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Advances in the In-Medium Active-Space CI

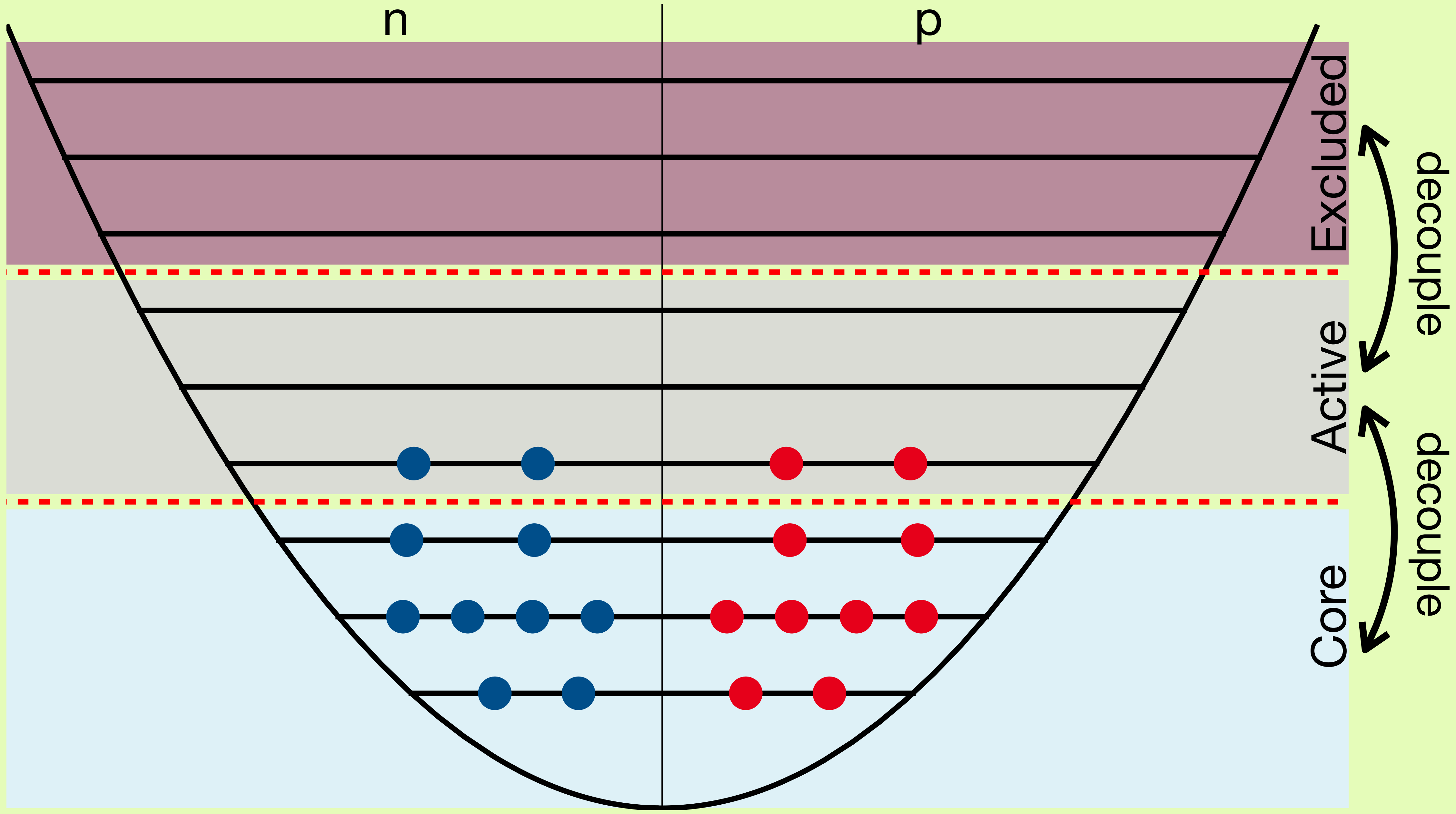
Cedric Wenz | AG R. Roth | IKP @ TU Darmstadt

Hessisches Kompetenzzentrum für Hochleistungsrechnen

IM-ASCI

Workflow

- Define partitioning of single-particle basis into core, active and excluded states
- Constrained HF with small CI run to construct multi-det. reference state $|\psi_{\text{ref}}\rangle$
- Normal order 2B approx. w.r.t. $|\psi_{\text{ref}}\rangle$
- Decouple active-space in MR-IM-SRG(2)
- Diagonalize decoupled active-space in final CI calculation to extract observables



$$\frac{\mathrm{d}}{\mathrm{d}s}H(s) = [\eta(s), H(s)]$$

IM-ASCI vs VS-IMSRG

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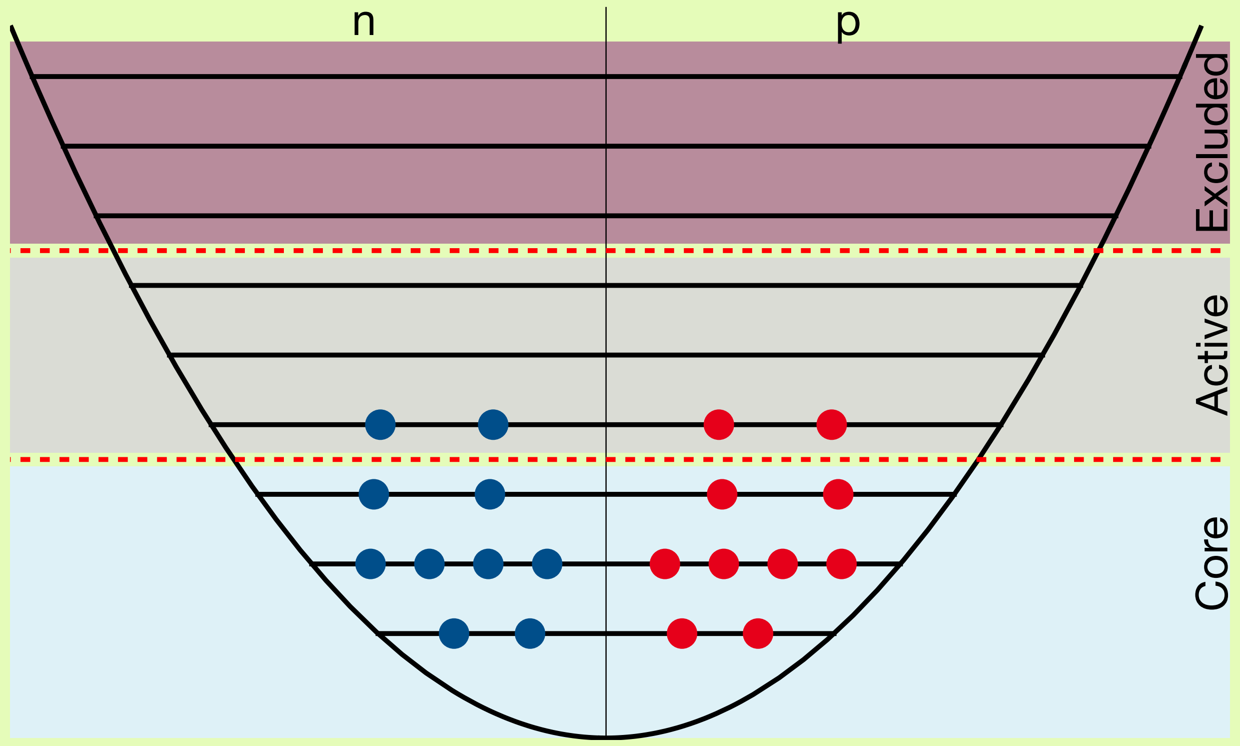
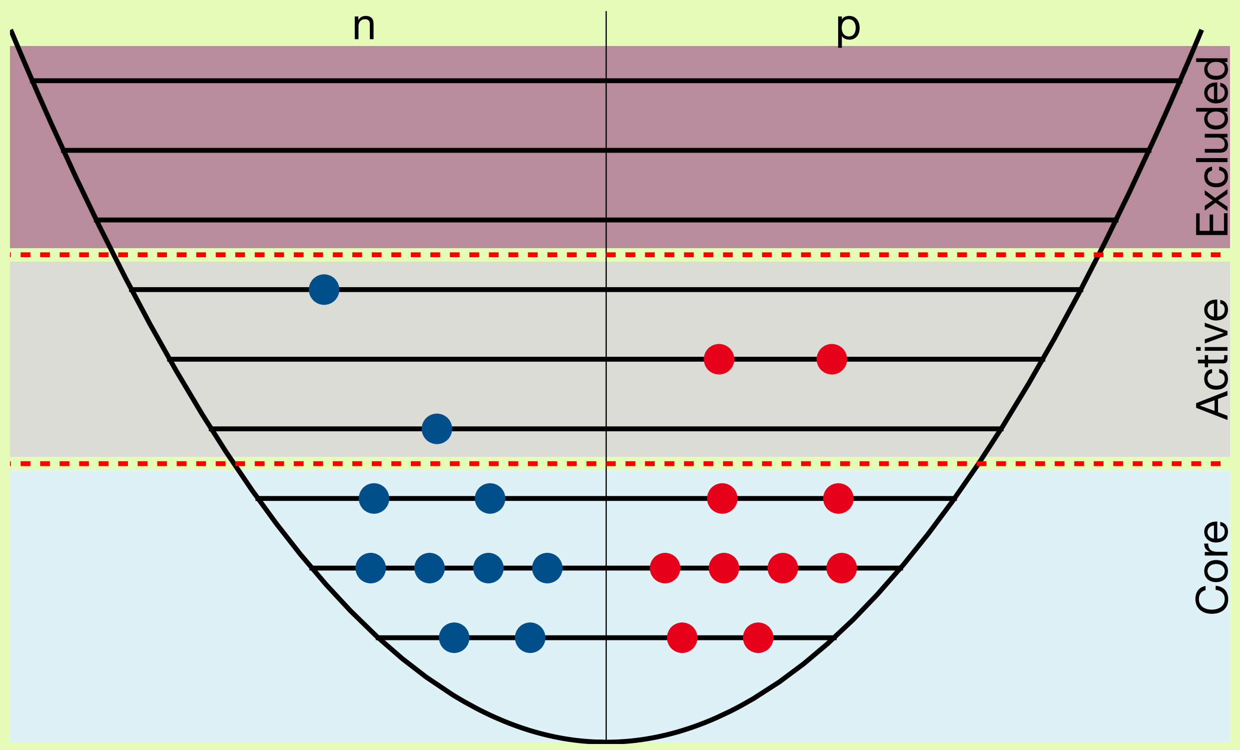
IM-ASCI	VS-IMSRG
• Multi-determinantal reference state $\|\psi_{\mathrm{ref}}\rangle$	• Single Slater determinant $\|\psi_{\mathrm{ref}}\rangle$
• $\|\psi_{\mathrm{ref}}\rangle$ is the nucleus of interest	• $\|\psi_{\mathrm{ref}}\rangle$ is closest closed-shell nucleus
• Irreducible densities $\lambda^{[1]}, \lambda^{[2]}$	• Ensemble normal ordering
• MR-IMSRG framework	• SR-IMSRG framework
• Multi-shell decoupling possible	• Multi-shell decoupling only artificially

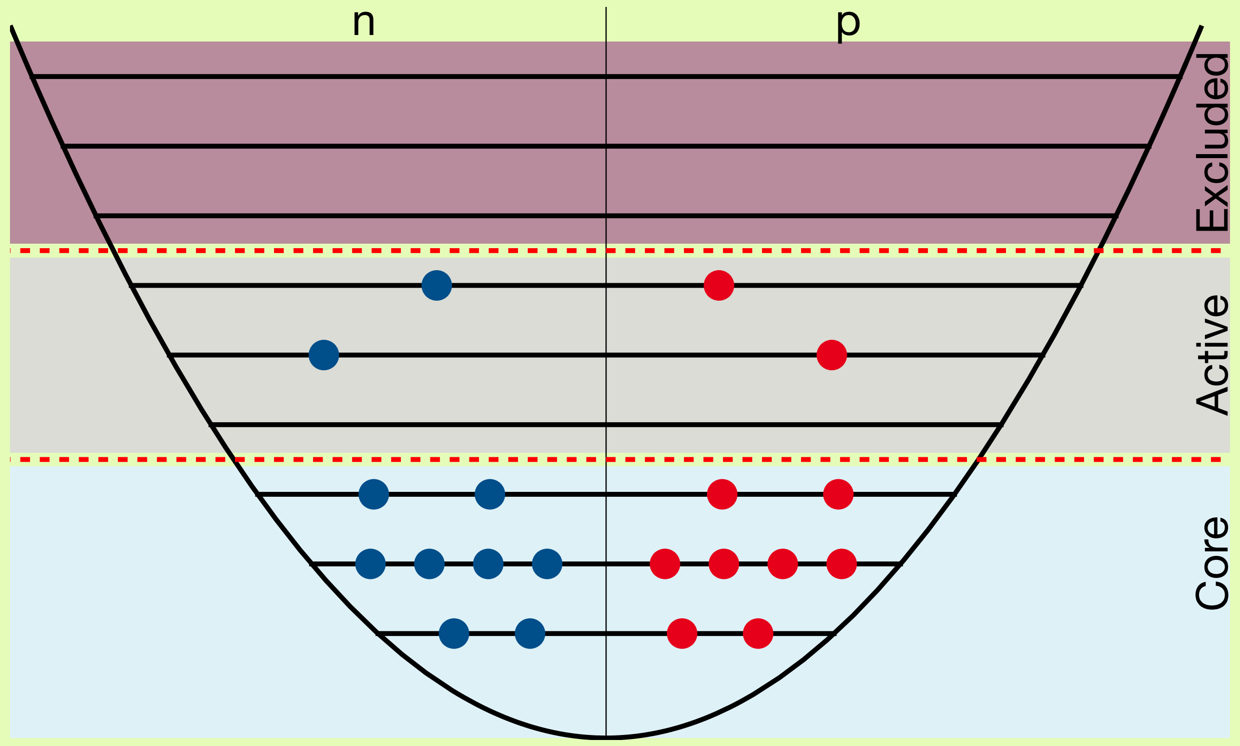
$|\psi_{\mathrm{ref}}\rangle_{\mathrm{AS}} = \mathcal{N}_1 \cdot$



$+ \mathcal{N}_2 \cdot$



$+ \mathcal{N}_3 \cdot$



$+ \ldots$

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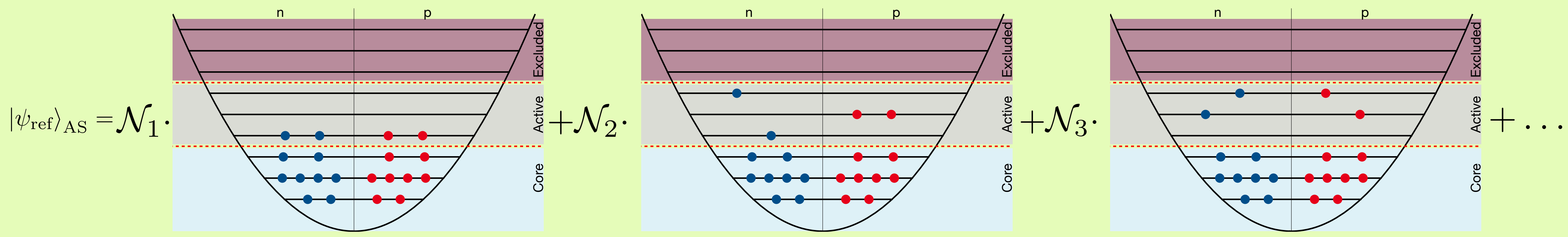
IM-ASCI vs VS-IMSRG

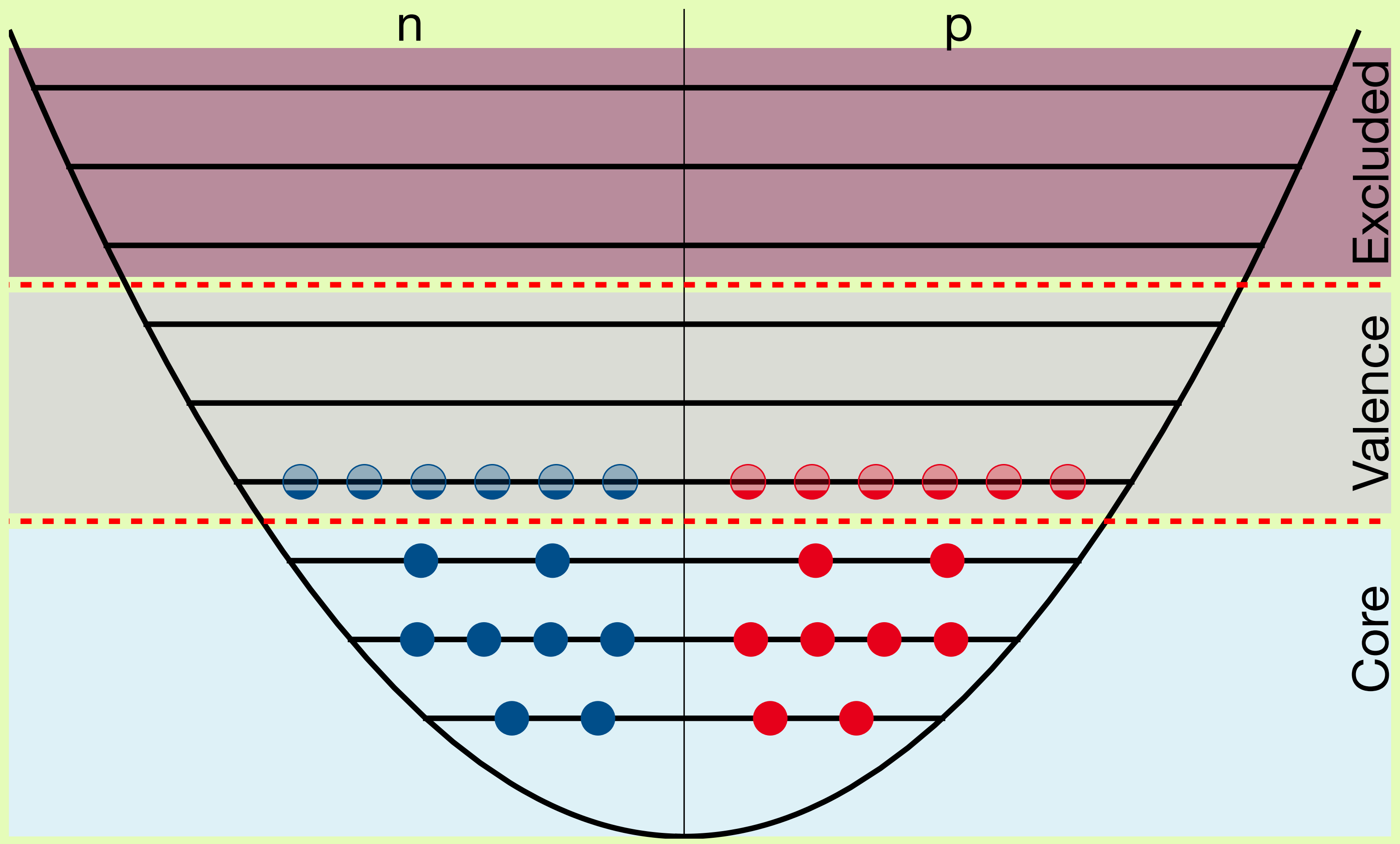
- Multi-determinantal reference state $|\psi_{\mathrm{ref}}\rangle$
- $|\psi_{\mathrm{ref}}\rangle$ is the nucleus of interest
- Irreducible densities $\lambda^{[1]}$, $\lambda^{[2]}$
- MR-IMSRG framework
- Multi-shell decoupling possible



- Single Slater determinant $|\psi_{\mathrm{ref}}\rangle$
- $|\psi_{\mathrm{ref}}\rangle$ is closest closed-shell nucleus
- Ensemble normal ordering
- SR-IMSRG framework
- Multi-shell decoupling only artificially

T. Miyagi, S. R. Stroberg, et al. Phys. Rev. C 102, 034320 (2020)

$|\psi_{\mathrm{ref}}\rangle_{\mathrm{VS}} =$

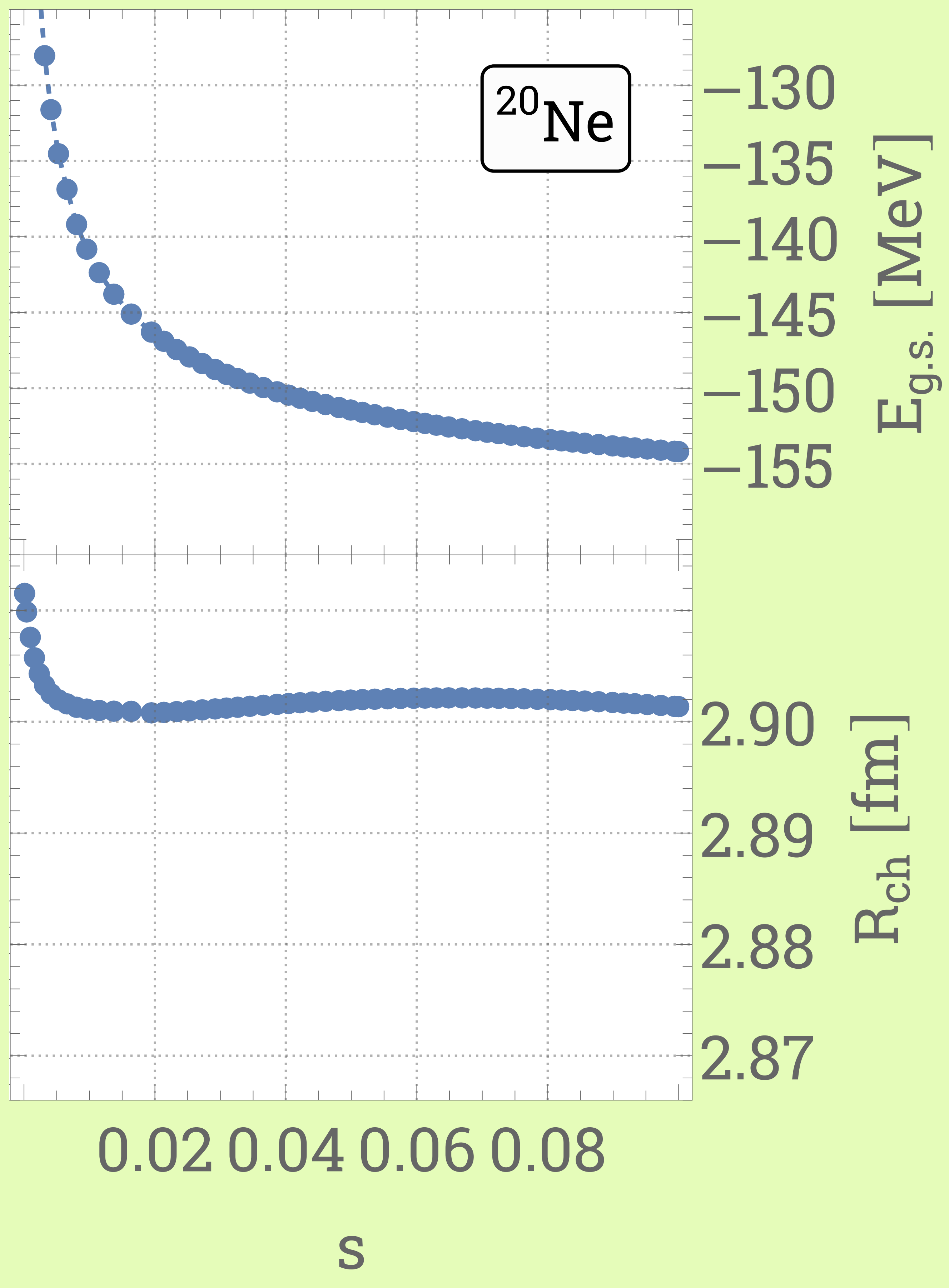


Decoupling

Generator construction

- Previous implementation „Occ“ used occupation numbers in generator construction

$$\eta_v^x = \bar{n}_x n_v f_v^x \mathcal{F}(\Delta_v^x)$$
$$\eta_{vw}^{xy} = \bar{n}_x \bar{n}_y n_v n_w \Gamma_{vw}^{xy} \mathcal{F}(\Delta_{vw}^{xy})$$



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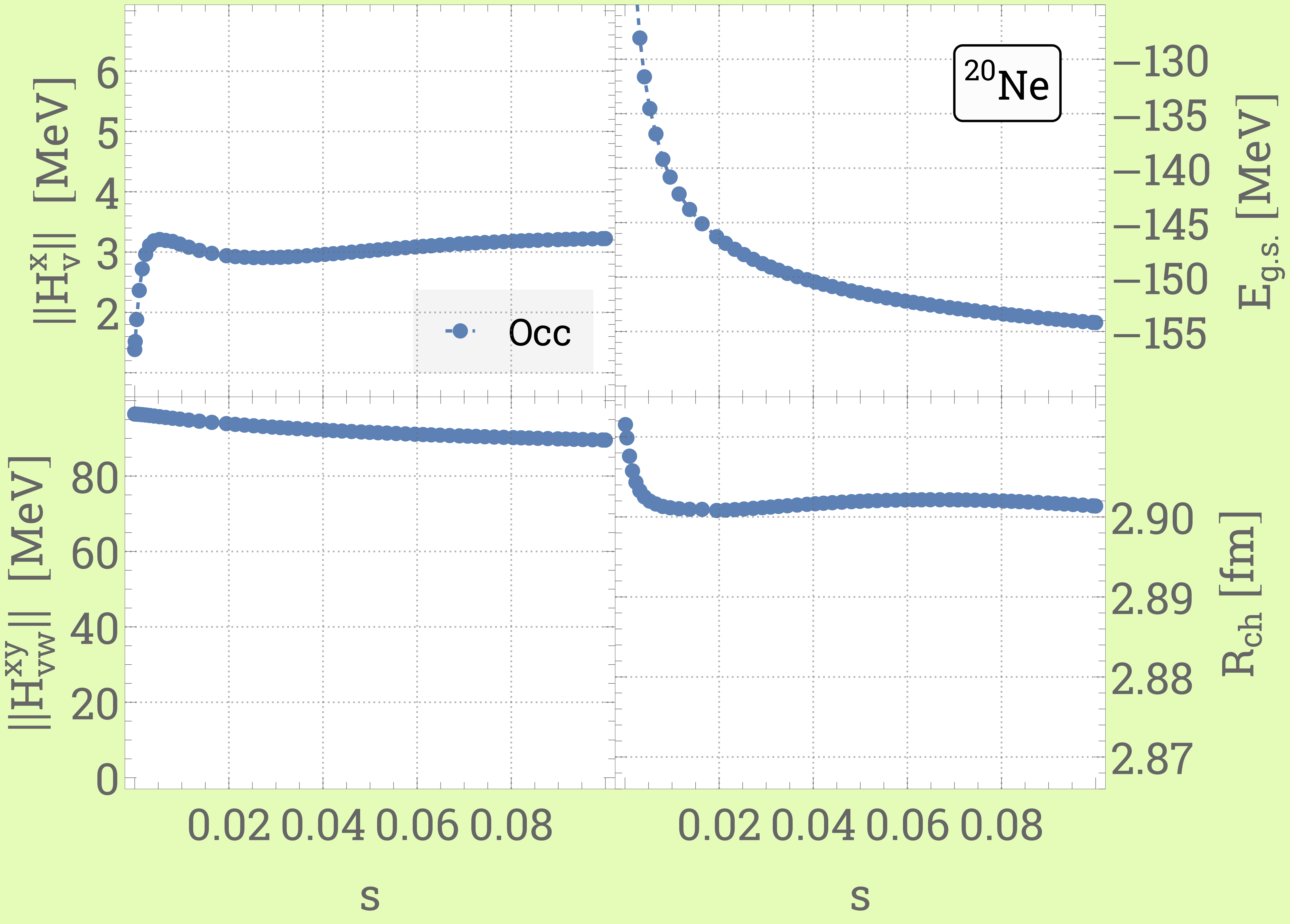
- Was *not* successful in decoupling all off-diagonal blocks!

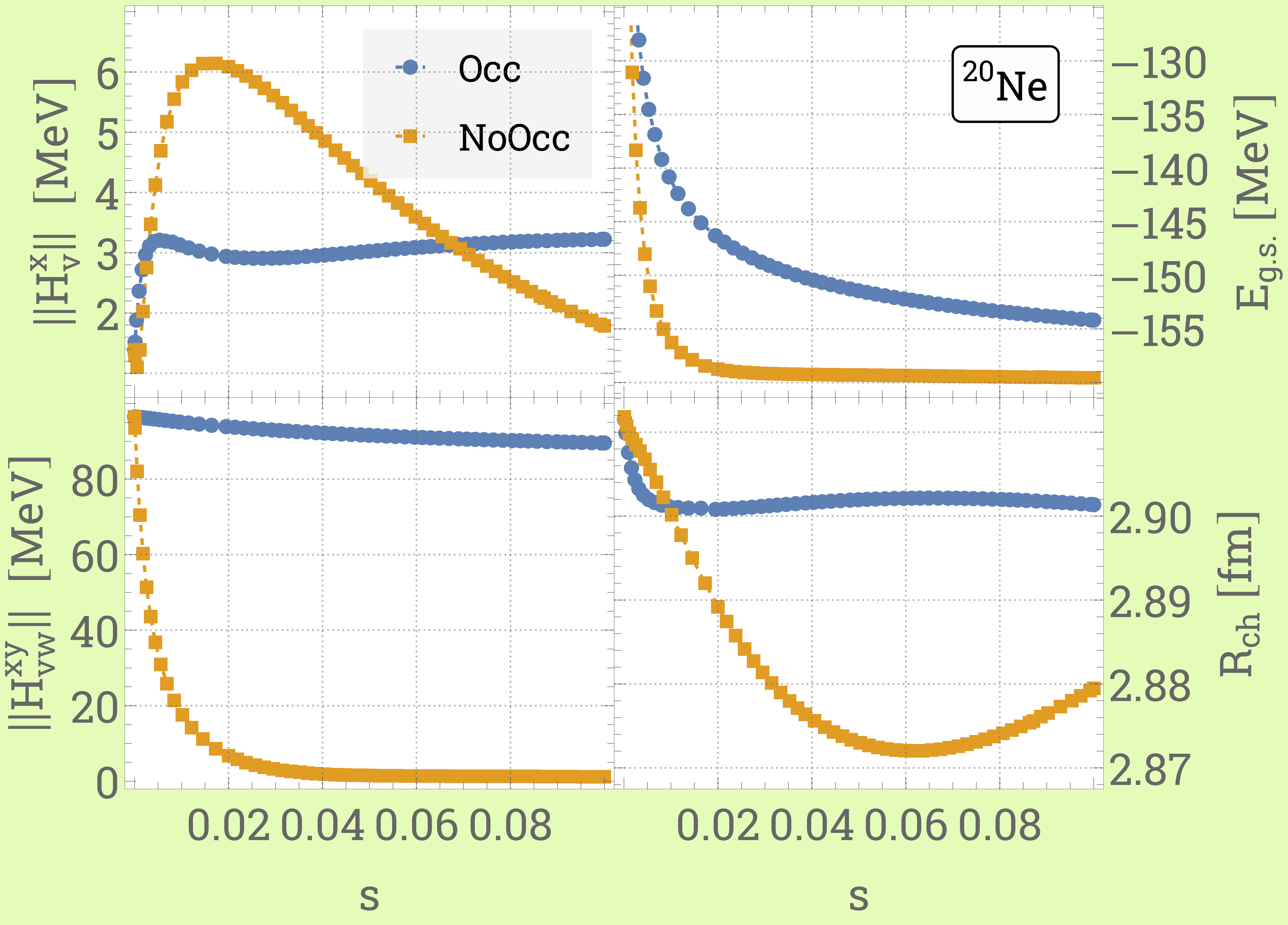


Decoupling
Generator construction

- Refined implementation „NoOcc" omits occupation numbers in generator matrix elements

$$\eta_v^x = \cancel{\bar{n}_x n_v} f_v^x \mathcal{F}(\Delta_v^x)$$
$$\eta_{vw}^{xy} = \cancel{\bar{n}_x \bar{n}_y n_v n_w} \Gamma_{vw}^{xy} \mathcal{F}(\Delta_{vw}^{xy})$$

- Decouples all off-diagonal blocks



Decoupling

Generator construction

- Refined implementation „NoOcc" omits occupation numbers in generator matrix elements

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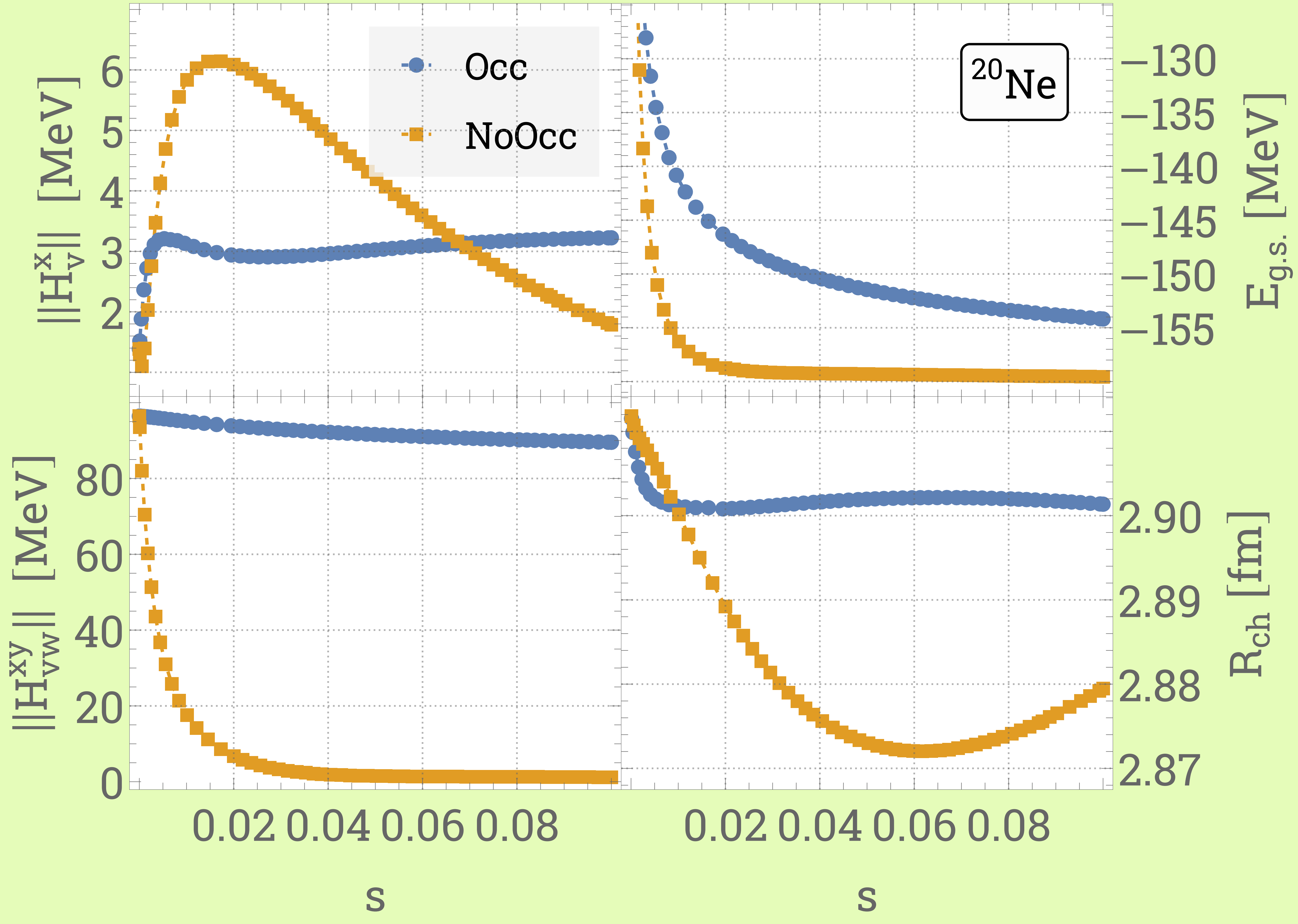
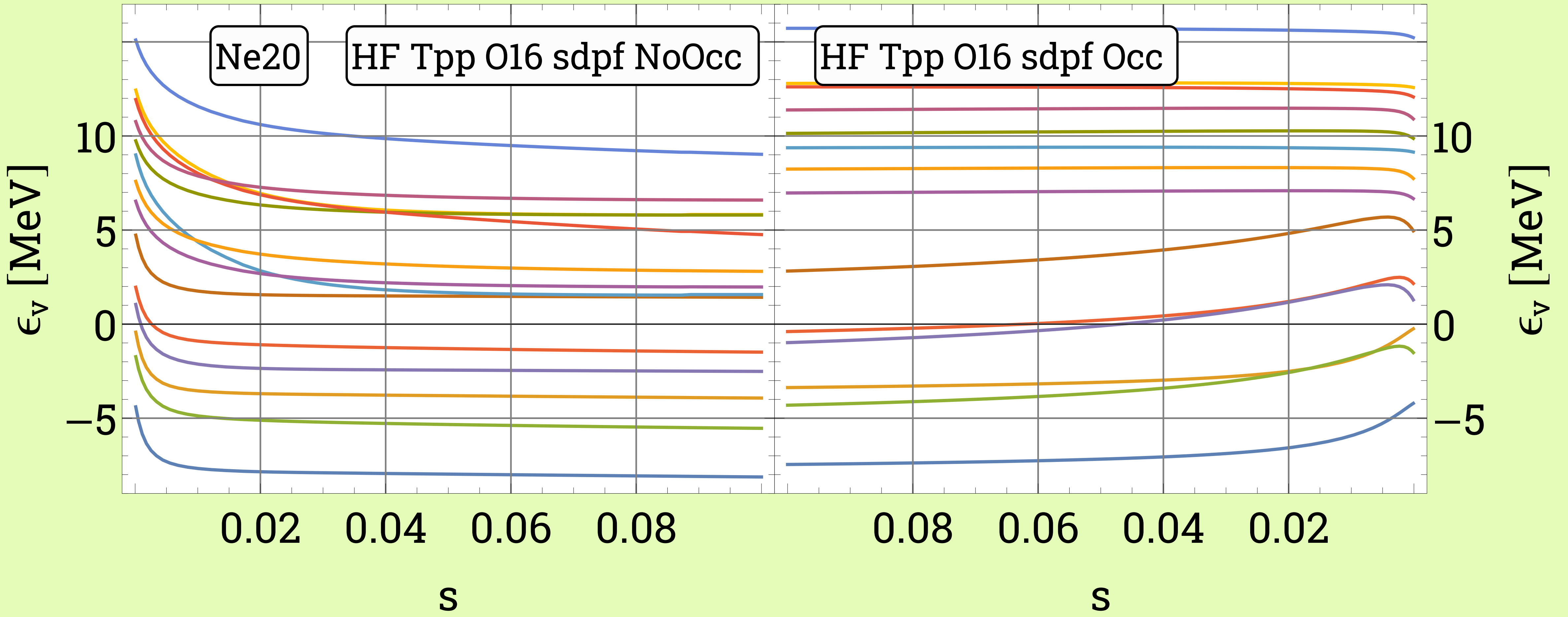
$$\eta_{vw}^{xy} = \cancel{\bar{n}_x \bar{n}_y n_v n_w} \Gamma_{vw}^{xy} \mathcal{F}(\Delta_{vw}^{xy})$$

- Decouples all off-diagonal blocks
- Higher single-particle states (with small occupation numbers) are decoupled now





Flow analysis

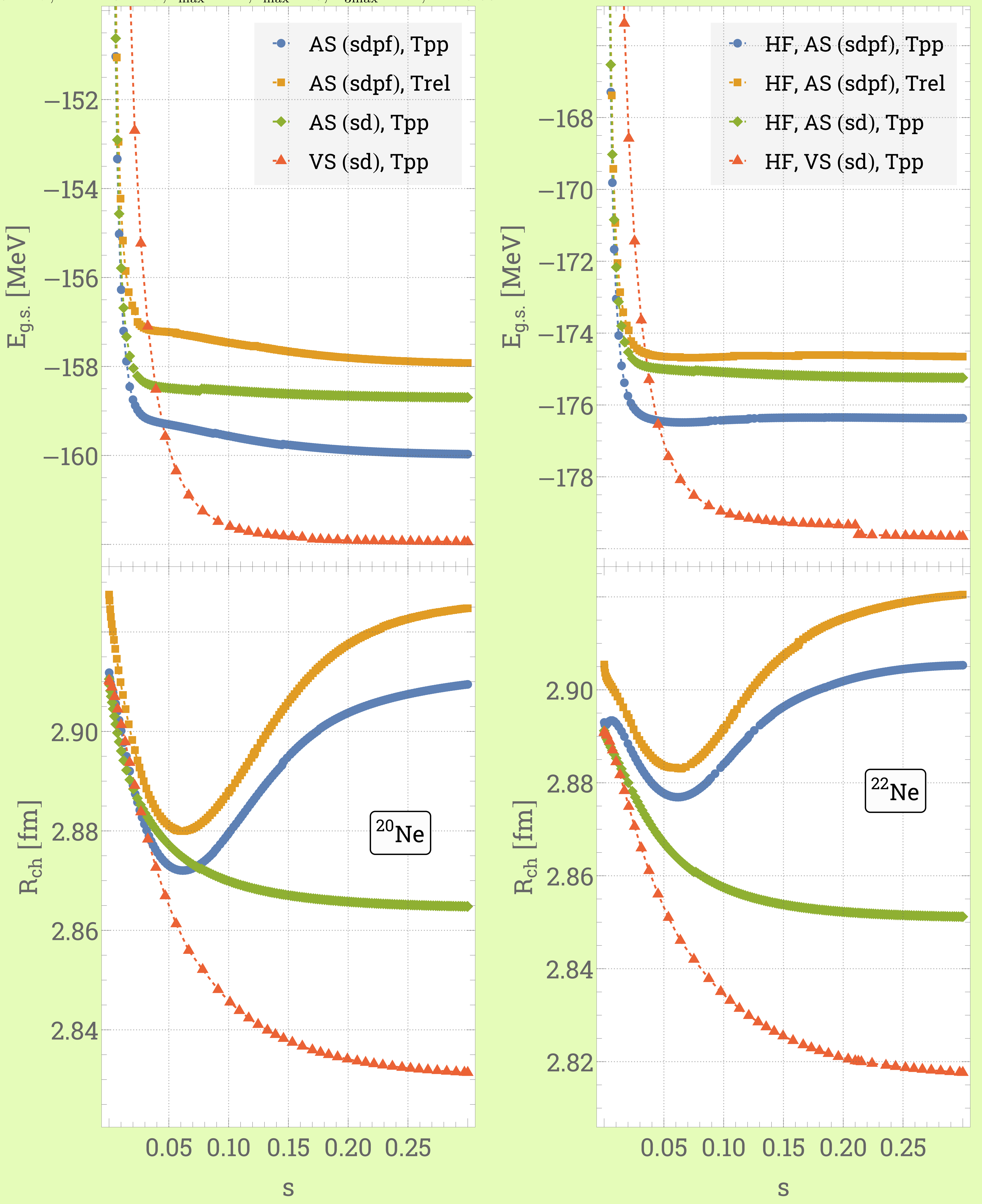
^{20}Ne & ^{22}Ne

- Fast and stable convergence of $E_{\text{g.s.}}$ in IM-ASCI
- Unexpected structures in R_{ch} flow makes long term evolution necessary for IM-ASCI
- Formulation of kinetic energy, $T_{\text{pp}}/T_{\text{rel}}$, has small influence on result but not flow behavior
- Geometrically larger single-particle states in *pf*-shell may contribute stronger to R_{ch} in final $|\psi_{\text{ref}}\rangle$

Non-local NN+3N @ N^{3}LO

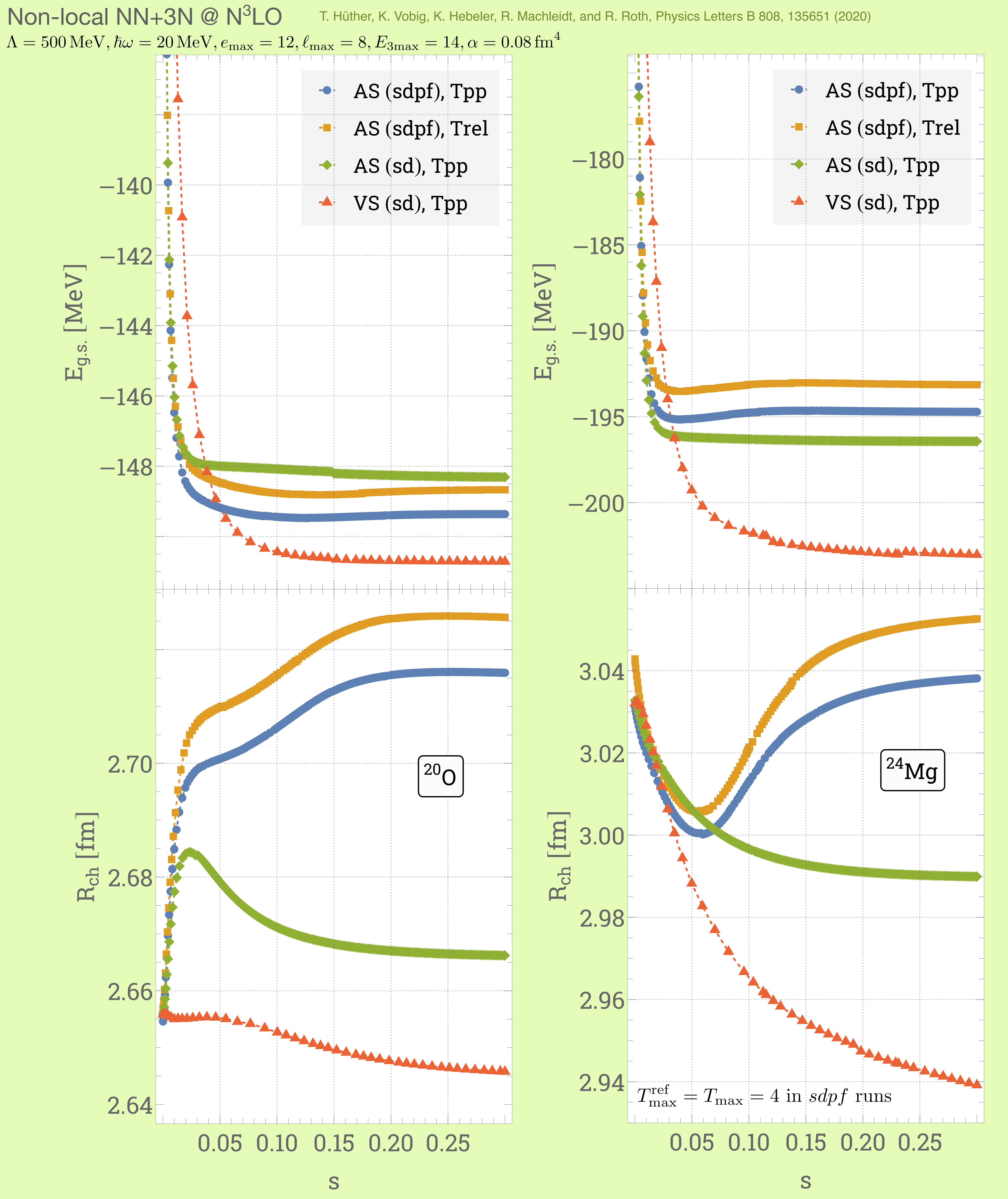
$\Lambda = 500\,\text{MeV}, \hbar\omega = 20\,\text{MeV}, e_{\max} = 12, \ell_{\max} = 8, E_{3\max} = 14, \alpha = 0.08\,\text{fm}^4$

T. Hüther, K. Vobig, K. Hebeler, R. Machleidt, and R. Roth, Physics Letters B 808, 135651 (2020)



Flow analysis
^{20}O & ^{24}Mg

- Fast and stable convergence of $E_{g.s.}$ in IM-ASCI
- Unexpected structures in R_{ch} flow makes long term evolution necessary for IM-ASCI
- Formulation of kinetic energy, T_{pp}/T_{rel}, has small influence on result but not flow behavior
- Geometrically larger single-particle states in *pf*-shell may contribute stronger to R_{ch} in final $|\psi_{\text{ref}}\rangle$
- ^{20}O undergoes different flow pattern in R_{ch} than ^{20}Ne, ^{22}Ne and ^{24}Mg - potentially resulting from only Neutrons in active space



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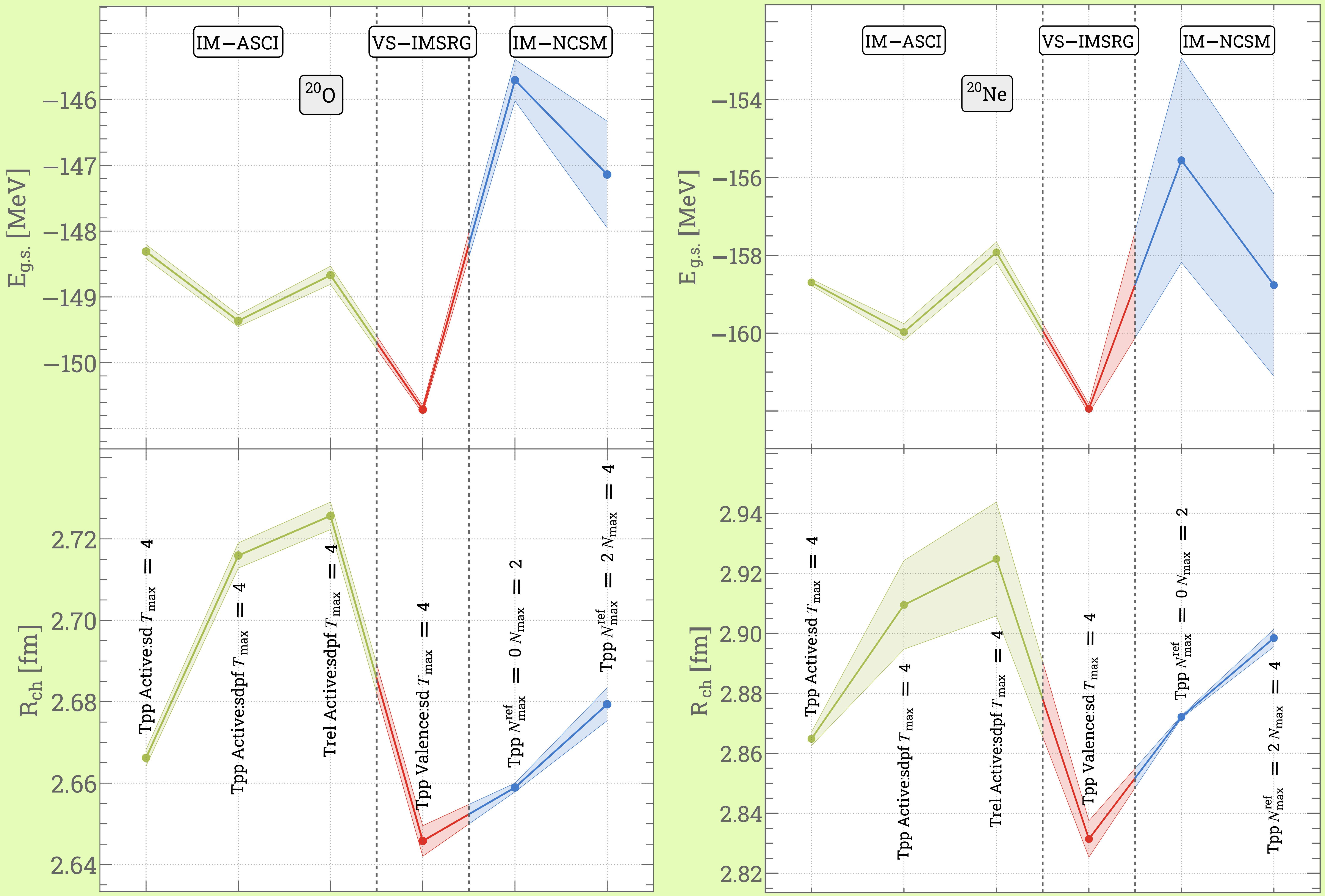
Result comparison

^{20}O & ^{20}Ne

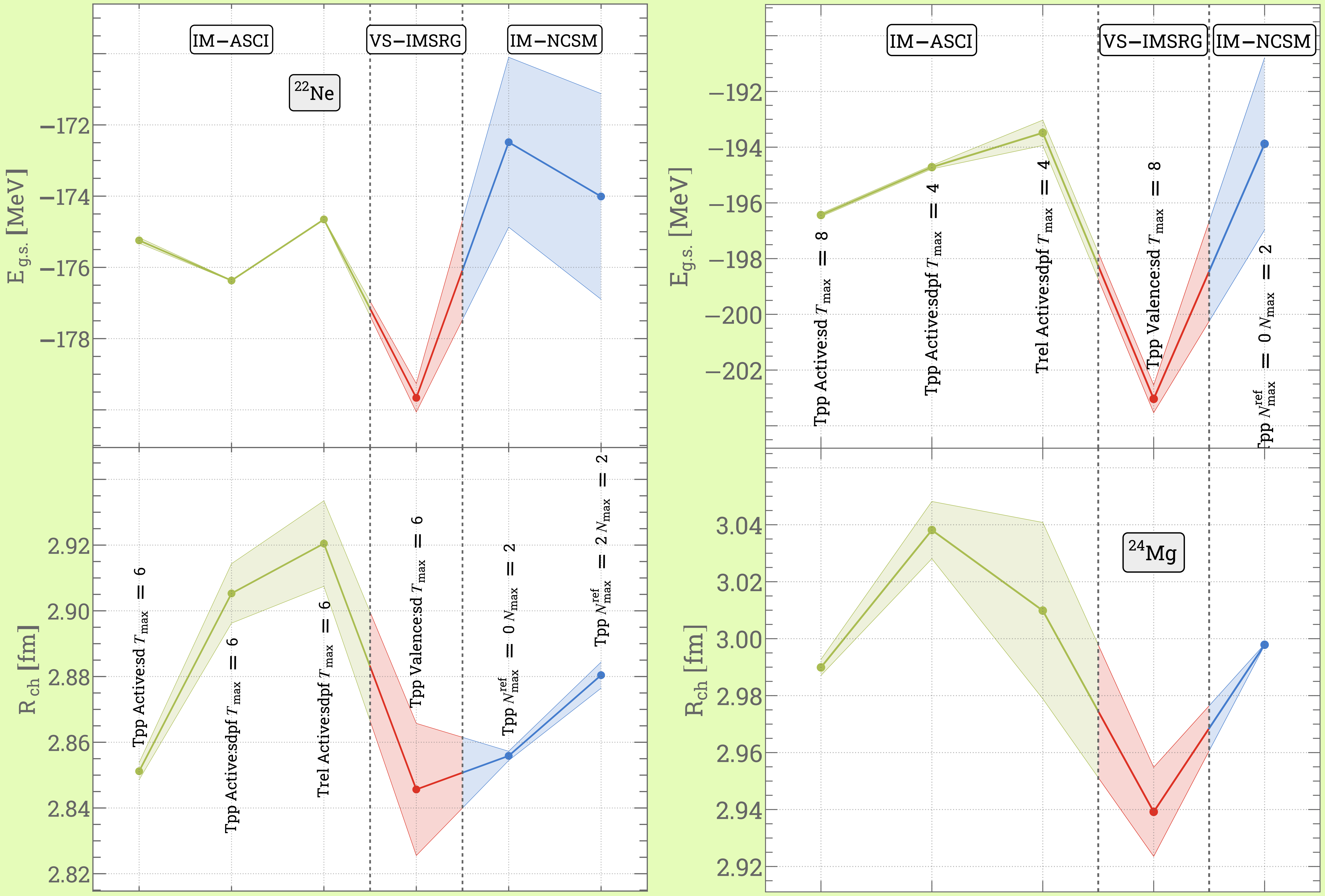
- Final results $O(s_\infty = 0.3)$ with symmetric uncertainty bands from $|O(s_\infty) - O(s_\infty/2)|$
- Energies for different active spaces are consistent
- Radii systematically larger for larger active spaces



Result comparison

^{22}Ne & ^{24}Mg

- Final results $O(s_\infty = 0.3)$ with symmetric uncertainty bands from $|O(s_\infty) - O(s_\infty/2)|$
- Energies for different active spaces are consistent
- Radii systematically larger for larger active spaces
- More flexible than IM-NCSM - scalable to heavier nuclei



Summary

- IM-ASCI is a powerful, new multi-reference decoupling
- Refined previous decoupling
- Conceptional improvement over VS-IMSRG
- Full flexibility in choice of active space
- More versatile than IM-NCSM
- *pf*-single-particle states relevant to R_{ch} but less for $E_{g.s.}$

Outlook

- Optimize generator construction
- Construct uncertainty estimation
- Investigate non-scalar observables
- Benchmark in Carbon isotopes against high-precision extrapolated NCSM results
- Larger active spaces
- Heavier isotopes

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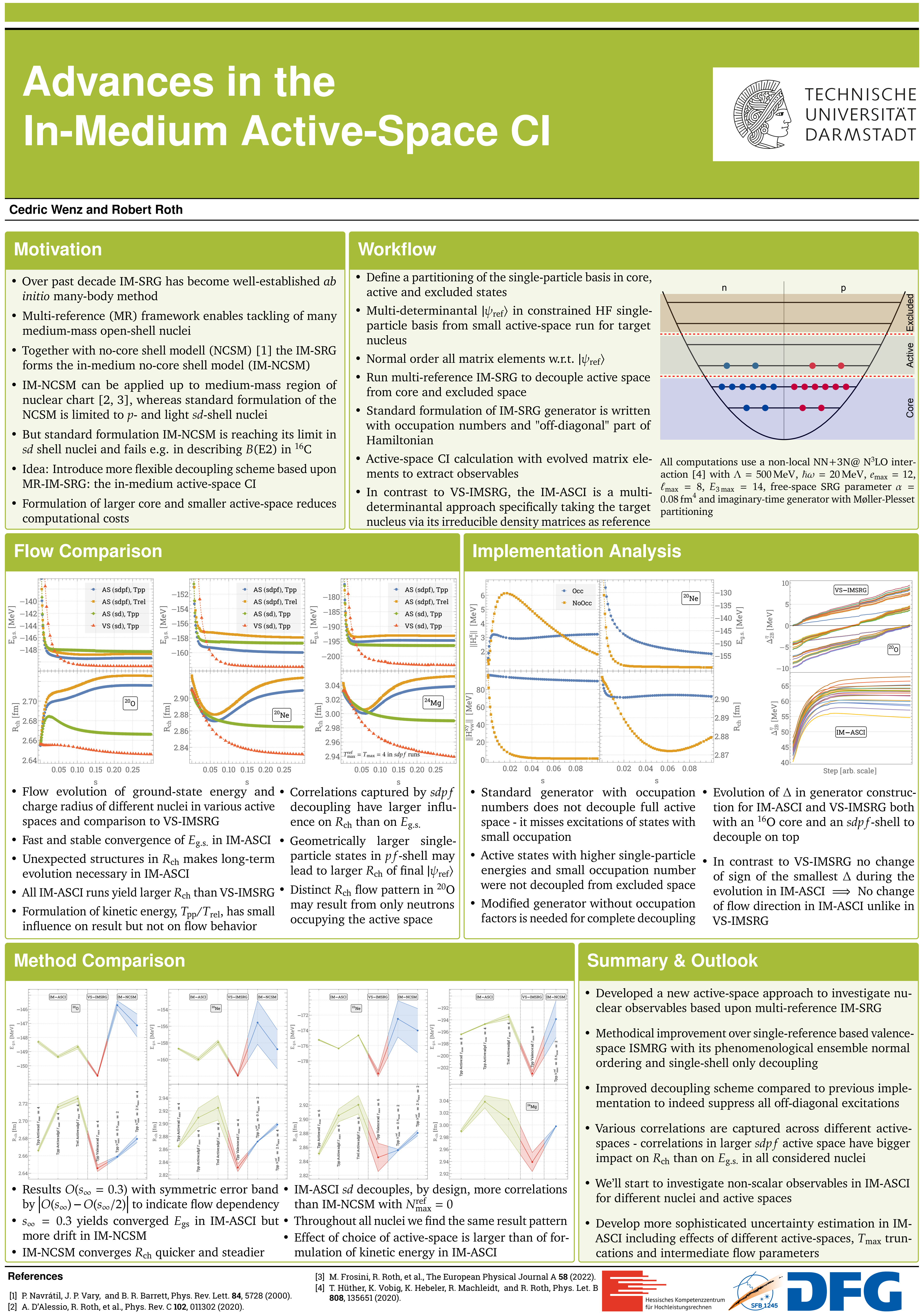

Advances in the In-Medium Active-Space CI

Cedric Wenz and Robert Roth

Motivation

- Over past decade IM-SRG has become well-established *ab initio* many-body method
- Multi-reference (MR) framework enables tackling of many medium-mass open-shell nuclei
- Together with no-core shell modell (NCSM) [1] the IM-SRG forms the in-medium no-core shell model (IM-NCSM)
- IM-NCSM can be applied up to medium-mass region of nuclear chart [2, 3], whereas standard formulation of the NCSM is limited to p- and light sd-shell nuclei
- But standard formulation IM-NCSM is reaching its limit in sd shell nuclei and fails e.g. in describing $B(E2)$ in ^{16}C
- Idea: Introduce more flexible decoupling scheme based upon MR-IM-SRG: the in-medium active-space CI
- Formulation of larger core and smaller active-space reduces computational costs

Workflow

- Define a partitioning of the single-particle basis in core, active and excluded states
- Multi-determinantal $|\psi_{\text{ref}}\rangle$ in constrained HF single-particle basis from small active-space run for target nucleus
- Normal order all matrix elements w.r.t. $|\psi_{\text{ref}}\rangle$
- Run multi-reference IM-SRG to decouple active space from core and excluded space
- Standard formulation of IM-SRG generator is written with occupation numbers and "off-diagonal" part of Hamiltonian
- Active-space CI calculation with evolved matrix elements to extract observables
- In contrast to VS-IMSRG, the IM-ASCI is a multi-determinantal approach specifically taking the target nucleus via its irreducible density matrices as reference

All computations use a non-local NN+3N@ N^{3}LO interaction [4] with Λ = 500 MeV, $\hbar\omega$ = 20 MeV, $e_{\max}$ = 12, $\ell_{\max}$ = 8, $E_{3\max}$ = 14, free-space SRG parameter α = 0.08 fm^4 and imaginary-time generator with Møller-Plesset partitioning

Flow Comparison

- Flow evolution of ground-state energy and charge radius of different nuclei in various active spaces and comparison to VS-IMSRG
- Fast and stable convergence of $E_{\text{g.s.}}$ in IM-ASCI
- Unexpected structures in R_{ch} makes long-term evolution necessary in IM-ASCI
- All IM-ASCI runs yield larger R_{ch} than VS-IMSRG
- Formulation of kinetic energy, $T_{\text{pp}}/T_{\text{rel}}$, has small influence on result but not on flow behavior
- Correlations captured by $sdpf$ decoupling have larger influence on R_{ch} than on $E_{\text{g.s.}}$
- Geometrically larger single-particle states in pf-shell may lead to larger R_{ch} of final $|\psi_{\text{ref}}\rangle$
- Distinct R_{ch} flow pattern in ^{20}O may result from only neutrons occupying the active space

Implementation Analysis

- Standard generator with occupation numbers does not decouple full active space - it misses excitations of states with small occupation
- Active states with higher single-particle energies and small occupation number were not decoupled from excluded space
- Modified generator without occupation factors is needed for complete decoupling
- Evolution of Δ in generator construction for IM-ASCI and VS-IMSRG both with an ^{16}O core and an $sdpf$-shell to decouple on top
- In contrast to VS-IMSRG no change of sign of the smallest Δ during the evolution in IM-ASCI $\implies$ No change of flow direction in IM-ASCI unlike in VS-IMSRG

Method Comparison

- Results $O(s_\infty = 0.3)$ with symmetric error band by $|O(s_\infty) - O(s_\infty/2)|$ to indicate flow dependency
- s_∞ = 0.3 yields converged E_{gs} in IM-ASCI but more drift in IM-NCSM
- IM-NCSM converges R_{ch} quicker and steadier
- IM-ASCI sd decouples, by design, more correlations than IM-NCSM with $N^{\text{ref}}_{\max}$ = 0
- Throughout all nuclei we find the same result pattern
- Effect of choice of active-space is larger than of formulation of kinetic energy in IM-ASCI

Summary & Outlook

- Developed a new active-space approach to investigate nuclear observables based upon multi-reference IM-SRG
- Methodical improvement over single-reference based valence-space ISMRG with its phenomenological ensemble normal ordering and single-shell only decoupling
- Improved decoupling scheme compared to previous implementation to indeed suppress all off-diagonal excitations
- Various correlations are captured across different active-spaces - correlations in larger $sdpf$ active space have bigger impact on R_{ch} than on $E_{\text{g.s.}}$ in all considered nuclei
- We'll start to investigate non-scalar observables in IM-ASCI for different nuclei and active spaces
- Develop more sophisticated uncertainty estimation in IM-ASCI including effects of different active-spaces, $T_{\max}$ truncations and intermediate flow parameters

References

[1] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. 84, 5728 (2000).
[2] A. D'Alessio, R. Roth, et al., Phys. Rev. C 102, 011302 (2020).
[3] M. Frosini, R. Roth, et al., The European Physical Journal A 58 (2022).
[4] T. Hüther, K. Vobig, K. Hebeler, R. Machleidt, and R. Roth, Phys. Lett. B 808, 135651 (2020).

Thank you for your attention!

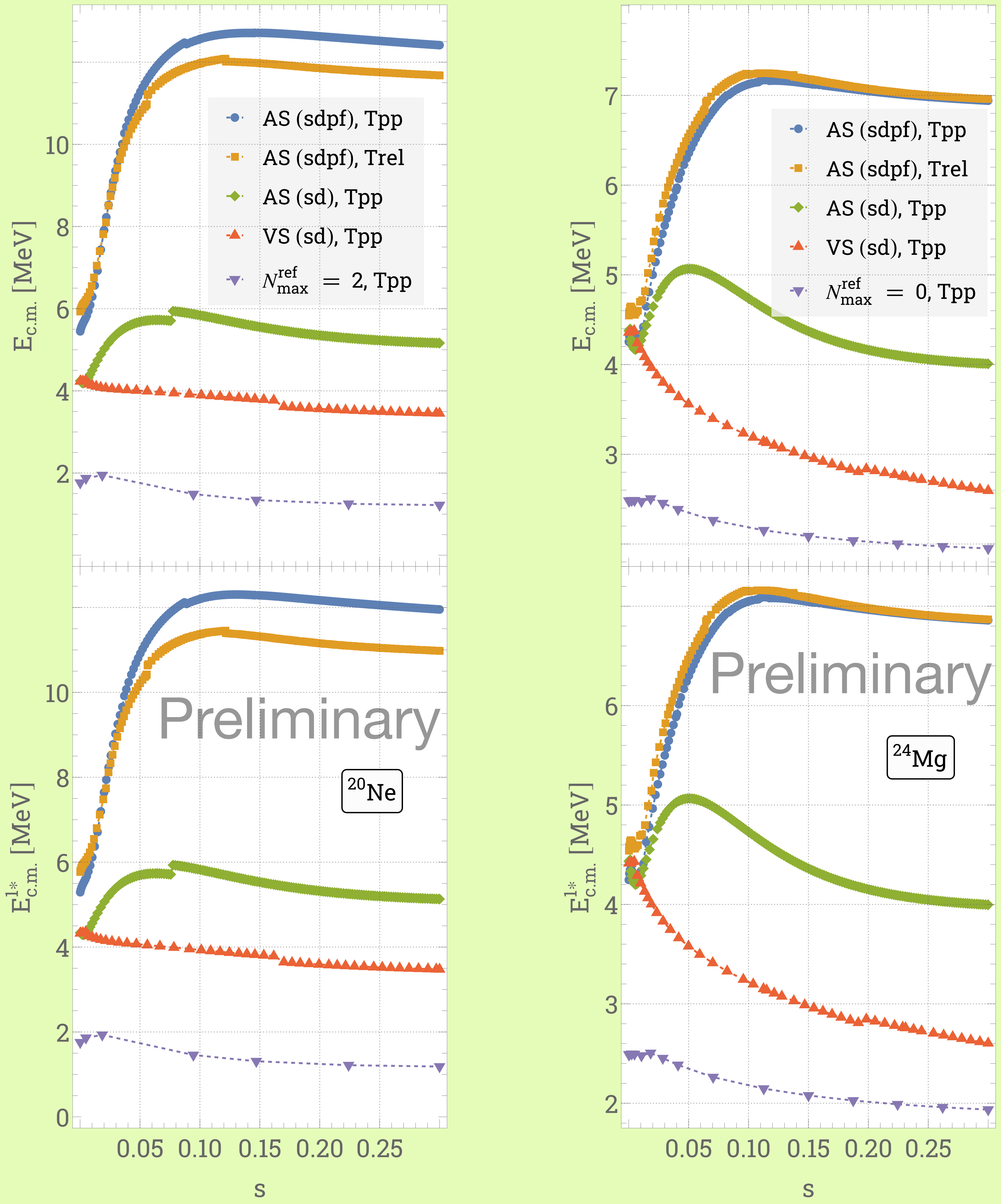
Looking forward to lively discussions

← at my poster

BACK UP

$E_{c.m.}$ flow
^{20}Ne & ^{24}Mg

- Flow of $E_{c.m.}$ of ground-state and first excited state
- We see increase in $E_{c.m.}$ with growing active space
- All of this still has to be understood in detail - this is preliminary!!



All workflows

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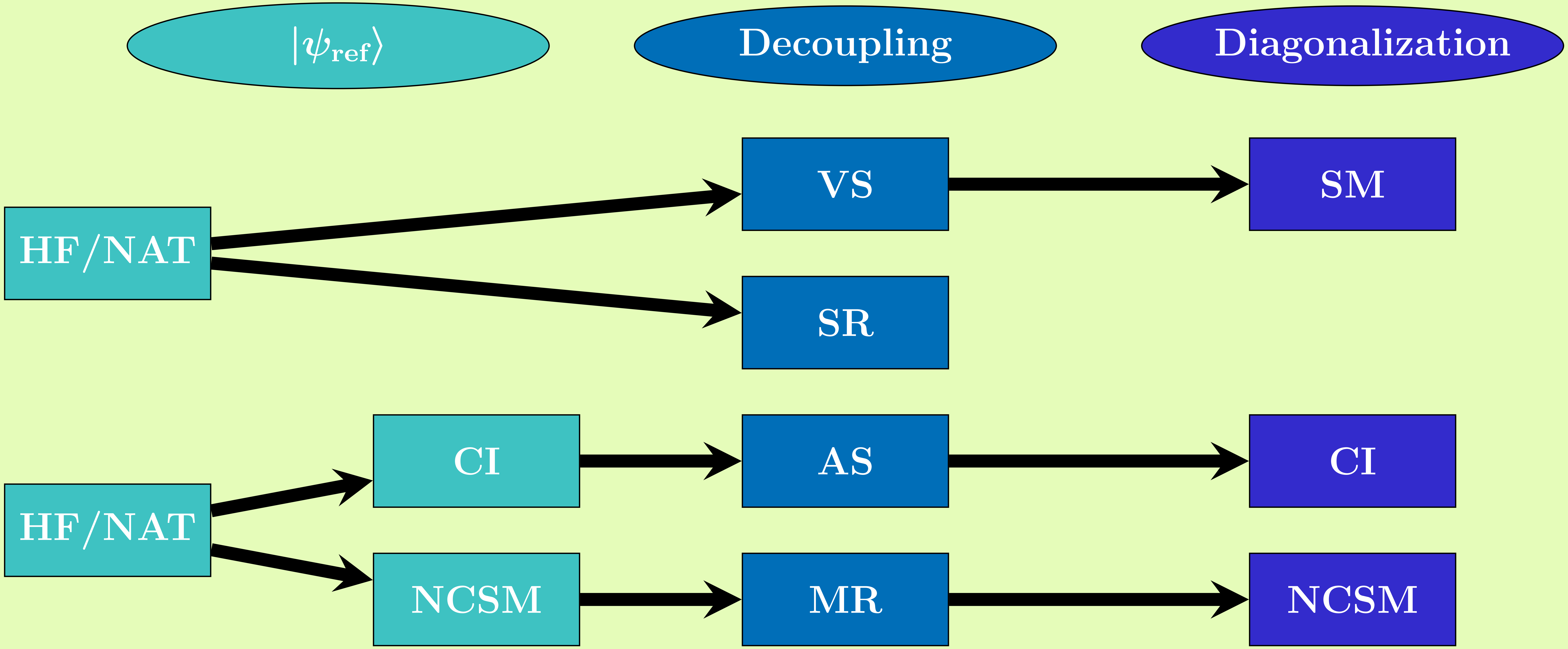


VS-IMSRG

SR-IMSRG

IM-ASCI

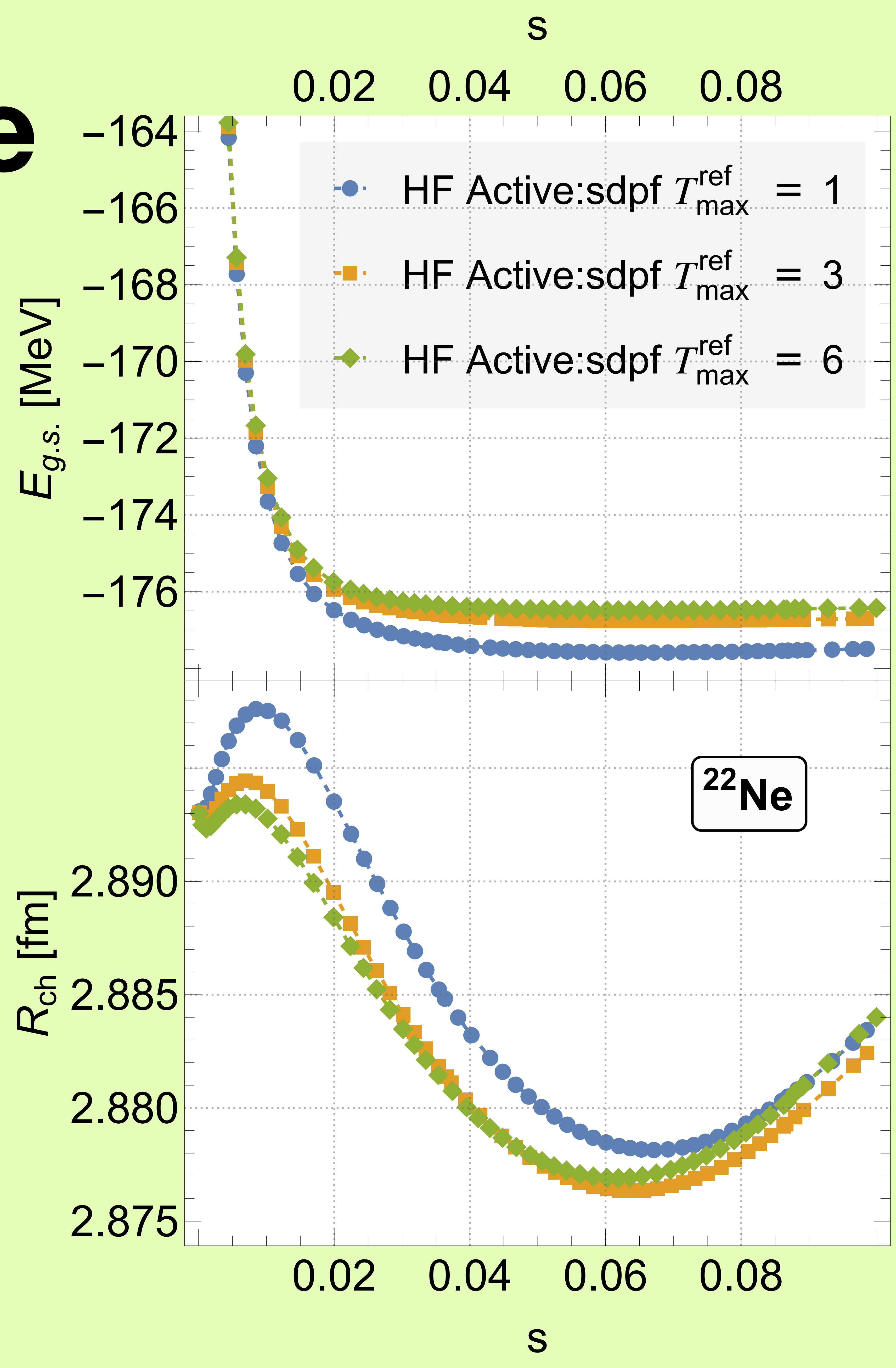
IM-NCSM

Reference state dependence

Ne22

- $T^{\mathrm{ref}}_{\mathrm{max}} = 3$ fully sufficient in reference to capture same flow behavior as full $T^{\mathrm{ref}}_{\mathrm{max}} = 6$ run

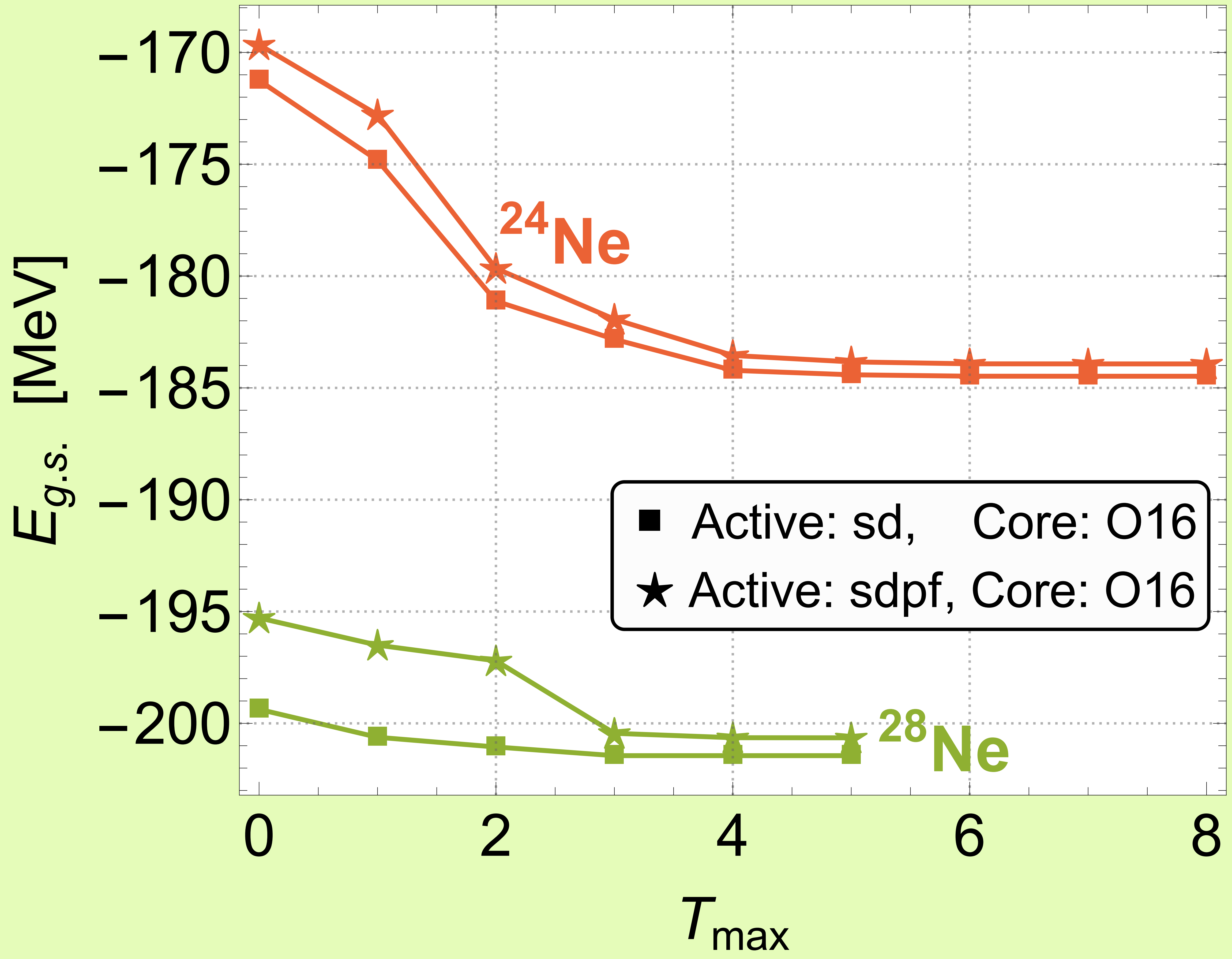
- Conclusion: $T^{\mathrm{ref}}_{\mathrm{max}} = 4$ is sufficient in ^{24}Mg *sdpf* run as well, but much cheaper



T_{max} convergence

In old „Occ“ implementation

- For old IM-ASCI version with occupation numbers in generator construction
- T_{Max}=4 sufficient in both cases
- Conclusion: T_{Max}=4 also good enough for ^{24}Mg



Epsilon convergence

In BCH series for s=0.1 Omega

- Take initial Hamiltonian *H*(0)
- Evolve it in BCH series with $\Omega(s = 0.1)$
- Until convergence is reached $\frac{\| \frac{1}{k!} \left[\Omega(s), O(0)\right]_k \|}{\sum_{i=0}^{k} \frac{1}{i!} \left[\Omega(s), O(0)\right]_i} < \epsilon_{\mathrm{BCH}}$
- $\epsilon_{\mathrm{BCH}} = 10^{-3}$ sufficient -> Next, test if $\epsilon_{\mathrm{BCH}} = 10^{-2}$ is also enough in flow - would lead to less terms in BCH series and thus speed up in flow