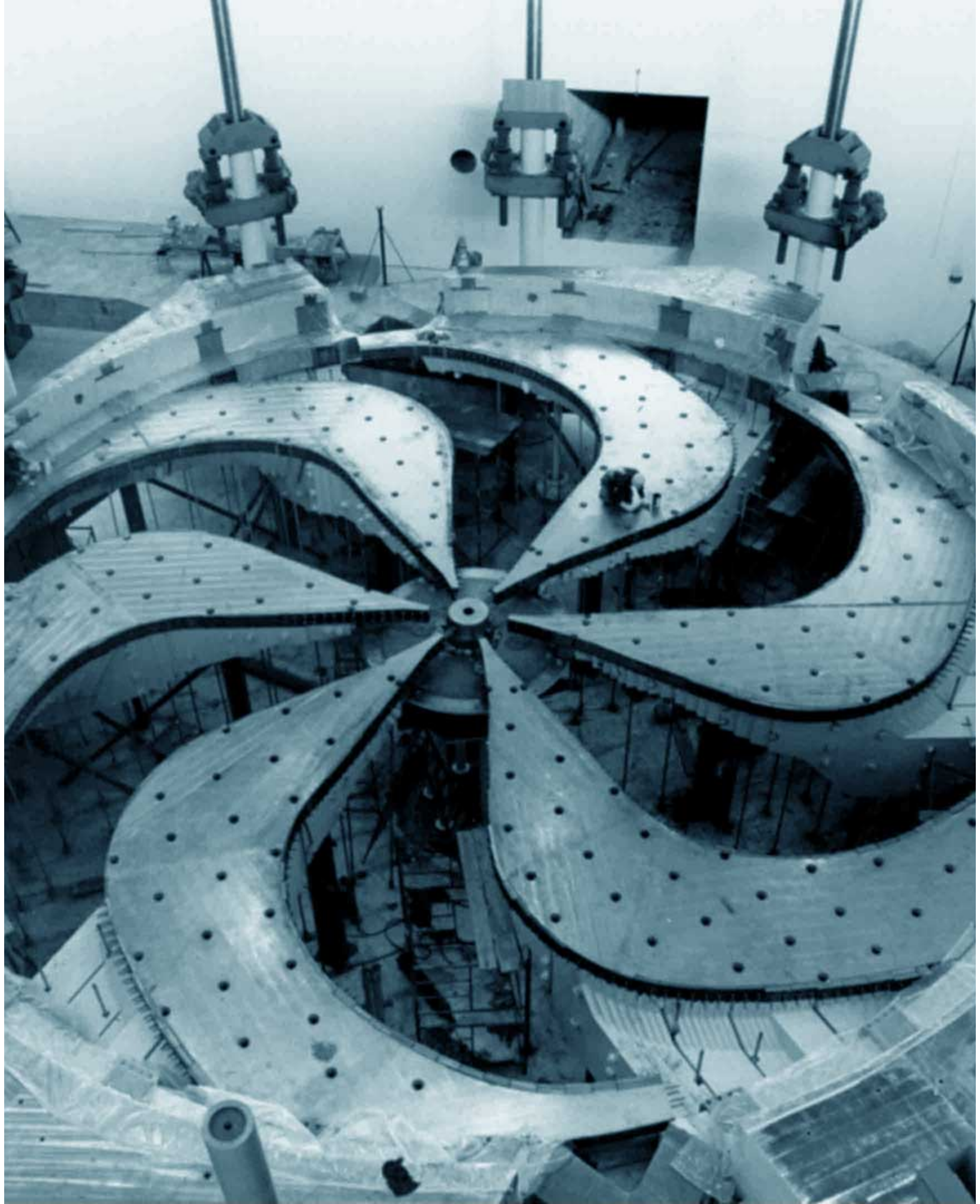
TRIUMF

Towards multi-major-shell effective hamiltonian from IMSRG



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Progress in Ab Initio Techniques in Nuclear Physics
February 26 - March 1, 2019

Discovery, accelerated

Motivation

- Ab initio extension to shell-model calculation is a powerful tool.
- CCM+SM
  - G. R. Jansen, M. D. Schuster, A. Signoracci, G. Hagen, and P. Navrátil, Phys. Rev. C **94**, 011301 (2016).
  - Z. H. Sun, T. D. Morris, G. Hagen, G. R. Jansen, and T. Papenbrock, Phys. Rev. C **98**, 054320 (2018).
- IM-SRG+SM
  - S. R. Stroberg, H. Hergert, J. D. Holt, S. K. Bogner, and A. Schwenk, Phys. Rev. C **93**, 051301 (2016).
  - S. R. Stroberg, A. Calci, H. Hergert, J. D. Holt, S. K. Bogner, R. Roth, and A. Schwenk, Phys. Rev. Lett. **118**, 032502 (2017).

Motivation

- Two-major-shell effective Hamiltonian is required:
  - ✦For unnatural parity state
  - ✦For excitation spectra for doubly closed (^{16}O, ^{40}Ca, …)
  - ✦For exotic nuclei far from stability (Island of inversion, …)
  - ✦…

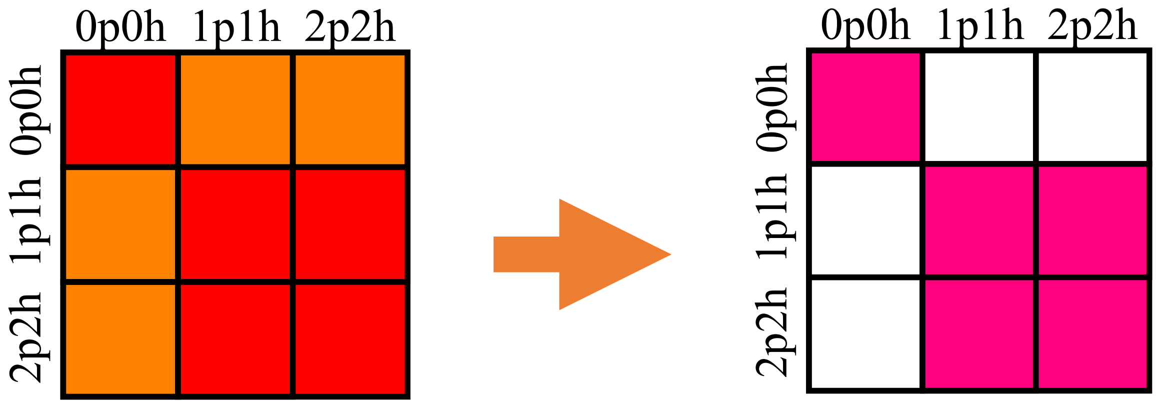
Motivation

- Shell-model effective Hamiltonian across the major shells:
  - Phenomenological
    - *psd*-shell, *sdpf*-shell, …
  - Ab initio
    - Many-body perturbation theory
    - IM-SRG (this work)

H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tsukiyama, Phys. Rep. **621**, 165 (2016).
S. R. Stroberg, A. Calci, H. Hergert, J. D. Holt, S. K. Bogner, R. Roth, and A. Schwenk, Phys. Rev. Lett. **118**, 032502 (2017).

IM-SRG (Quick reminder)

- In-medium similarity renormalization group:



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

s: flow parameter

$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\eta_{ab} f_{ba} + \frac{1}{2}\sum_{abcd} \eta_{abcd}\Gamma_{cdab} n_a n_b \overline{n}_c \overline{n}_d$$

$$\frac{df_{12}}{ds} = \sum_a (1+P_{12})\eta_{1a} f_{a2} + \frac{1}{2}\sum_{ab}(n_a - n_b)(\eta_{ab}\Gamma_{b1a2} - f_{ab}\eta_{b1a2}) + \frac{1}{2}\sum_{abc}(n_a n_b \overline{n}_c + \overline{n}_a \overline{n}_b n_c)(1+P_{12})\eta_{c1ab}\Gamma_{abc2}$$

$$\frac{d\Gamma_{1234}}{ds} = \sum_a [(1-P_{12})(\eta_{1a}\Gamma_{a234} - f_{1a}\eta_{a234}) - (1-P_{34})(\eta_{a3}\Gamma_{12a4} - f_{a3}\eta_{12a3})] + \frac{1}{2}\sum_{ab}(1 - n_a - n_b)(\eta_{12ab}\Gamma_{ab34} - \Gamma_{12ab}\eta_{ab34}) - \sum_{ab}(n_a - n_b)(1-P_{12})(1-P_{34})\eta_{b2a4}\Gamma_{a1b3}$$

n_a : occupation number

$\overline{n}_a = 1 - n_a$

H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tsukiyama, Phys. Rep. **621**, 165 (2016).
S. R. Stroberg, A. Calci, H. Hergert, J. D. Holt, S. K. Bogner, R. Roth, and A. Schwenk, Phys. Rev. Lett. **118**, 032502 (2017).

IM-SRG (Quick reminder)

- In-medium similarity renormalization group:

Generator is chosen to suppress the off diagonal component:

$$\eta_{12} = \frac{f_{12}}{f_{11} - f_{22} + \Gamma_{1212}}$$

$$\eta_{1234} = \frac{\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234}}$$

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

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

$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\eta_{ab} f_{ba} + \frac{1}{2}\sum_{abcd}\eta_{abcd}\Gamma_{cdab} n_a n_b \overline{n}_c \overline{n}_d$$

$$\frac{df_{12}}{ds} = \sum_{a}(1 + P_{12})\eta_{1a} f_{a2} + \frac{1}{2}\sum_{ab}(n_a - n_b)(\eta_{ab}\Gamma_{b1a2} - f_{ab}\eta_{b1a2}) + \frac{1}{2}\sum_{abc}(n_a n_b \overline{n}_c + \overline{n}_a \overline{n}_b n_c)(1 + P_{12})\eta_{c1ab}\Gamma_{abc2}$$

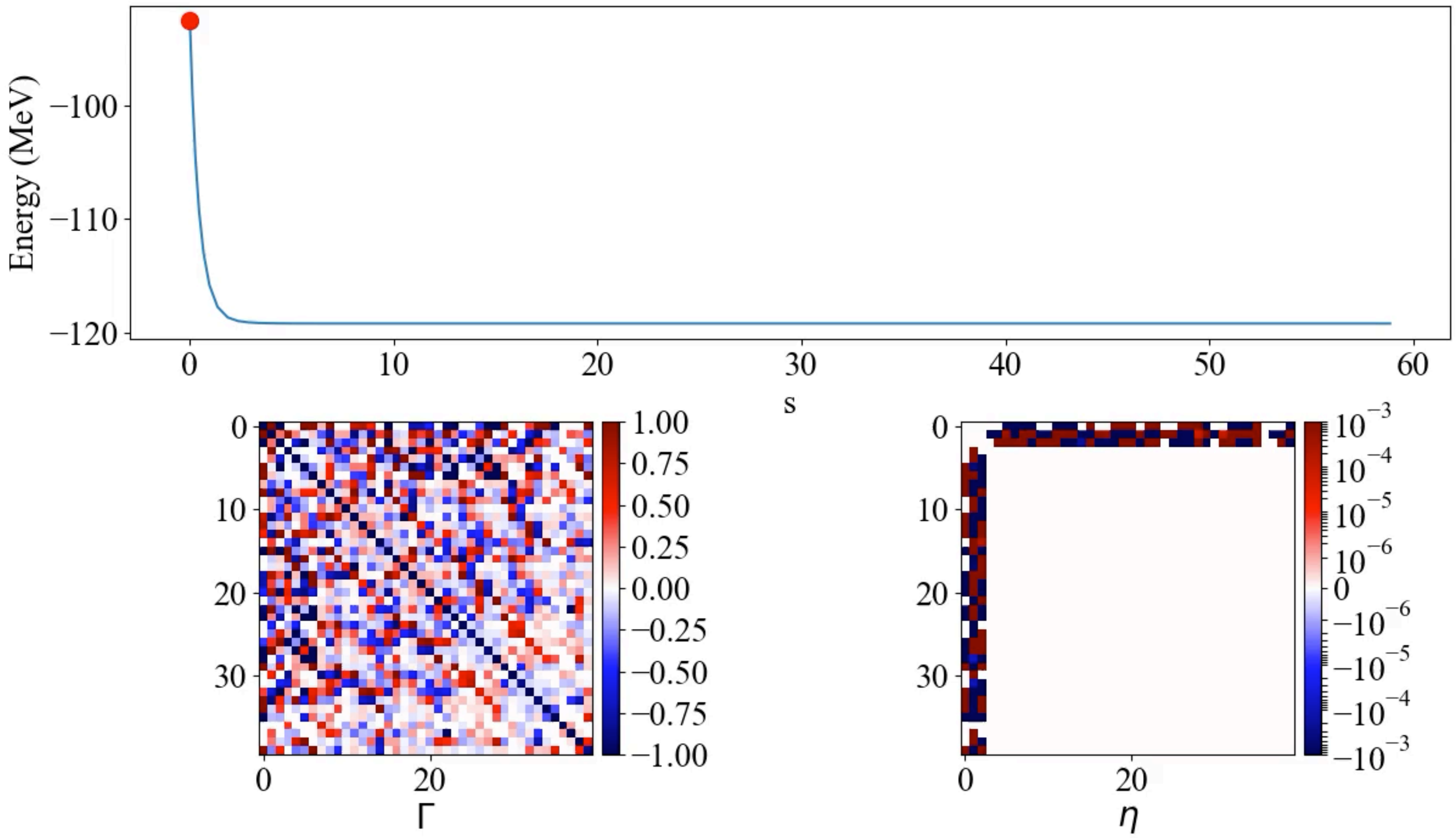
$$\frac{d\Gamma_{1234}}{ds} = \sum_{a}[(1 - P_{12})(\eta_{1a}\Gamma_{a234} - f_{1a}\eta_{a234}) - (1 - P_{34})(\eta_{a3}\Gamma_{12a4} - f_{a3}\eta_{12a3})] + \frac{1}{2}\sum_{ab}(1 - n_a - n_b)(\eta_{12ab}\Gamma_{ab34} - \Gamma_{12ab}\eta_{ab34}) - \sum_{ab}(n_a - n_b)(1 - P_{12})(1 - P_{34})\eta_{b2a4}\Gamma_{a1b3}$$

n_a : occupation number

$\overline{n}_a = 1 - n_a$

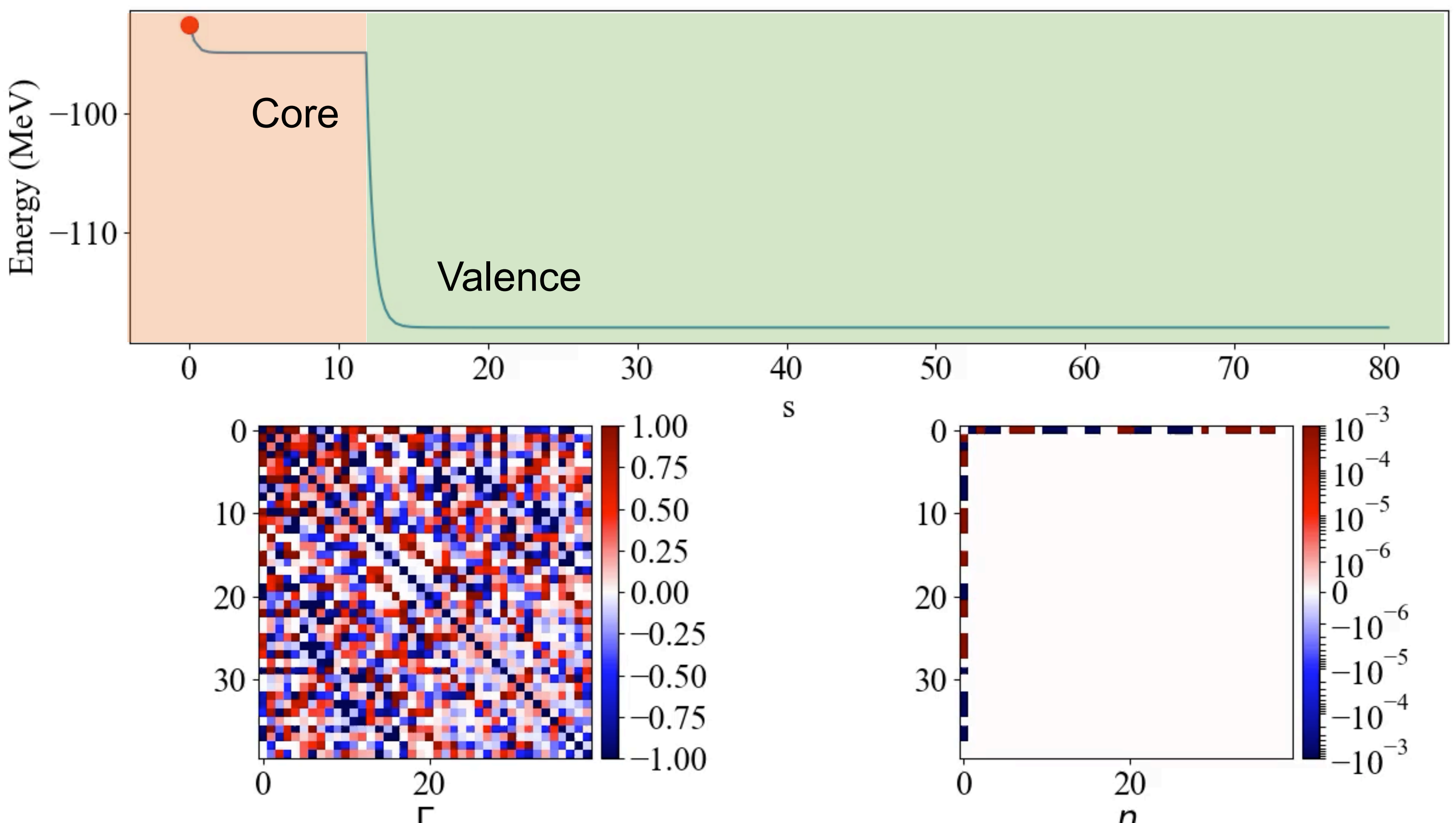
IM-SRG (Quick reminder)

Evolution for single reference problem (^{14}C w/ SRG evolved NN-only)



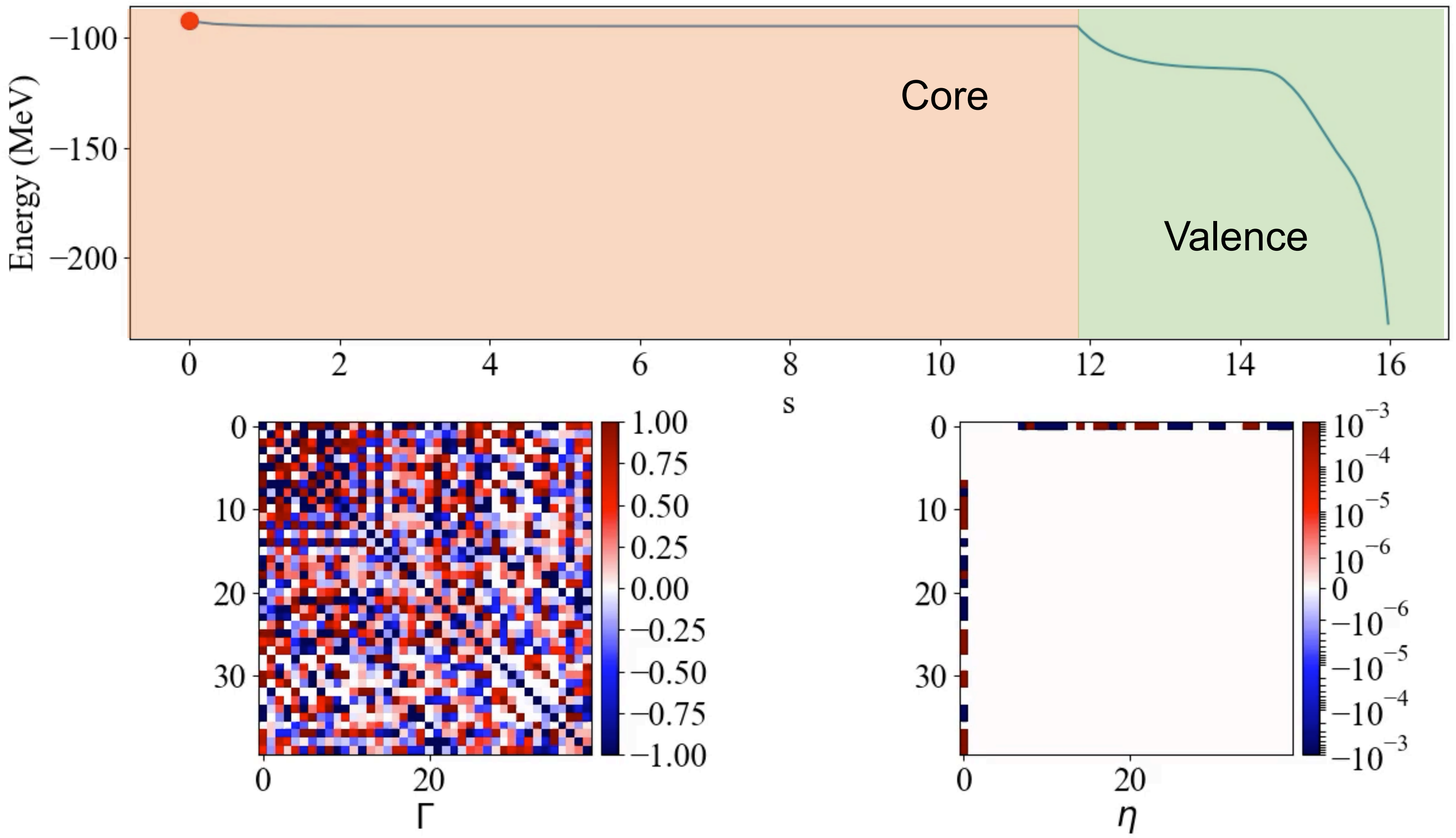
IM-SRG (Quick reminder)

Evolution for p-shell problem (^{14}C [^{4}He core] w/ SRG evolved NN-only)



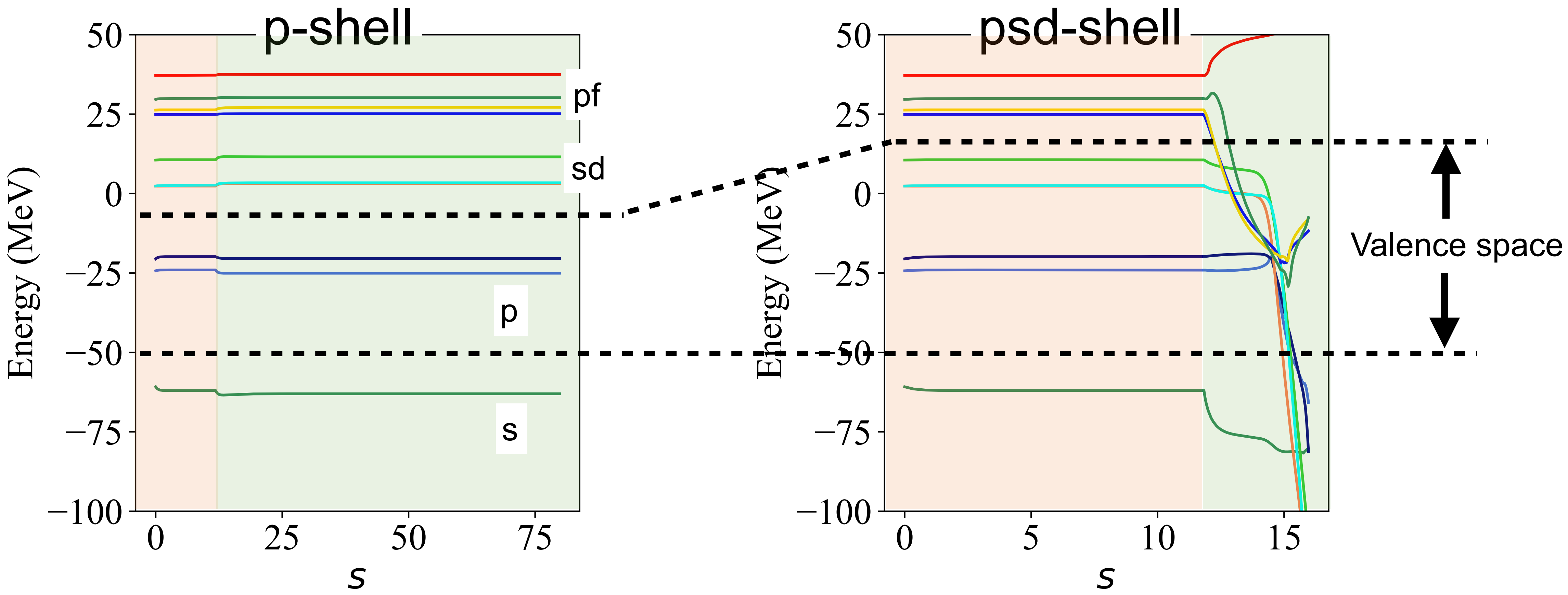
IM-SRG for two-major shell valence space problem

Evolution for psd-shell problem (^{14}C [^{4}He core] w/ SRG evolved NN-only)



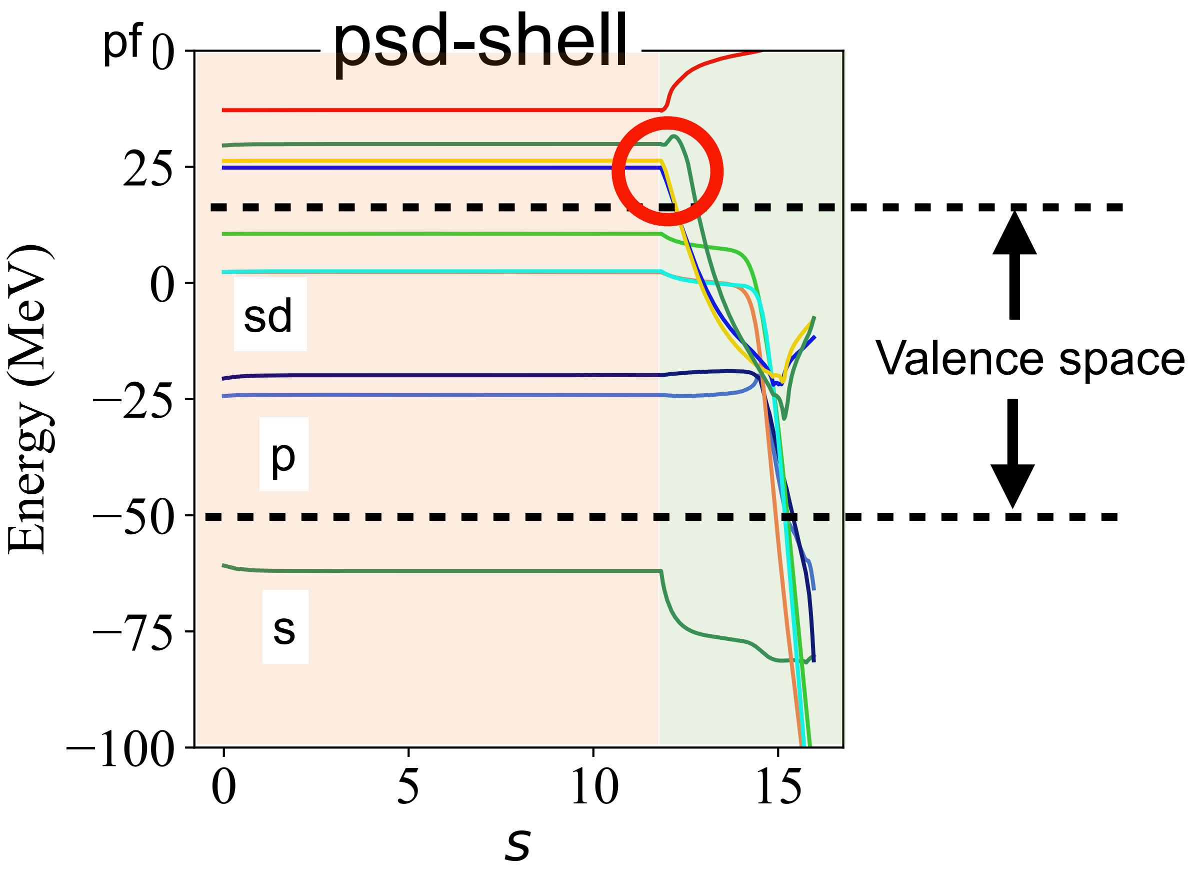
How it fail

- Flow of single-particle energies



How it fail

- Flow of single-particle energies
  - At the very beginning of valence-decoupling flow, some of pf-shell orbits come down.
  - Intuitively, we expect that P- and Q-space single particle energies do not mix.
  - At the beginning of the flow, the slope of single-particle energies (df/ds) seems to be crucial.



Flow equation for single-particle energies

- Flow equation for S.P.Es:

$$\frac{df_{pp}}{ds} = 2\sum_{a}\eta_{pa}f_{ap} + \frac{1}{2}\sum_{ab}(n_a - n_b)(\eta_{ab}\Gamma_{bpap} - f_{ab}\eta_{bpap})$$
$$+ \sum_{abc}(n_a n_b \overline{n}_c + \overline{n}_a \overline{n}_b n_c)\eta_{cpab}\Gamma_{abcp}$$

- Assuming White generator:

$$\eta_{12} = \frac{f_{12}}{f_{11} - f_{22}}$$
$$\eta_{1234} = \frac{\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44}}$$

Flow equation for single-particle energies

- Assuming HF basis:

$$\frac{df_{pp}}{ds} \sim \sum_{p'} \sum_{hh'} \frac{|\Gamma_{hh'pp'}|^2}{f_{pp} + f_{p'p'} - f_{hh} - f_{h'h'}} + \sum_{p'p''} \sum_{h} \frac{|\Gamma_{php'p''}|^2}{f_{pp} + f_{hh} - f_{p'p'} - f_{p''p''}}$$

- We can modify the denominator so that $\frac{df_{pp}}{ds} \geq 0$

Flow equation for single-particle energies

- Modifying the generator
  - ✦Simple way is to give the constant shift to energy denominator

K. Suzuki, Prog. Theor. Phys. **58**, 1064 (1977).

N. Tsunoda, K. Takayanagi, M. Hjorth-Jensen, and T. Otsuka, Phys. Rev. C **89**, 024313 (2014).

$$\eta_{12} = \frac{f_{12}}{f_{11} - f_{22} + \Gamma_{1212}}$$

$$\eta_{1234} = \frac{\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234}}$$

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

→

$$\eta_{12} = \frac{f_{12}}{f_{11} - f_{22} + \Gamma_{1212} + \Delta}$$

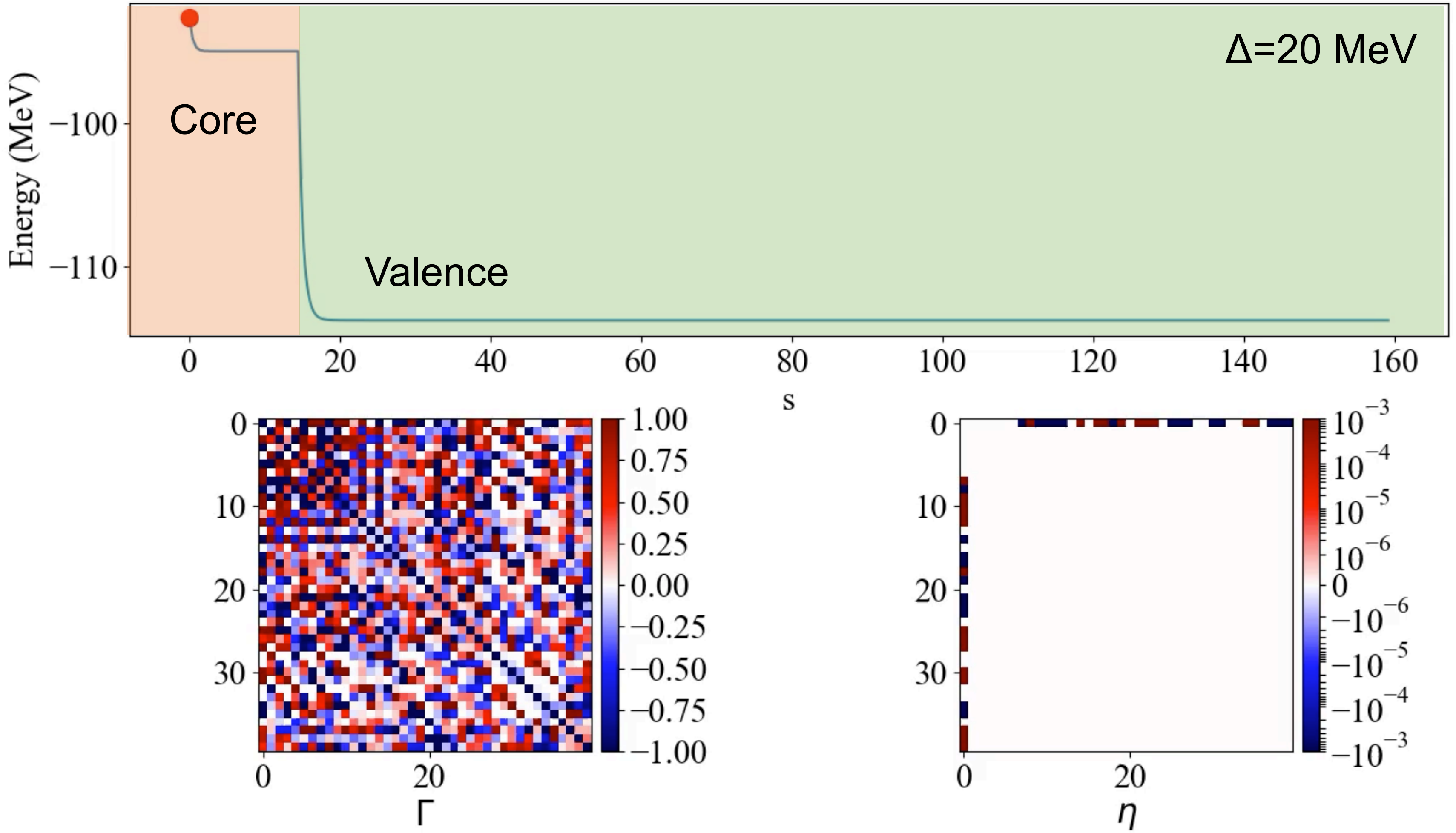
$$\eta_{1234} = \frac{\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234} + \Delta}$$

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

  - ✦For our purpose, suitable choice of Δ would be comparable to hw.

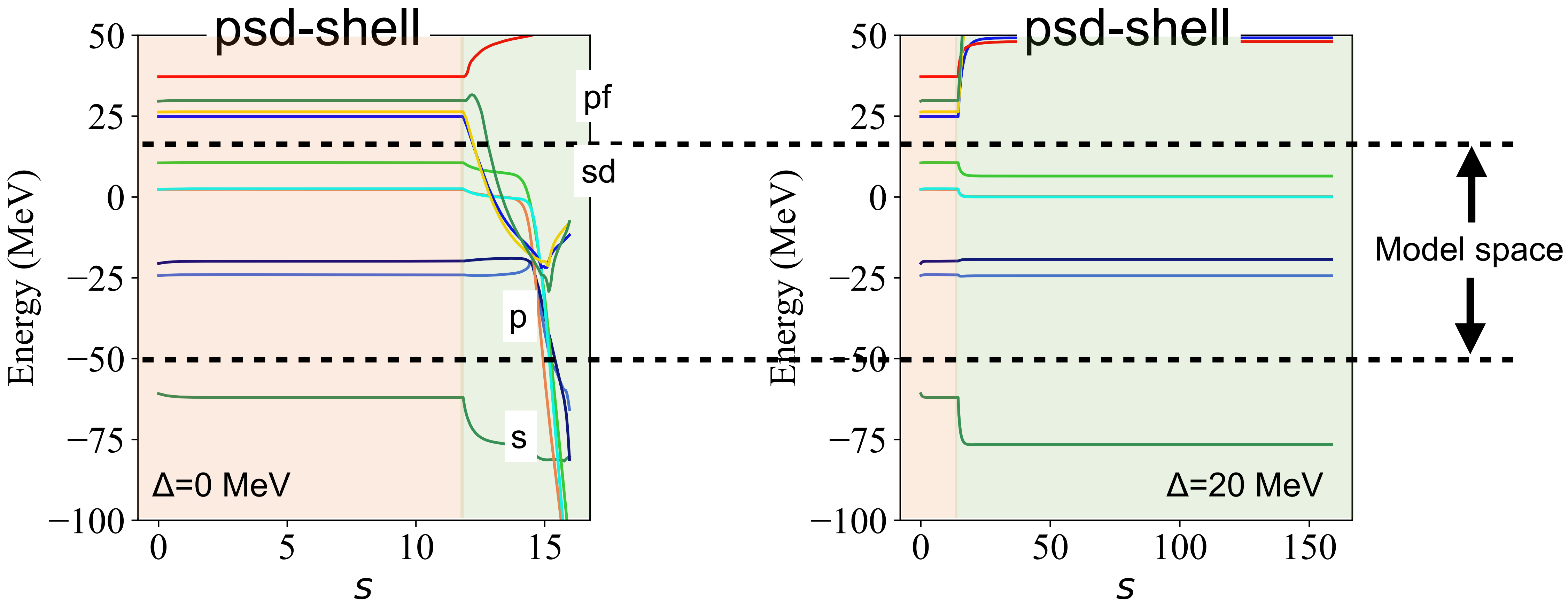
Does it really work?

Evolution for psd-shell problem (^{14}C [^{4}He core] w/ SRG evolved NN-only)



Does it really work?

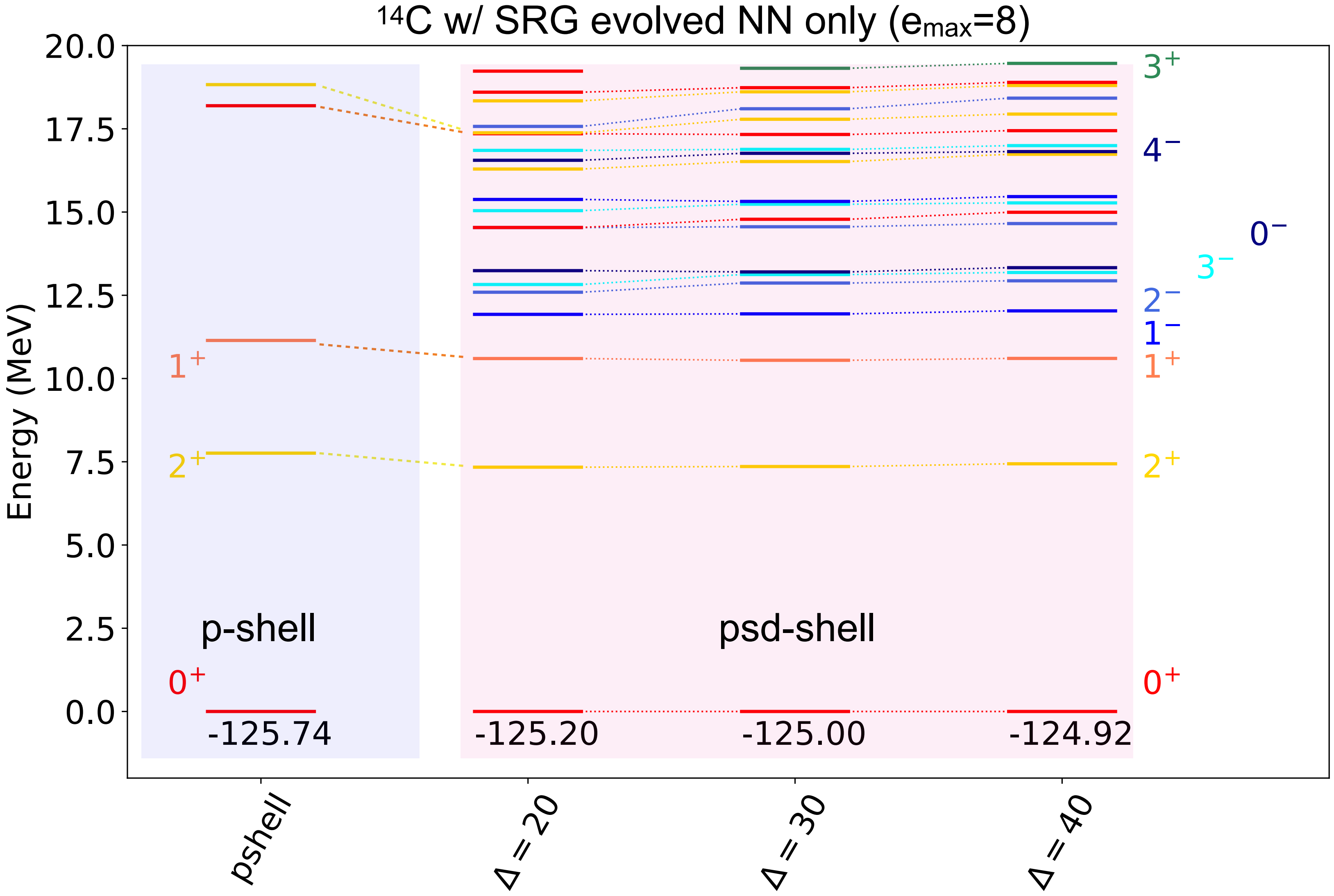
- Flow of single-particle energies



What is Δ?

- Introduction of Δ can be regarded as the choice of the generator.
  - There are some variations:
    - Wegner
    - White
    - Imaginary time
    - …
  - It can affect to the strength of induced many-body terms

Comparison with single major shell calculation

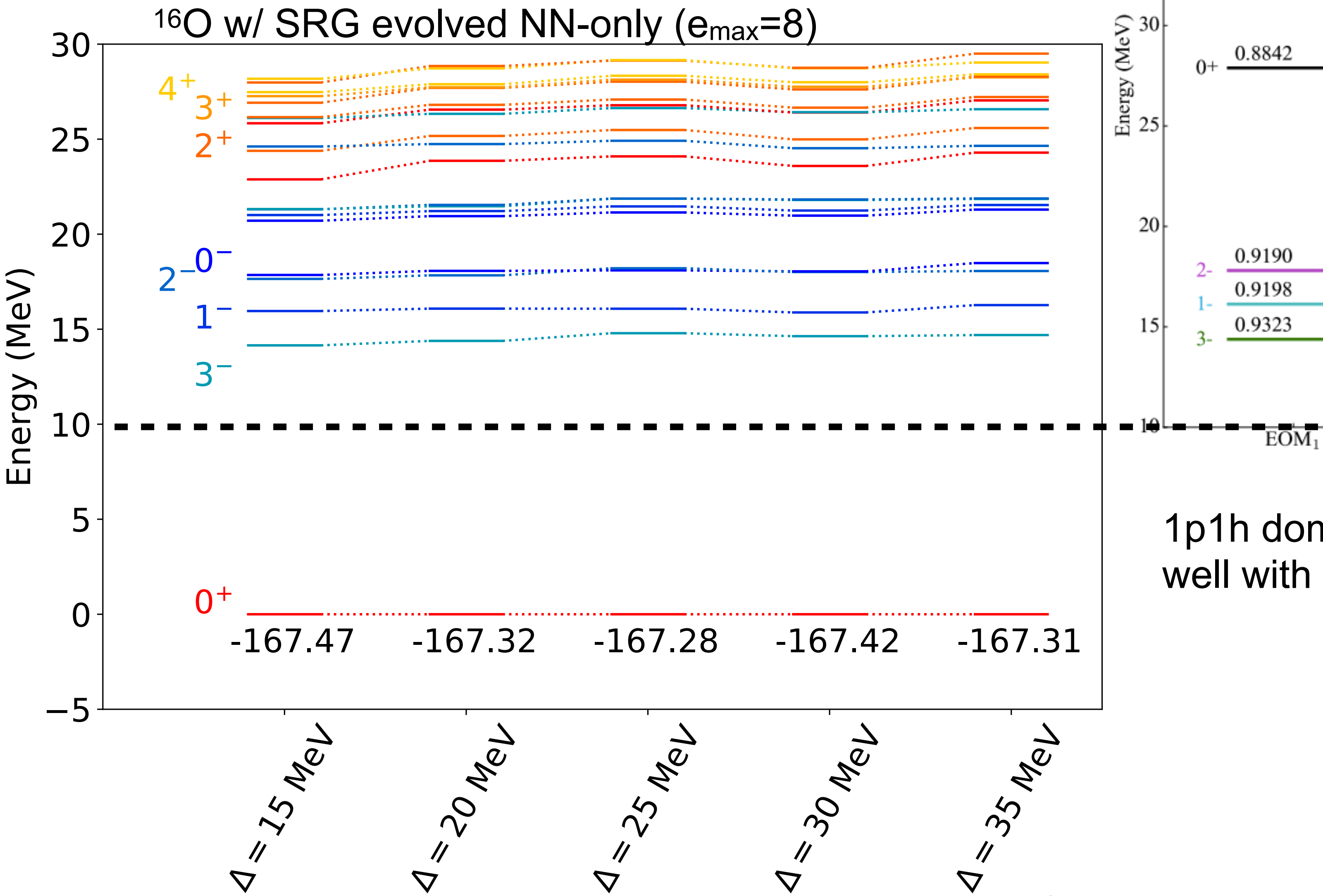


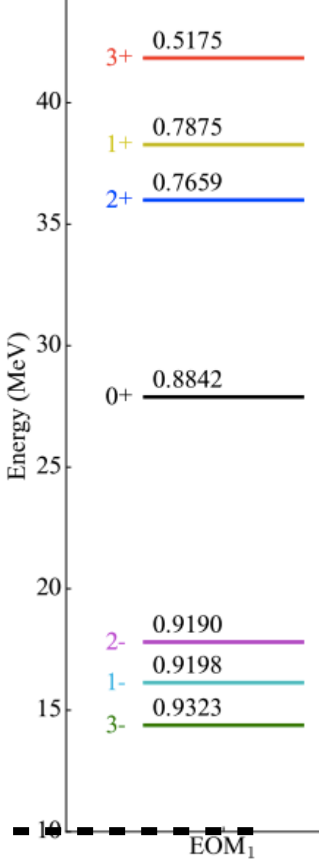
Including negative parity states, many states can appear from psd calculations.

For 0^+_1, 2^+_1, and 1^+_1, p-shell configurations are more than 90%. Also the energies are reasonably close to p-shell results.

Δ dependence is not unique

Comparison with EOM method



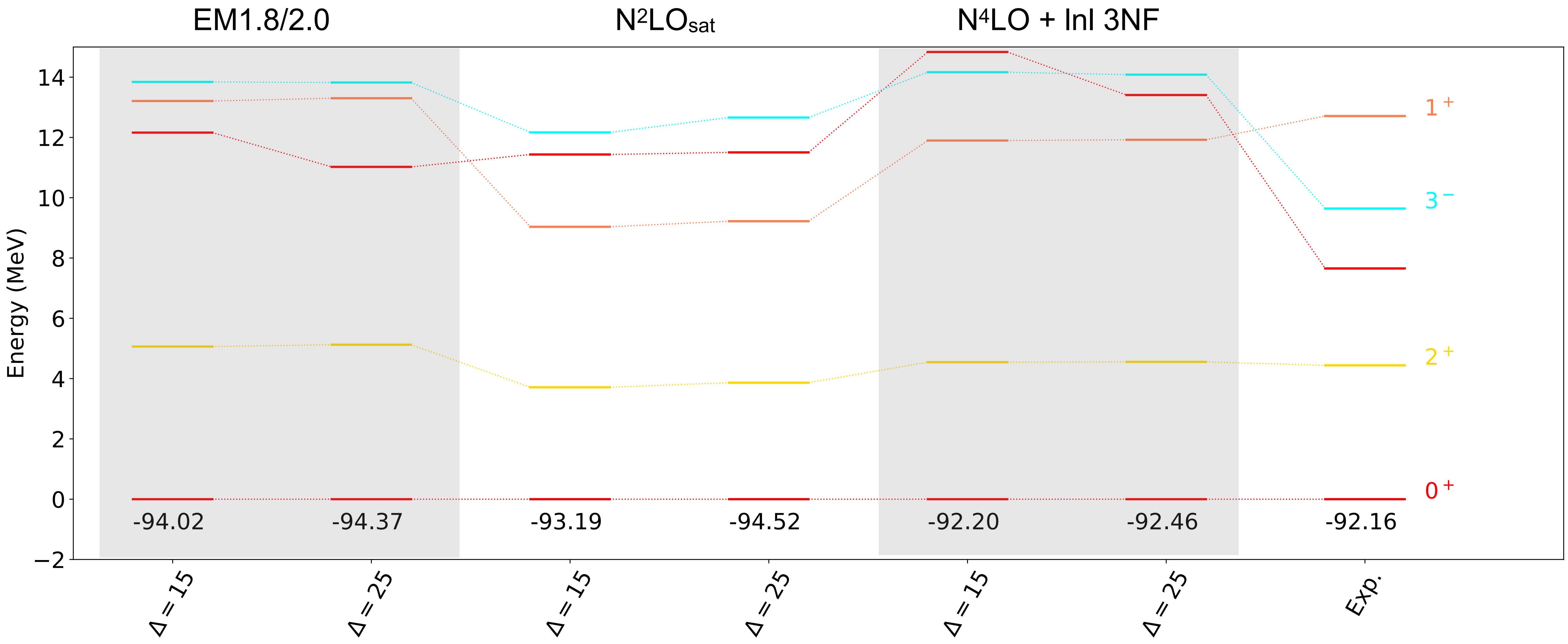


1p1h dominant lowest 3$^-$, 1$^-$, 2$^-$ agree well with the EOM-IMSRG results.

EOM-IMSRG results are take from N. M. Parzuchowski, T. D. Morris, and S. K. Bogner, Phys. Rev. C **95**, 044304 (2017).

^{12}C energies from *psd* calculations

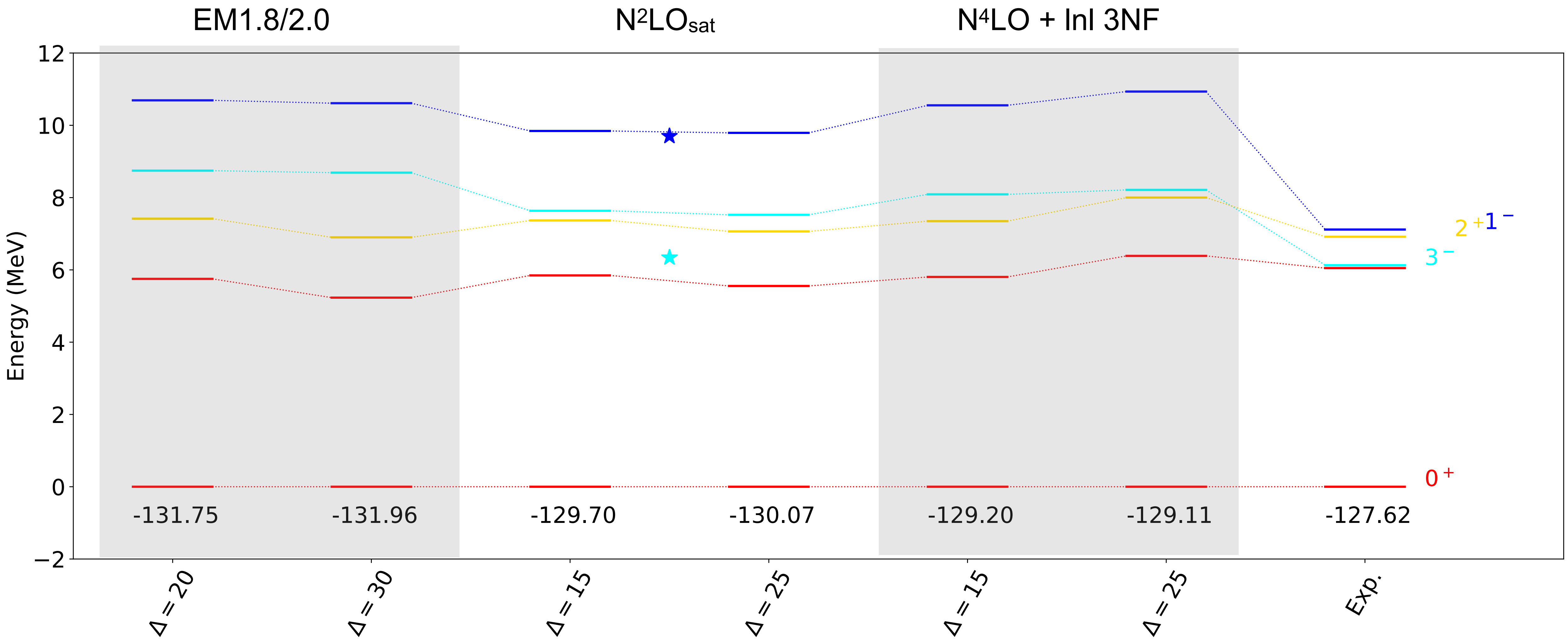
All calculation results are obtained @ e_{max}=10



★: EOM-CCM [A. Ekström,et al., Phys. Rev. C **91**, 051301 (2015).]

^{16}O energies from *psd* calculations

All calculation results are obtained @ e_{max}=10



Center-of-mass issue

- So far, we added the center-of-mass Hamiltonian at the shell-model calculation stage:

$$H \longrightarrow H_{\mathrm{VS}} + \beta H_{\mathrm{cm}} \longrightarrow \text{energies}$$

- But, H_{VS} is no longer represented in HO basis. We should add H_{cm} from the beginning:

$$H + \beta H_{\mathrm{cm}} \longrightarrow H_{\mathrm{VS}} \longrightarrow \text{energies}$$

Summary & Future work

- By adding the shift in energy denominator, the two-major shell-model effective Hamiltonian can be obtained.
- Obtained results are promising

- Treatment of center-of-mass motion
- Comparison with NCSM
- Application to island of inversion