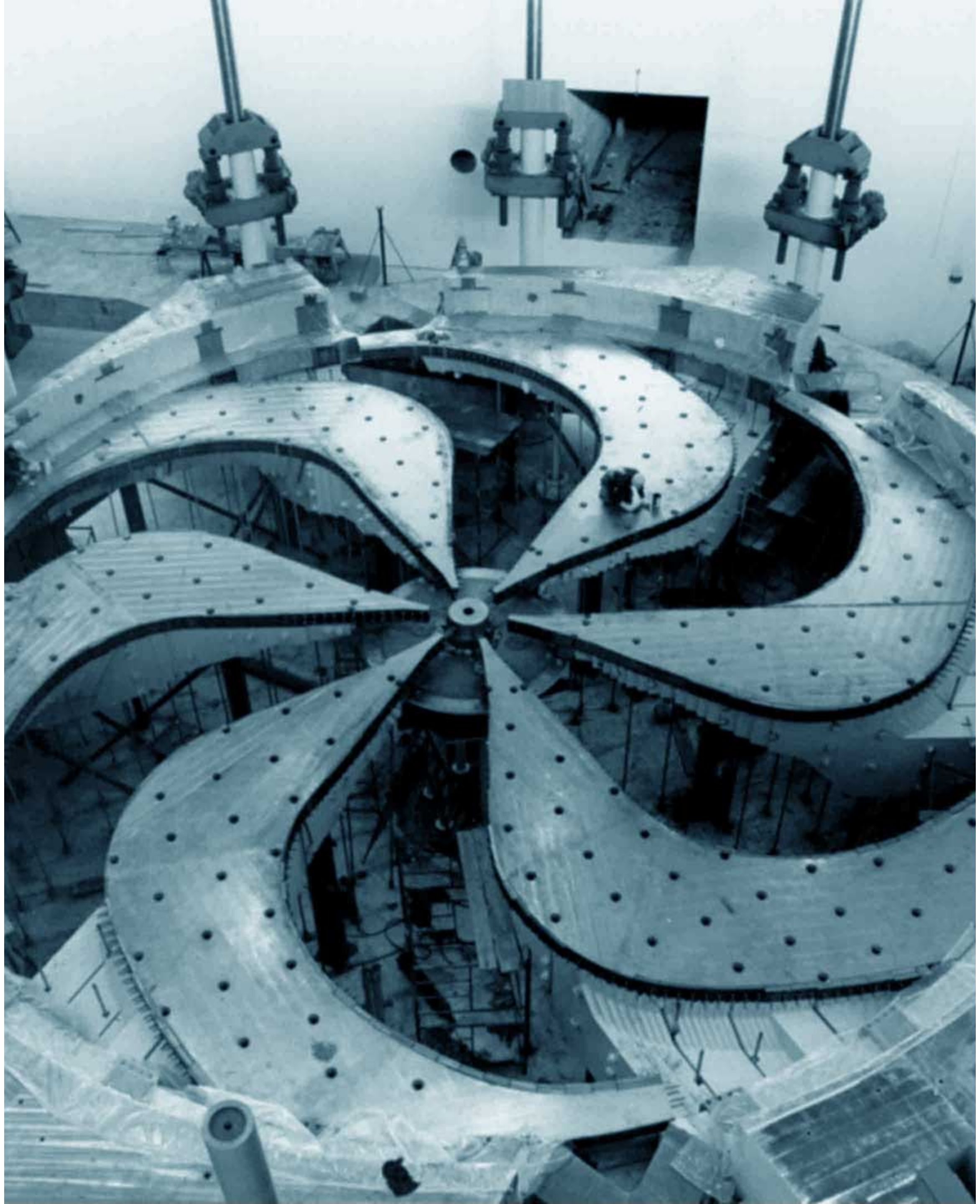
TRIUMF

Multi-major-shell effective hamiltonian from IMSRG

Takayuki Miyagi

Progress in Ab Initio Techniques in Nuclear Physics
March 3-6, 2020



Discovery,
accelerated

Outline

- The valence-space Hamiltonians across multiple major shells from IM-SRG

- Exploration of ^{208}Pb

Why we need multiple shell?

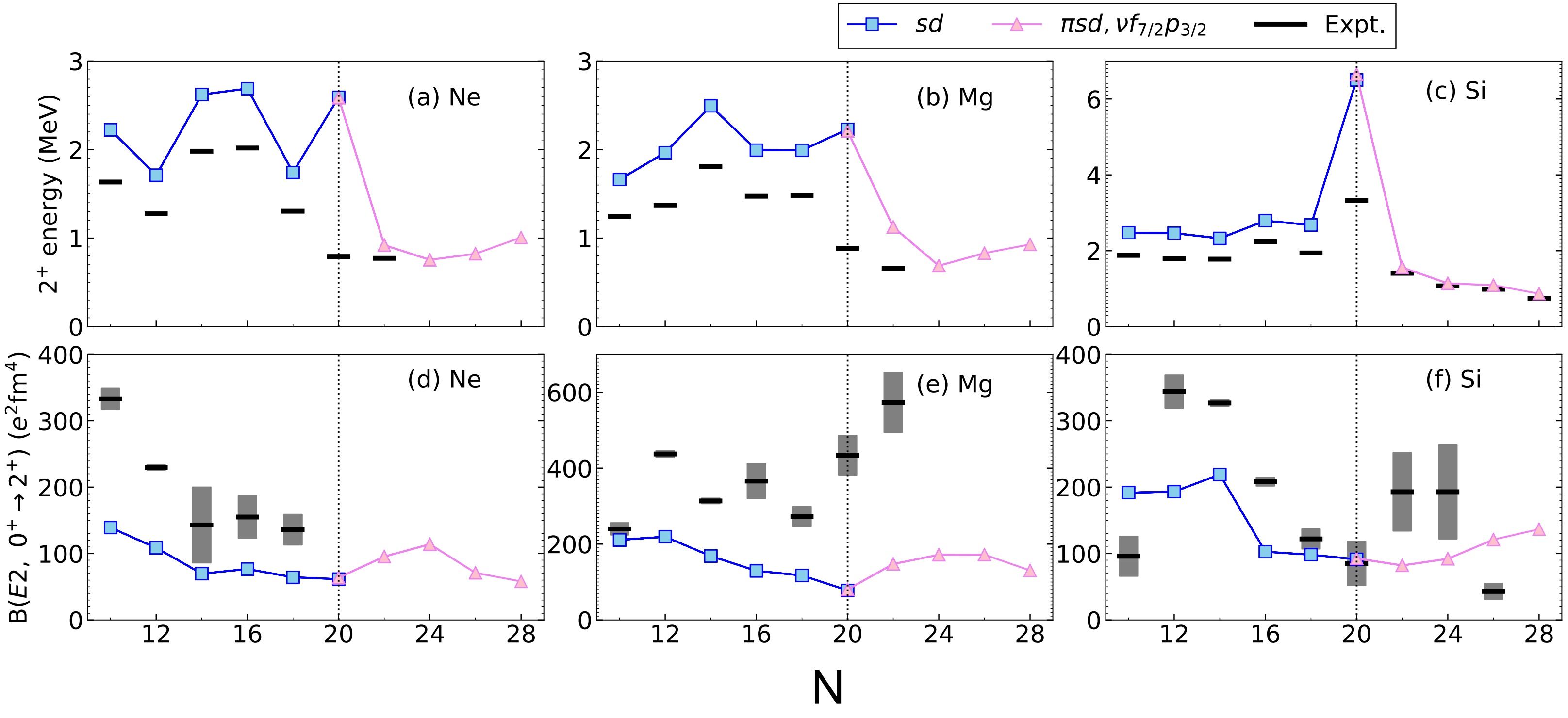
EM 1.8/2.0
e_{max}=12
e_{3max}=16

- N=20 island of inversion

IM-SRG(2) tends to give high excitation energies (see Ragnar's talk)

Small BE(2) is consistent with radii

Fail to reproduce the disappearance of N=20 magic



Starting from the multi-reference state* is another way.
*J. M. Yao et al., Phys. Rev. C **98**, 054311 (2018).

This is one of the many cases…

Valence-space interaction from nuclear force

- Many-body perturbation theory

M. Hjorth-Jensen et al., Phys. Rep. **261**, 125 (1995).
N. Tsunoda et al., Phys. Rev. C **95**, 021304 (2017).
…

- Coupled-cluster method

G. R. Jansen et al.. Rev. C **94**, 011301 (2016).
Z. H. Sun et al., Phys. Rev. C **98**, 054320 (2018).
…

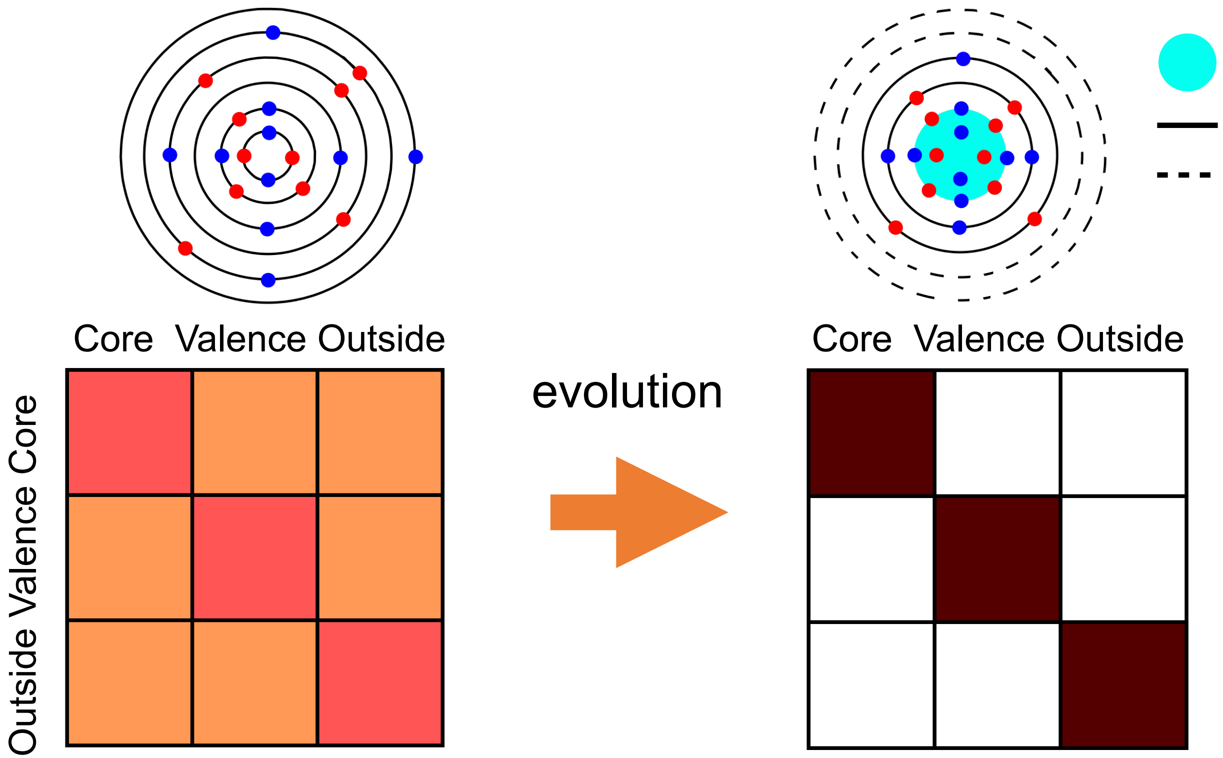
- IM-SRG

S. K. Bogner, et al., Phys. Rev. Lett. **113**, 142501 (2014).
S. R. Stroberg et al., Annu. Rev. Nucl. Part. Sci. **69**, 307 (2019).
…

- …

H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tsukiyama, Phys. Rep. **621**, 165 (2016).
S. R. Stroberg, H. Hergert, S. K. Bogner, and J. D. Holt, Annu. Rev. Nucl. Part. Sci. **69**, 307 (2019).

In-medium similarity renormalization group



Similarity transformation

$$H \qquad H(s) = e^{\Omega(s)} H e^{-\Omega(s)}$$

$$H(s) \approx E(s) + \sum_{12} f_{12}(s)\{a_1^\dagger a_2\} + \frac{1}{4}\sum_{1234} \Gamma_{1234}(s)\{a_1^\dagger a_2^\dagger a_4 a_3\}$$

s: flow parameter

$$\frac{d\Omega}{ds} = \eta(s) - \frac{1}{2}[\Omega(s), \eta(s)] + \cdots$$

$$\eta(s) = \sum_{12} \eta_{12}(s)\{a_1^\dagger a_2\} + \sum_{1234} \eta_{1234}(s)\{a_1^\dagger a_2^\dagger a_4 a_3\}$$

$$\eta_{12} = \frac{1}{2}\arctan\left(\frac{2f_{12}}{f_{11} - f_{22} + \Gamma_{1212} + \Delta}\right)$$

$$\eta_{1234} = \frac{1}{2}\arctan\left(\frac{2\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234} + \Delta}\right)$$

$$A_{1234} = \Gamma_{1212} + \Gamma_{3434} - \Gamma_{1313} - \Gamma_{2424} - \Gamma_{1414} - \Gamma_{2323}$$

f_{12}, Γ_{1234} : matrix element we want to suppress

Δ : newly introduced parameter

H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tsukiyama, Phys. Rep. **621**, 165 (2016).
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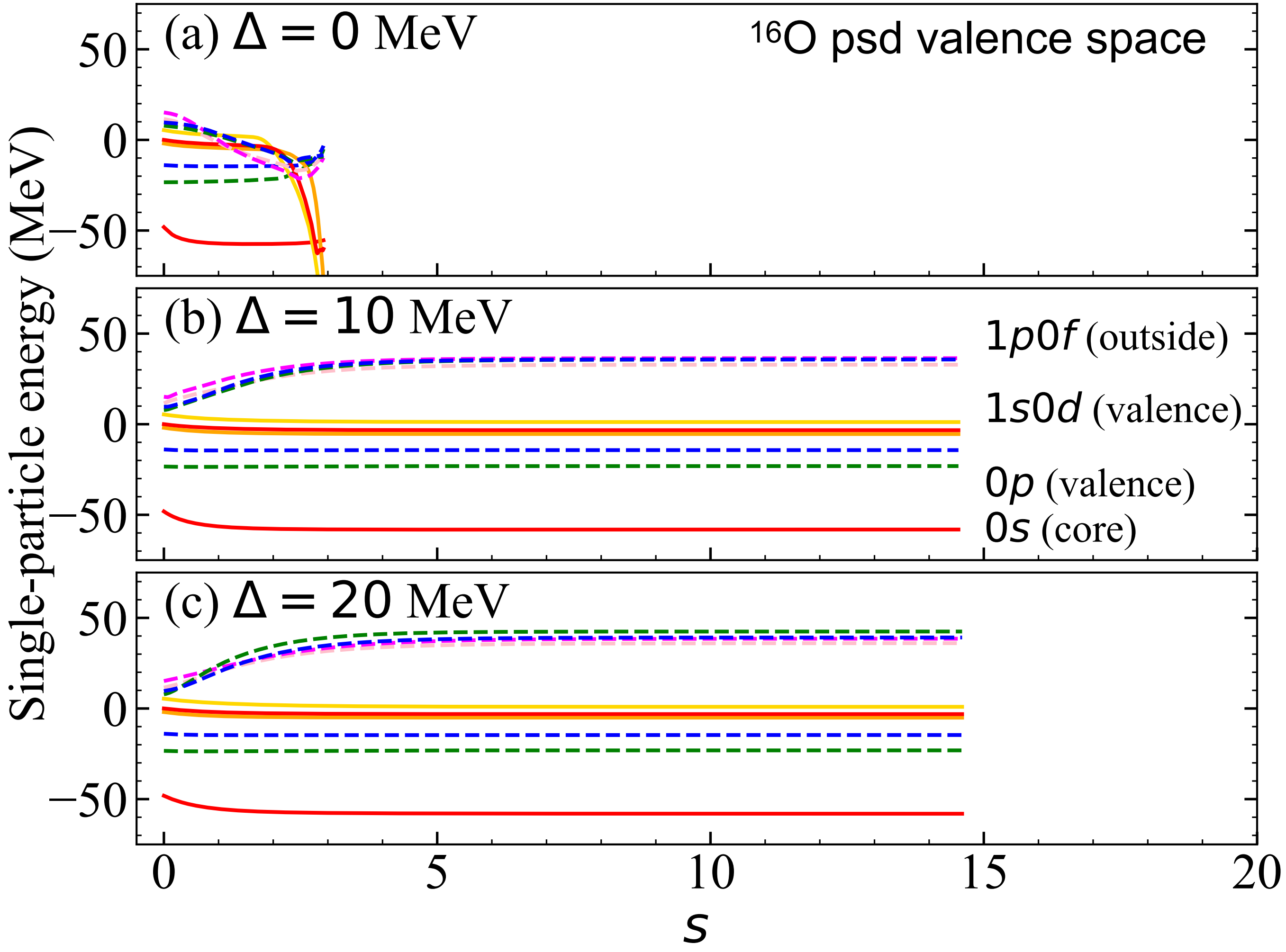
In-medium similarity renormalization group



$$\frac{d\Omega}{ds} = \eta(s) - \frac{1}{2}[\Omega(s), \eta(s)] + \cdots$$

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Center of mass motion

- Add before shell-model diagonalization

No longer HO basis representation.
CM Hamiltonian induces undesired coupling.

$$H_{\mathrm{SM}} = e^{\Omega(s,0)} H e^{-\Omega(s,0)} + \beta H_{\mathrm{cm}}$$

- Add consistently evolved cm Hamiltonian

CM Hamiltonian induces undesired coupling.

$$H_{\mathrm{SM}} = e^{\Omega(s,0)} H e^{-\Omega(s,0)} + \beta e^{\Omega(s,0)} H_{\mathrm{cm}} e^{-\Omega(s,0)}$$

- Add cm Hamiltonian before the flow

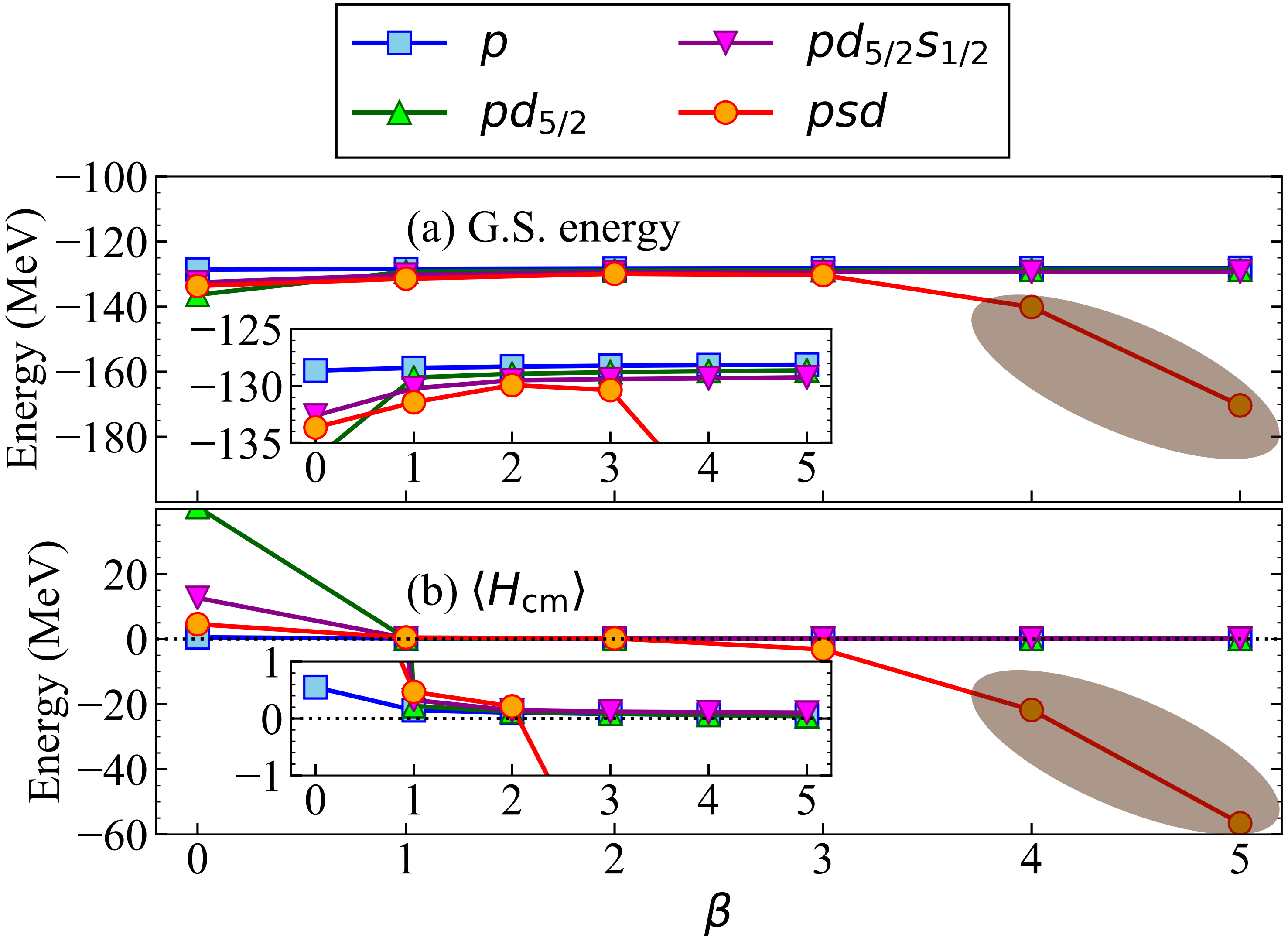
$$H_{\mathrm{SM}} = e^{\Omega(s,\beta)} (H + \beta H_{\mathrm{cm}}) e^{-\Omega(s,\beta)}$$

$$H_{\mathrm{cm}} = \frac{1}{2mA}\left(\sum_{i=1}^{A} \mathbf{p}_i\right)^2 + \frac{1}{2} m A \omega^2 \left(\sum_{i=1}^{A} \frac{1}{A}\mathbf{r}_i\right)^2 - \frac{3}{2}\hbar\omega$$

Center of mass motion

- IM-SRG(2) breaks down
- Valence-space choice is crucial

^{16}O @ e_{max}=8



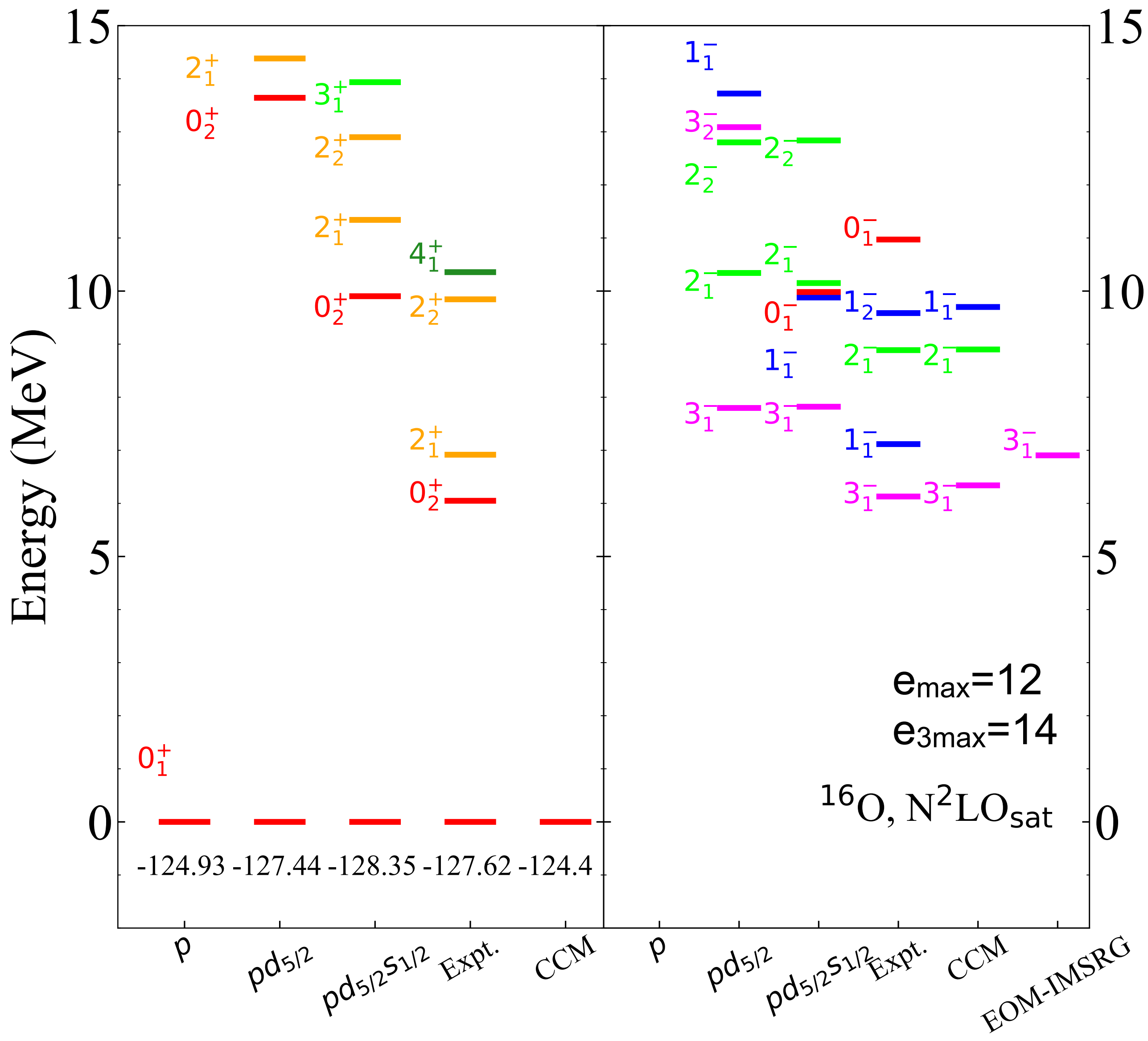
CCM: A. Ekström et al., Phys. Rev. C **91**, 051301 (2015).

EOM-IMSRG: N. M. Parzuchowski et al., Phys. Rev. C **95**, 044304 (2017).

First application: ^{16}O

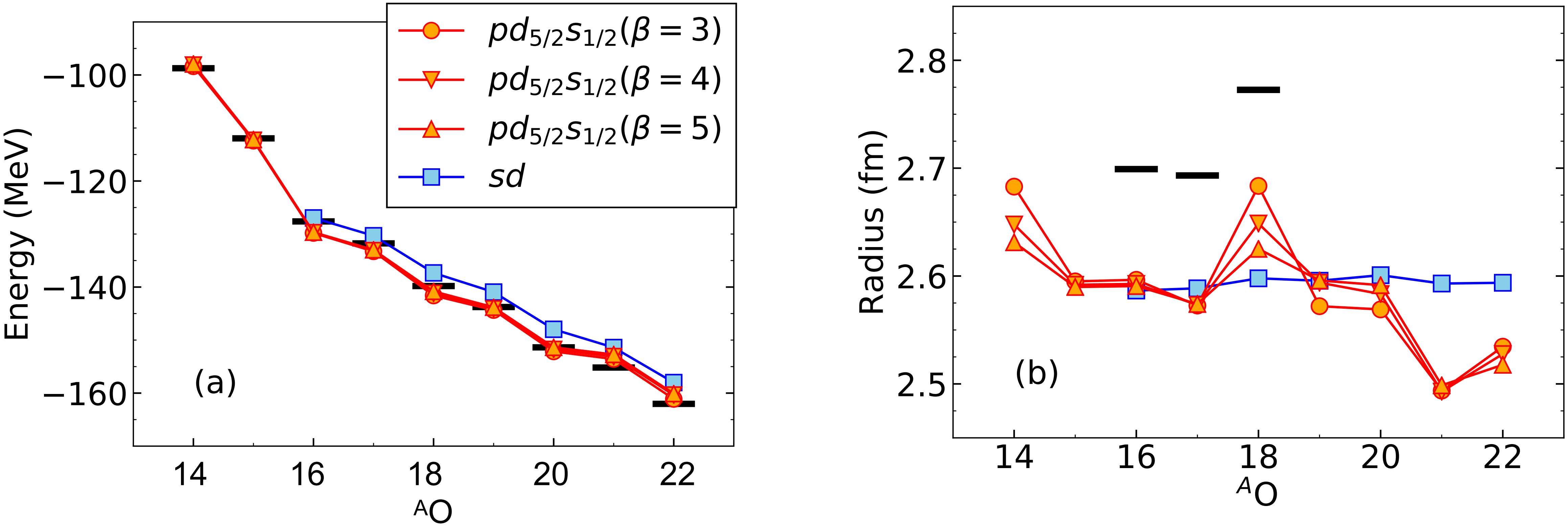
- Comparable to CCM results for negative parity states

- Not converged for positive parity excited states



First application: oxygen isotopes

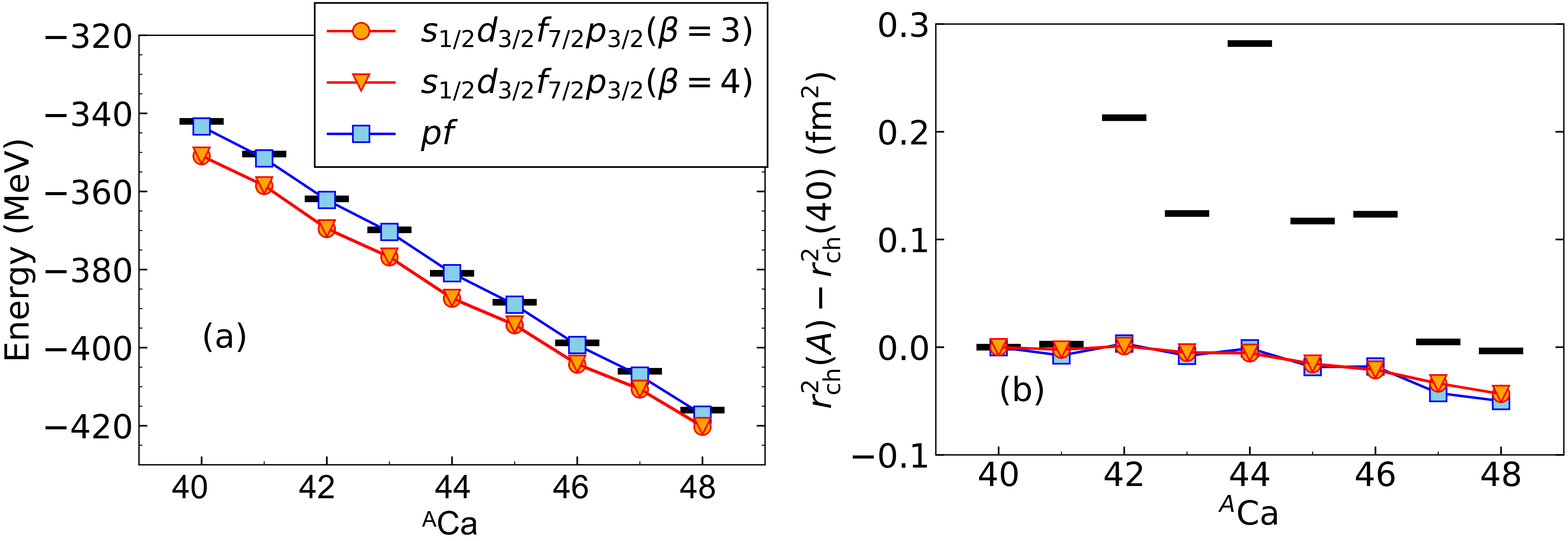
EM 1.8/2.0
e_{max}=12
e_{3max}=16



The excitation from p to sd seems essential to reproduce the trend of the radii.

First application: calcium isotopes

EM 1.8/2.0
e_{max}=12
e_{3max}=16

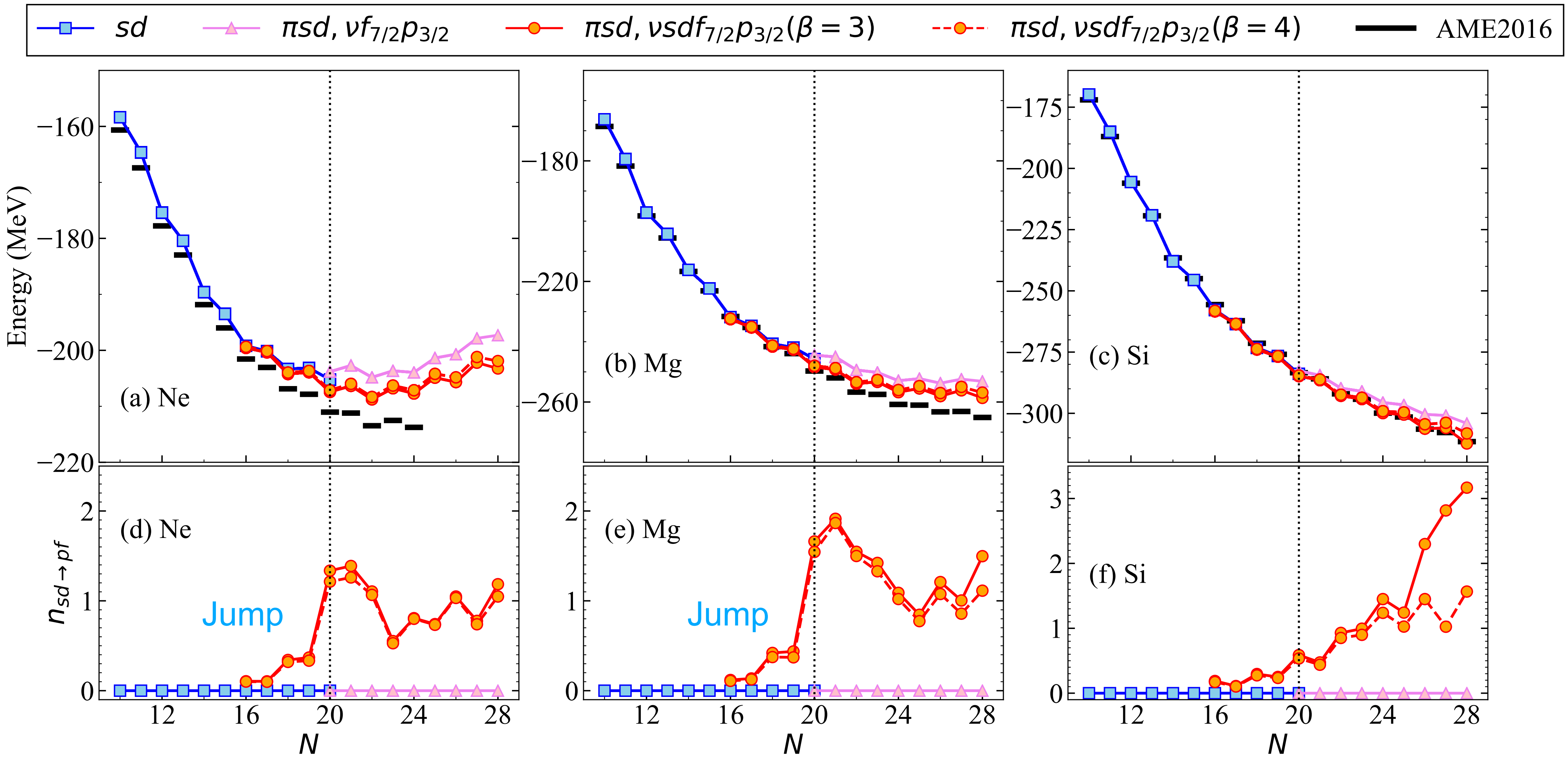


Still missing something in calcium isotopes

Phenomenological shell-model calculation study: E. Caurier et al., Phys. Lett. B **522**, 240 (2001).

EM 1.8/2.0
e_{max}=12
e_{3max}=16

First application: N=20 island of inversion



First application: N=20 island of inversion

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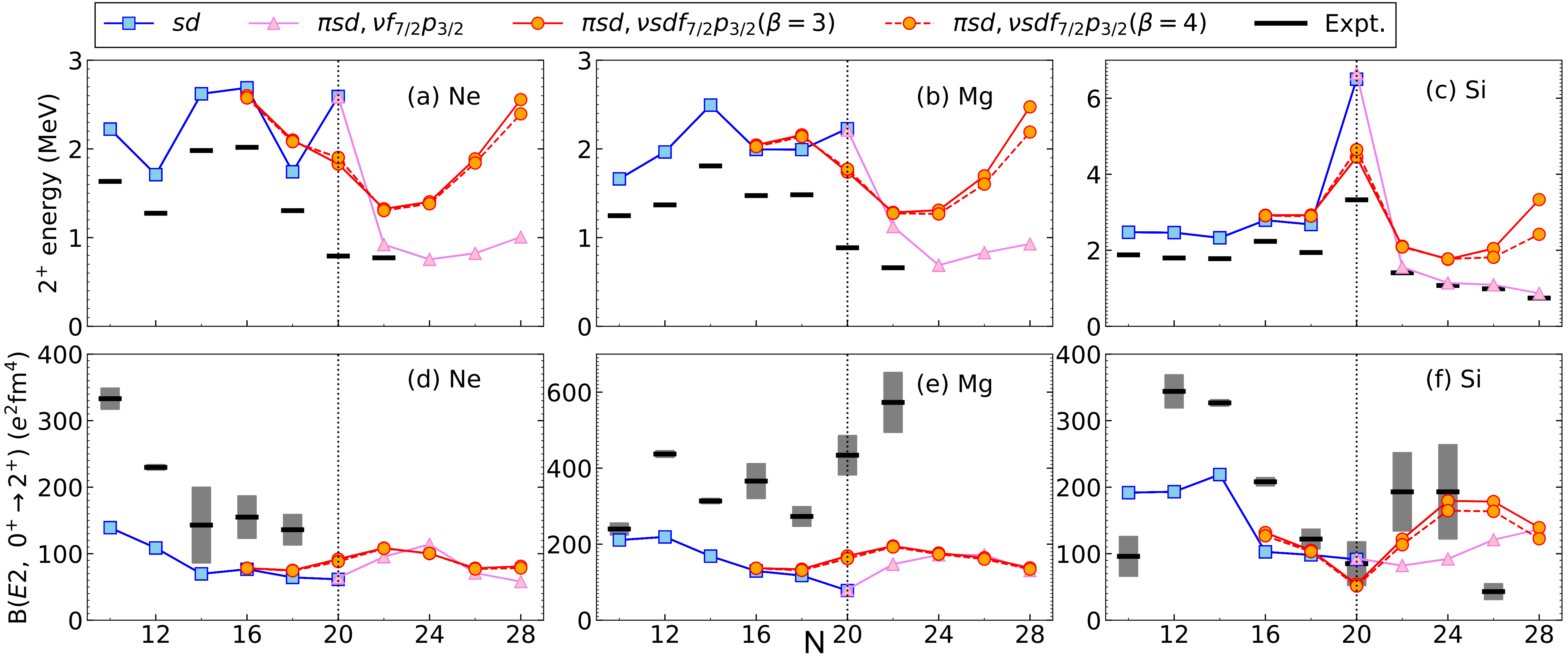


Need to optimize valence-space to discuss N=28 magic

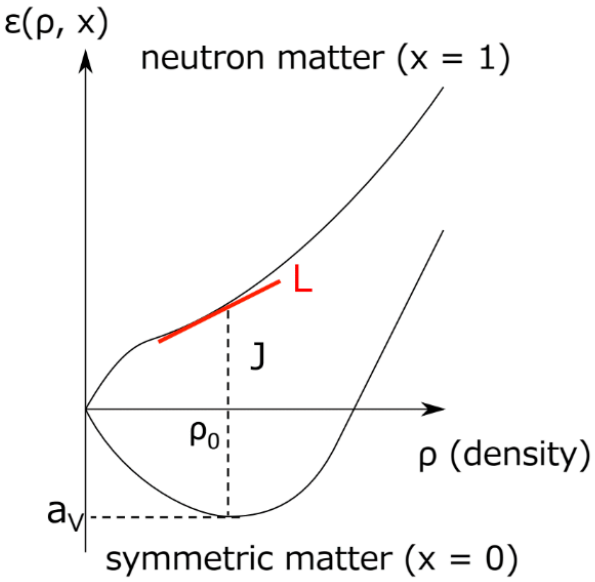
Second part

- Equation of state for nuclear matter

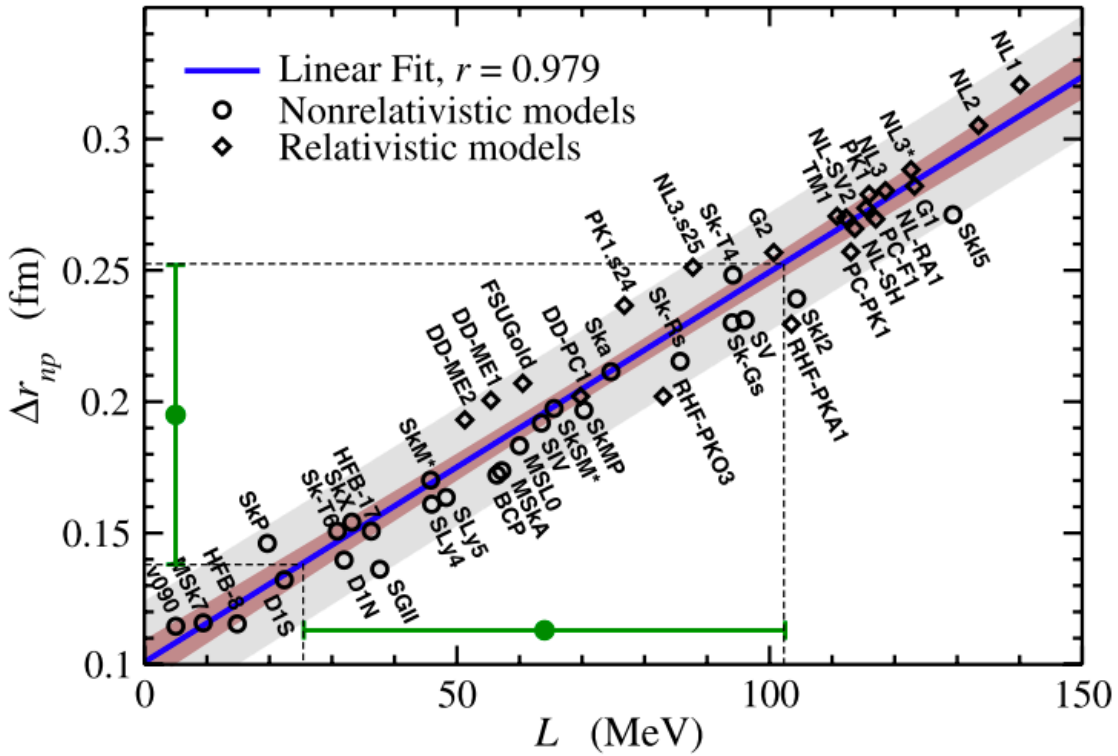
$$\epsilon(\rho, x) \sim a_V + \frac{1}{2}K_V\delta^2 + \left[J + L\delta + \frac{1}{2}K_{\rm sym}\delta^2\right]x^2$$

ϵ :Energy per particle, ρ : Nucleon density

x :Asymmetry parameter.



X. Roca-Maza et al., Phys. Rev. Lett. **106**, 252501 (2011).



Second part

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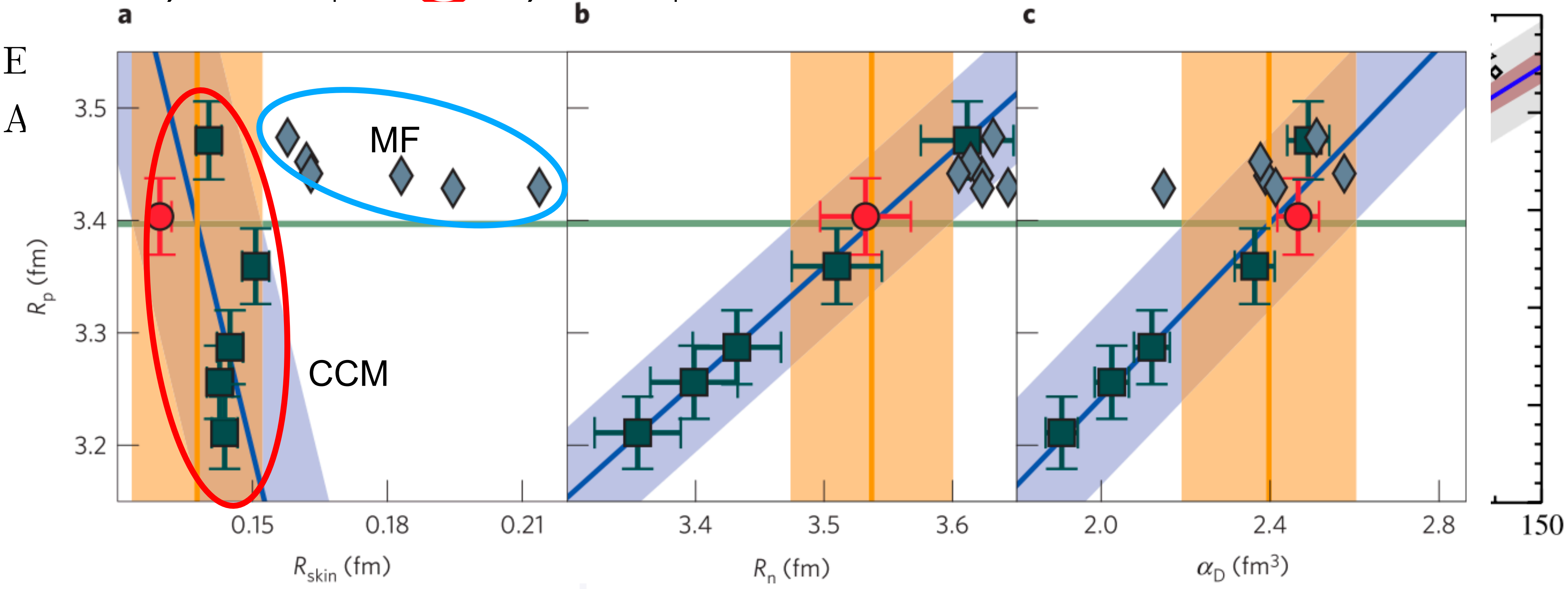
$$\epsilon(\rho, x) \sim a_V + \frac{1}{2}K_V\delta^2 + \left[J + L\delta + \frac{1}{2}K_{\text{sym}}\delta^2\right]x^2$$

G. Hagen et al., Nat. Phys. **12**, 186 (2016).

ϵ :E

x :A



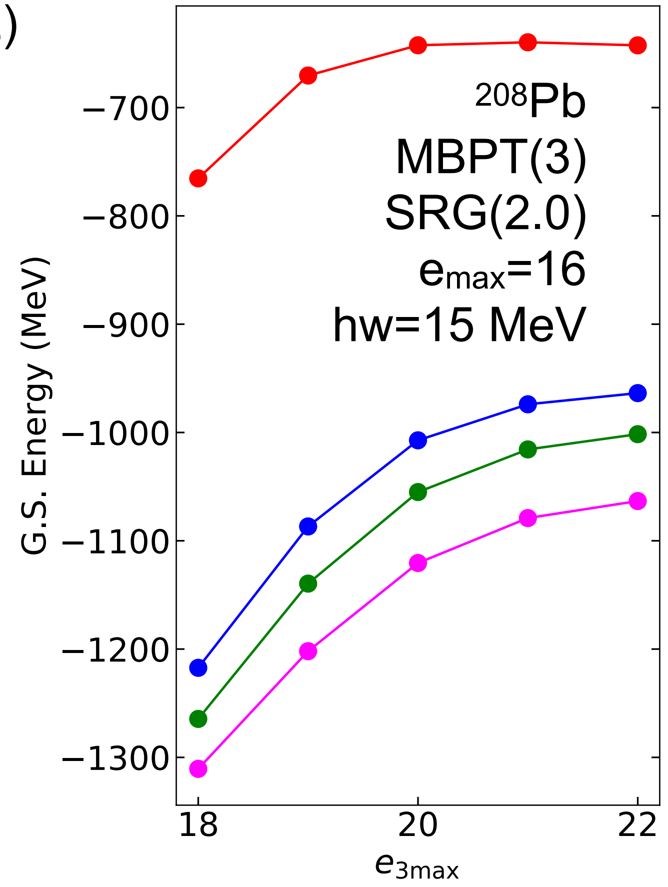
NN (N4LO) + 3N (N2LO, LNL)

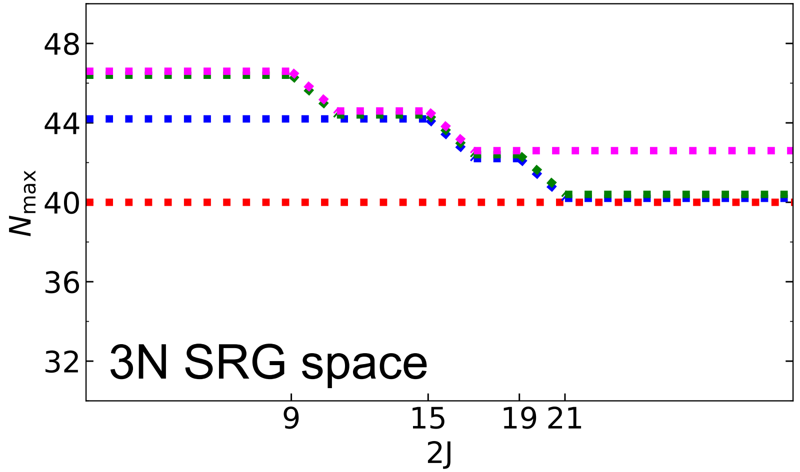
Issues

- Nuclear interaction
  - ✦Soft & perturbative
  - ✦3N SRG needs larger space (bare is better)

Delta full chiral NNLO interaction (394)

- Many-body calc.
  - ✦MBPT is enough to test the interactions
  - ✦More *e_{3max} needed





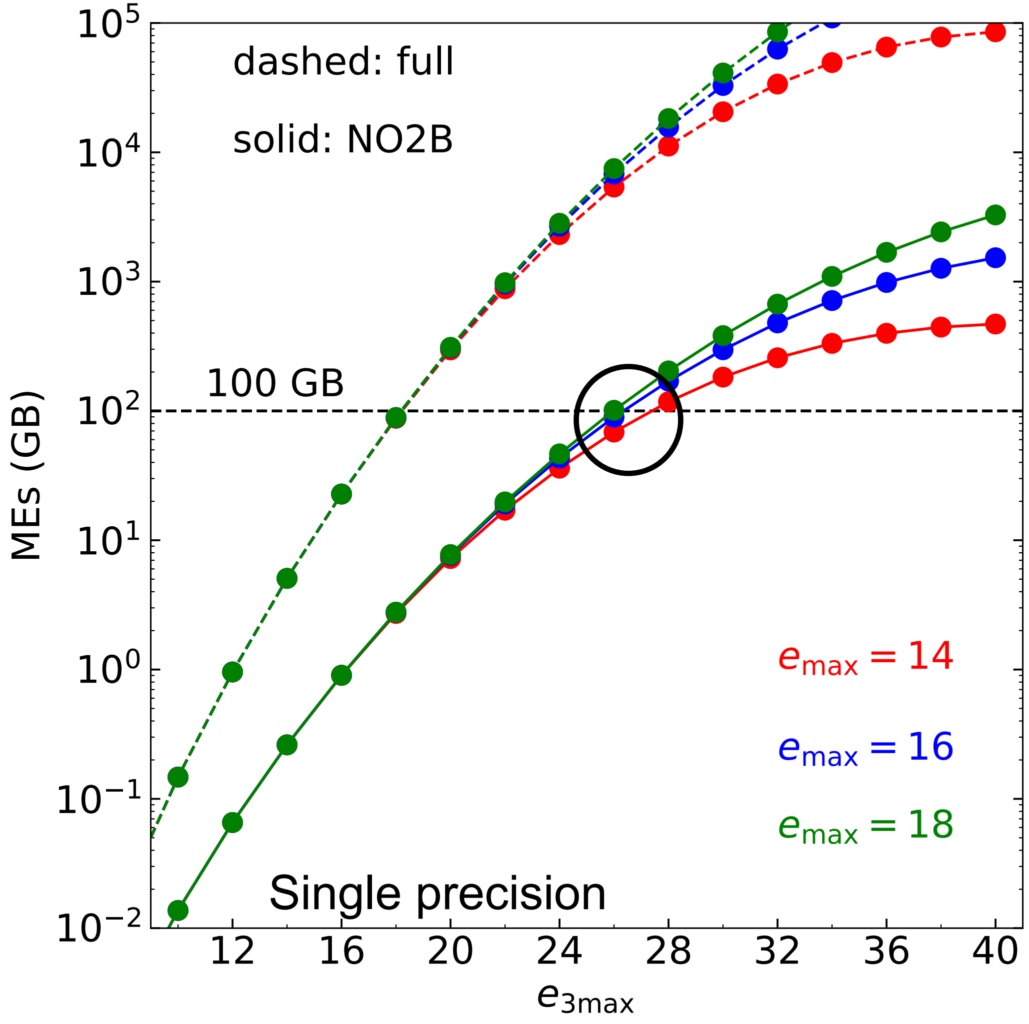
*$e_{3max} = \max(2n_1+l_1+2n_2+l_2+2n_3+l_3)$

Storing 3N matrix elements

- No need all 3N MEs!

$$\langle (a'b':j'_{ab}t'_{ab})c':T|V_{3N}|(ab:j_{ab}t_{ab})c:T\rangle$$
$$= \delta_{j'_{ab}j_{ab}}\delta_{l_{c'}l_c}\delta_{j_{c'}j_c}\sum_J (2J+1)$$
$$\times \langle (a'b':j'_{ab}t'_{ab})c':JT|V_{3N}|(ab:j_{ab}t_{ab})c:JT\rangle$$

- e_{3max}=26 is possible



3N Jacobi => Laboratory frame

- Matrix multiplication form:

$$\langle (a'b':j'_{ab}t'_{ab})c':JT|V_{3N}|(ab:j_{ab}t_{ab})c:JT\rangle$$
$$= 6 \sum_{N_{\rm cm}L_{\rm cm}J_{\rm rel}} \sum_{E'i'} \sum_{Ei} \langle (a'b':j'_{ab}t'_{ab})c':JT|N_{\rm cm}L_{\rm cm}E'i':J_{\rm rel}T\rangle$$
$$\times \langle E'i':J_{\rm rel}T|V_{3N}|Ei:J_{\rm rel}T\rangle$$
$$\times \langle N_{\rm cm}L_{\rm cm}Ei:J_{\rm rel}T|(ab:j_{ab}t_{ab})c:JT\rangle$$

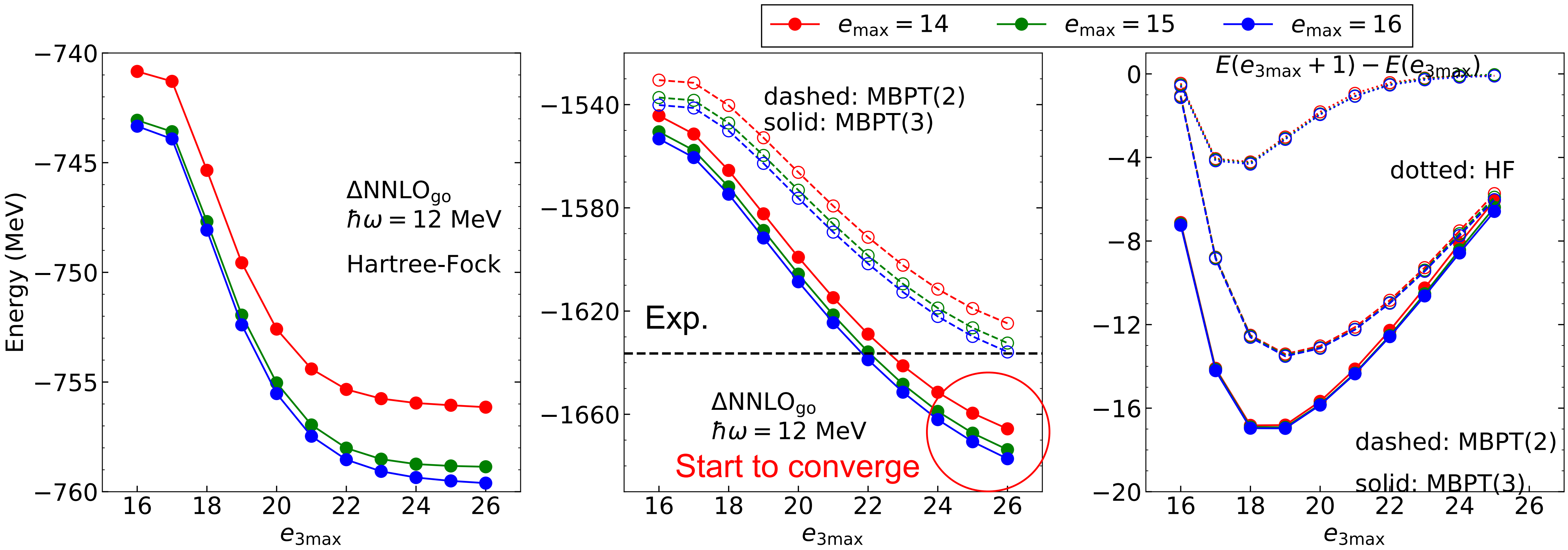
$$\langle N_{\rm cm}L_{\rm cm}Ei:JT|(ab:j_{ab}t_{ab})c:JT\rangle$$
$$= \sum_{\alpha} \langle Ei:JT|E\alpha:JT\rangle$$
$$\times \langle N_{\rm cm}L_{\rm cm}E\alpha:JT|(ab:j_{ab}t_{ab})c:JT\rangle$$
$$\alpha = \{n_{12}, l_{12}, s_{12}, j_{12}.t_{12}, n_3, l_3, j_3\},\ \ (t_{ab}=t_{12})$$

Required RAM for typical channel (e_{3max}=26)

- :cfp ~ O(1) GB
- :T coef. (NAS => Lab) ~O(100) GB
- :T coef. (AS => Lab) ~O(10) GB
- : 3N int (Jacobi) ~O(1) GB
- : 3N int (Lab) ~O(0.1) GB

- Channel-by-channel MPI parallelization
  - ✦# of channels ~ 20000

Results for ^{208}Pb



Summary & Future work

- Due to the CM treatment, choice of the valence space is crucial
- Applicable to neutron-rich region.
- Application for other neutron-rich region.

- Data compression related NO2B approximation allow us to push up the e_{3max} limit.
- Half-precision float and/or additional truncation to reach convergence.

Collaborators:

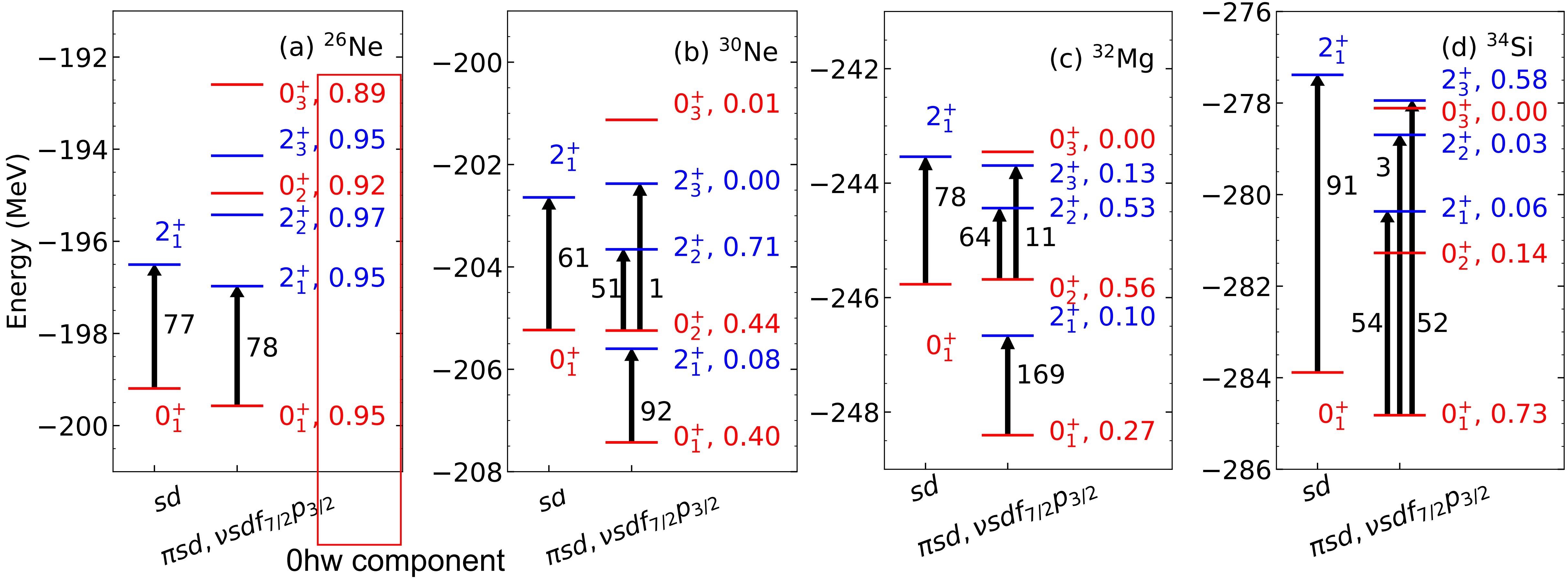
- R. Stroberg[1,2] (U Washington)
- J. D. Holt[1,2] (TRIUMF)
- N. Shimizu[1] (CNS, U Tokyo)
- A. Ekstrom[2] (Chalmers UT)
- C. Forssen[2] (Chalmers UT)
- G. Hagen[2] (ORNL)
- T. Papenbrock[2] (U Tennessee)

1: multi-shell application
2: Towards ^{208}Pb

Special thanks to J. Menendez[1], K. Hebeler[2], and P. Navratil[2]

Single- and multi-shell results

EM 1.8/2.0
e_{max}=12
e_{3max}=16



Single-shell calculations capture the excited states in the multi-shell calculations

3-body T coefficient

A. Nogga et al., Phys. Rev. C **73**, 064002 (2006).
R. Roth et al., Phys. Rev. C **90**, 024325 (2014).

- Basis LS-like method (6 summations):

$$\langle (ab:j_{ab}t_{ab})c:JT|N_{\rm cm}L_{\rm cm}(n_{12}l_{12}s_{12}j_{12}t_{12}n_3l_3j_3:J_{\rm rel}):JT\rangle$$

$$= \delta_{t_{ab}t_{12}}\sum_{l_{ab}}\sqrt{[j_a][j_b][l_{ab}][s_{12}]}\begin{Bmatrix} l_a & 1/2 & j_a \\ l_b & 1/2 & j_b \\ l_{ab} & s_{12} & j_{ab}\end{Bmatrix}\sum_{N_{12}L_{12}}\langle N_{12}L_{12},n_{12}l_{12}:l_{ab}|n_al_a,n_bl_b:l_{ab}\rangle_1$$

$$\times\sum_{LS}\sqrt{[j_{ab}][j_c][L][S]}\begin{Bmatrix} l_{ab} & s_{12} & j_{ab} \\ l_c & 1/2 & j_c \\ L & S & J\end{Bmatrix}\sum_{\lambda}(-1)^{l_{12}+l_c+l_{ab}+\lambda}\sqrt{[l_{ab}][\lambda]}\begin{Bmatrix} l_{12} & L_{12} & l_{ab} \\ l_c & L & \lambda\end{Bmatrix}$$

$$\times\langle N_{\rm cm}L_{\rm cm},n_3l_3:\lambda|N_{12}L_{12},n_cl_c:\lambda\rangle_2\sum_{\Lambda}(-1)^{L_{\rm cm}+l_3+l_{12}+L}\sqrt{[\lambda][\Lambda]}\begin{Bmatrix} L_{\rm cm} & l_3 & \lambda \\ l_{12} & L & \Lambda\end{Bmatrix}$$

$$\times(-1)^{L_{\rm cm}+\Lambda+S+J}\sqrt{[L][J_{\rm rel}]}\begin{Bmatrix} L_{\rm cm} & \Lambda & L \\ S & J & J_{\rm rel}\end{Bmatrix}(-1)^{l_3+l_{12}-\Lambda}\sqrt{[j_{12}][j_3][\Lambda][S]}\begin{Bmatrix} l_{12} & s_{12} & j_{12} \\ l_3 & 1/2 & j_3 \\ \Lambda & S & J_{\rm rel}\end{Bmatrix}$$

HO bracket convention is same as in G. P. Kamuntavičius, et al., Nucl. Phys. A **695**, 191 (2001).

3-body T coefficient

- More efficient jj-like method (4 summations):

$$
\begin{aligned}
&\langle (ab : j_{ab} t_{ab}) c : JT | N_{\rm cm} L_{\rm cm} (n_{12} l_{12} s_{12} j_{12} t_{12} n_3 l_3 j_3 : J_{\rm rel}) : JT \rangle \\
&= \delta_{t_{ab} t_{12}} \sum_{l_{ab}} \sqrt{[j_a][j_b][l_{ab}][s_{12}]} \begin{Bmatrix} l_a & 1/2 & j_a \\ l_b & 1/2 & j_b \\ l_{ab} & s_{12} & j_{ab} \end{Bmatrix} \sum_{N_{12} L_{12}} \langle N_{12} L_{12}, n_{12} l_{12} : l_{ab} | n_a l_a, n_b l_b : l_{ab} \rangle_1 \\
&\quad \times (-1)^{L_{12} + s_{12} + l_{12} + j_{ab}} \sqrt{[l_{ab}][j_{12}]} \begin{Bmatrix} L_{12} & l_{12} & l_{ab} \\ s_{ab} & j_{ab} & j_{12} \end{Bmatrix} \sum_{\Lambda} (-1)^{j_{12} + j_c + j_{ab} + \Lambda} \sqrt{[j_{ab}][\Lambda]} \begin{Bmatrix} j_{12} & L_{12} & j_{ab} \\ j_c & J & \Lambda \end{Bmatrix} \\
&\quad \times \sum_{\lambda} (-1)^{L_{12} + l_c + 1/2 + \Lambda} \sqrt{[\lambda][j_c]} \begin{Bmatrix} L_{12} & l_c & \lambda \\ 1/2 & \Lambda & j_c \end{Bmatrix} \langle N_{\rm cm} L_{\rm cm}, n_3 l_3 : \lambda | N_{12} L_{12}, n_c l_c : \lambda \rangle_2 \\
&\quad \times (-1)^{L_{\rm cm} + l_3 + 1/2 + \Lambda} \sqrt{[\lambda][j_3]} \begin{Bmatrix} L_{\rm cm} & l_3 & \lambda \\ 1/2 & \Lambda & j_3 \end{Bmatrix} (-1)^{L_{\rm cm} + j_3 + j_{12} + J} \sqrt{[\Lambda][J_{\rm rel}]} \begin{Bmatrix} L_{\rm cm} & j_3 & \Lambda \\ j_{12} & J & J_{\rm rel} \end{Bmatrix} \\
&\quad \times (-1)^{j_{12} + j_3 - J_{\rm rel}}
\end{aligned}
$$

*four 6j symbols can be one 12j symbol.

HO bracket convention is same as in G. P. Kamuntavičius, et al., Nucl. Phys. A **695**, 191 (2001).