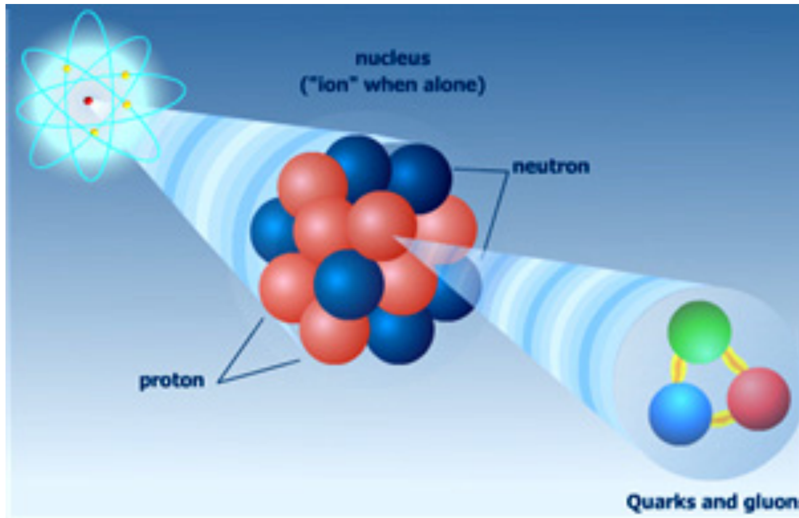


KHuK annual meeting, December 10, 2021

Innovative many-body methods for nuclear structure

Caroline Robin

GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany
Fakultät für Physik, Universität Bielefeld, Germany

UNIVERSITÄT BIELEFELD

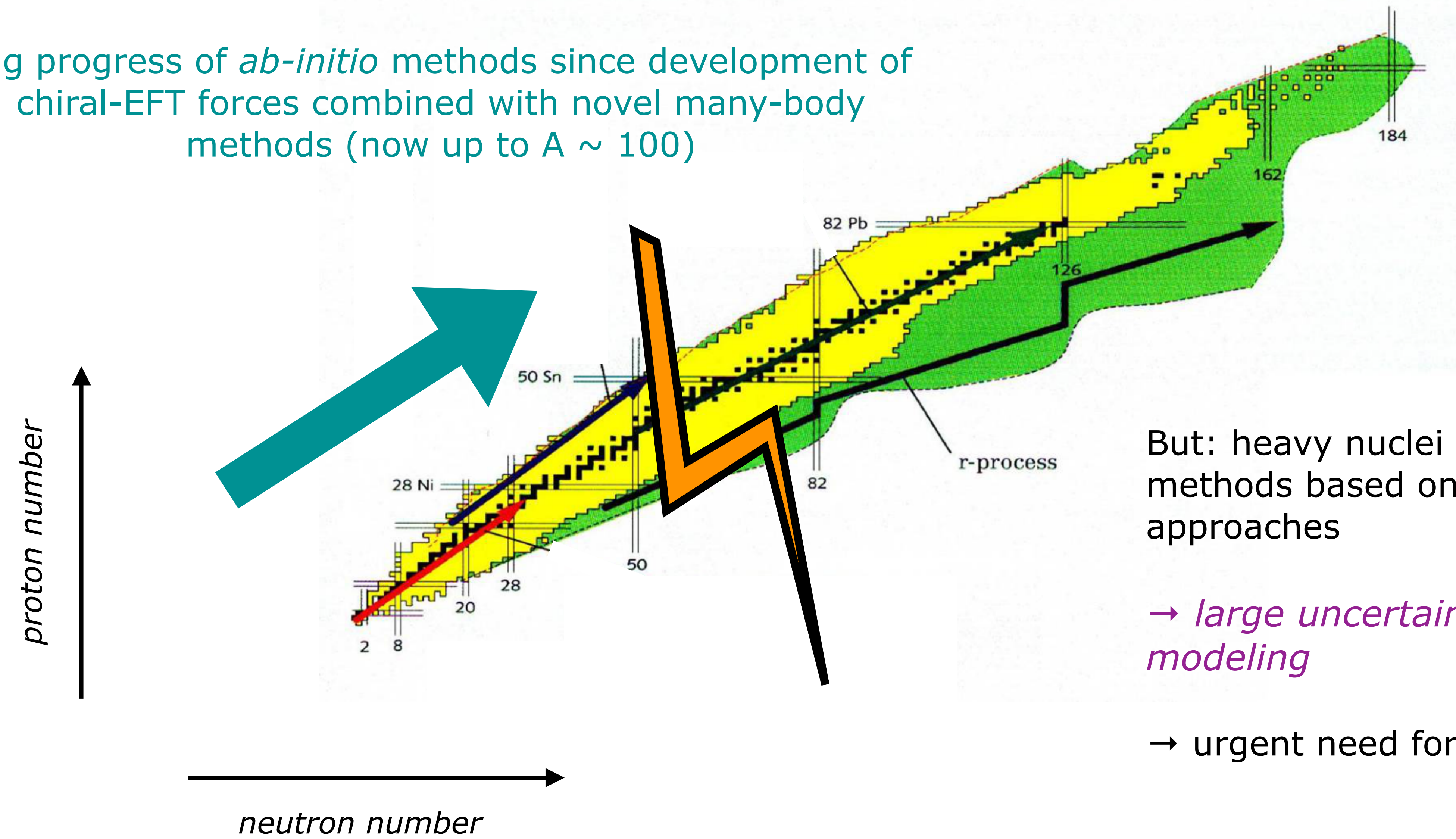
GSI

Goal of nuclear structure theory:

describe properties of all nuclei by solving the nuclear A-body problem

major issues: nuclear force? $2 \lesssim A \lesssim 300$

Big progress of *ab-initio* methods since development of chiral-EFT forces combined with novel many-body methods (now up to A ~ 100)



But: heavy nuclei still only accessible by methods based on “phenomenological” approaches

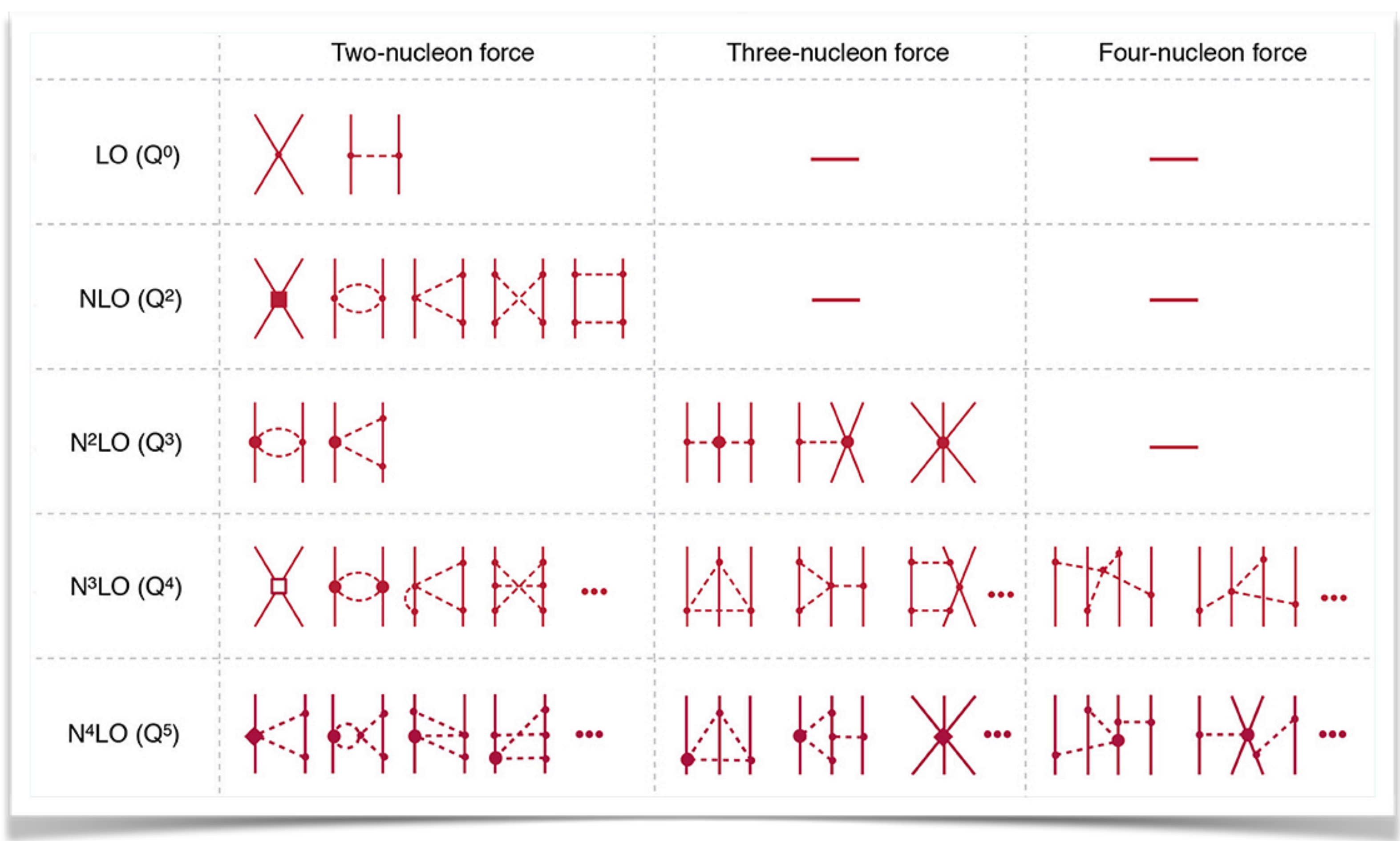
→ *large uncertainties in astrophysical modeling*

→ urgent need for improvement

Ab-initio methods for light and mid-mass nuclei

"ab-initio" = aim at solving the nuclear many-body problem based on n-nucleon forces derived from chiral EFT and fitted to n-nucleon data

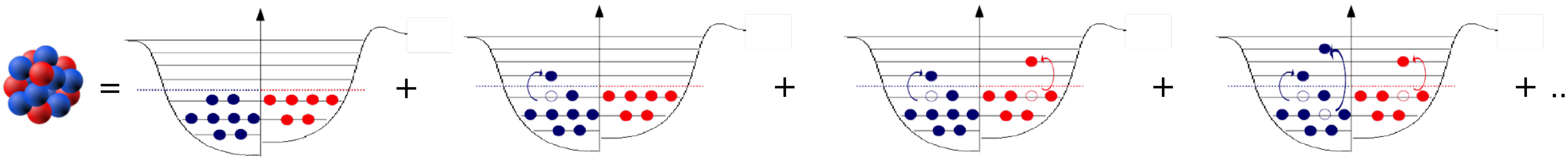
→ controlled approximations, systematically improvable, theoretical uncertainties can be assessed



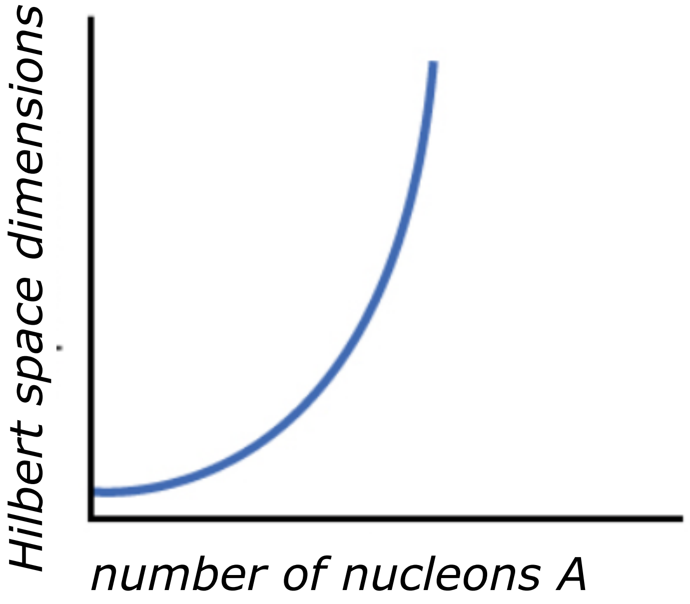
Hierarchy of nuclear forces at increasing orders in chiral expansion
Epelbaum, Krebs, Reinert, Front. Phys. 8, 98 (2020)

Configuration-space methods

$$|\Psi\rangle = A_{0p0h}|\Phi_{0p0h}\rangle + \sum_{1p1h} A_{1p1h}|\Phi_{1p1h}\rangle + \sum_{2p2h} A_{2p2h}|\Phi_{2p2h}\rangle + \sum_{3p3h} A_{3p3h}|\Phi_{3p3h}\rangle + \dots$$



Issue: factorial growth of the number of configurations

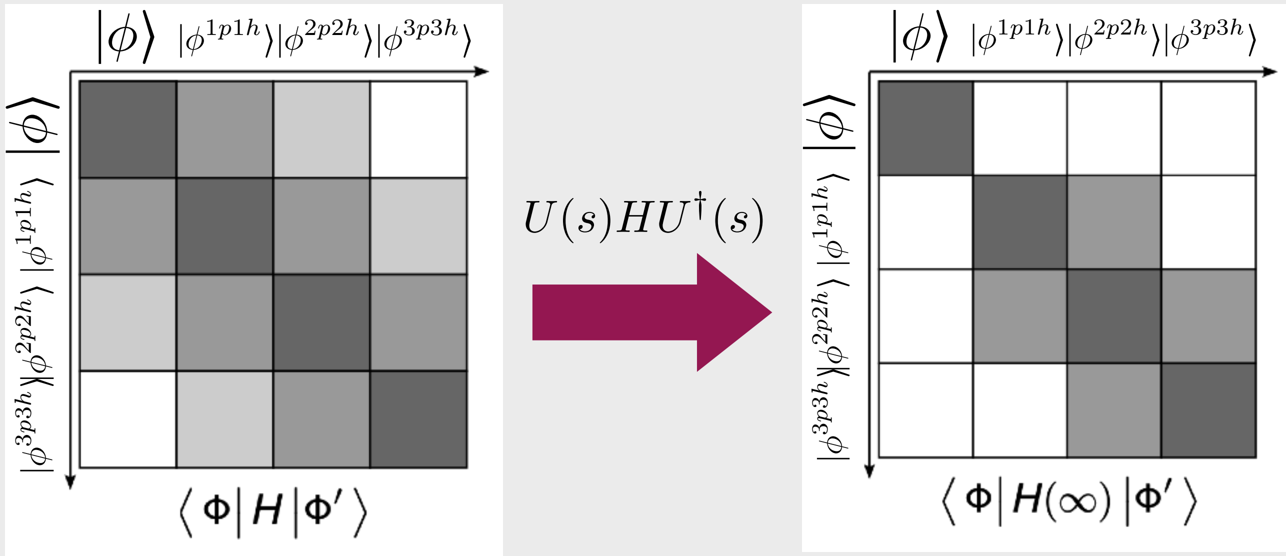


➡ How to account for np-nh correlations, while keeping the problem tractable?

In-Medium Similarity Renormalization group

IMSRG group for nuclei,
K. Tsukiyama, S. K. Bogner, and A. Schwenk, PRL106, 222502 (2011)

decouple reference state |ϕ> from excitations:



$$E = \langle\Psi|H|\Psi\rangle = \langle\phi|H(\infty)\phi\rangle$$

balance between |ϕ> and Hamiltonian H(∞):

- ✳ valence space + core:
  Tsukiyama, Bogner, Schwenk PRC 85 C 85, 061304(R) (2012);
  Stroberg et al PRL 118, 032502 (2017)
- ✳ no-core: Gebrerufael, Vobig, Hergert, Roth PRL 118, 152503 (2017)

⇒ ground and excitation properties up to ~Ni

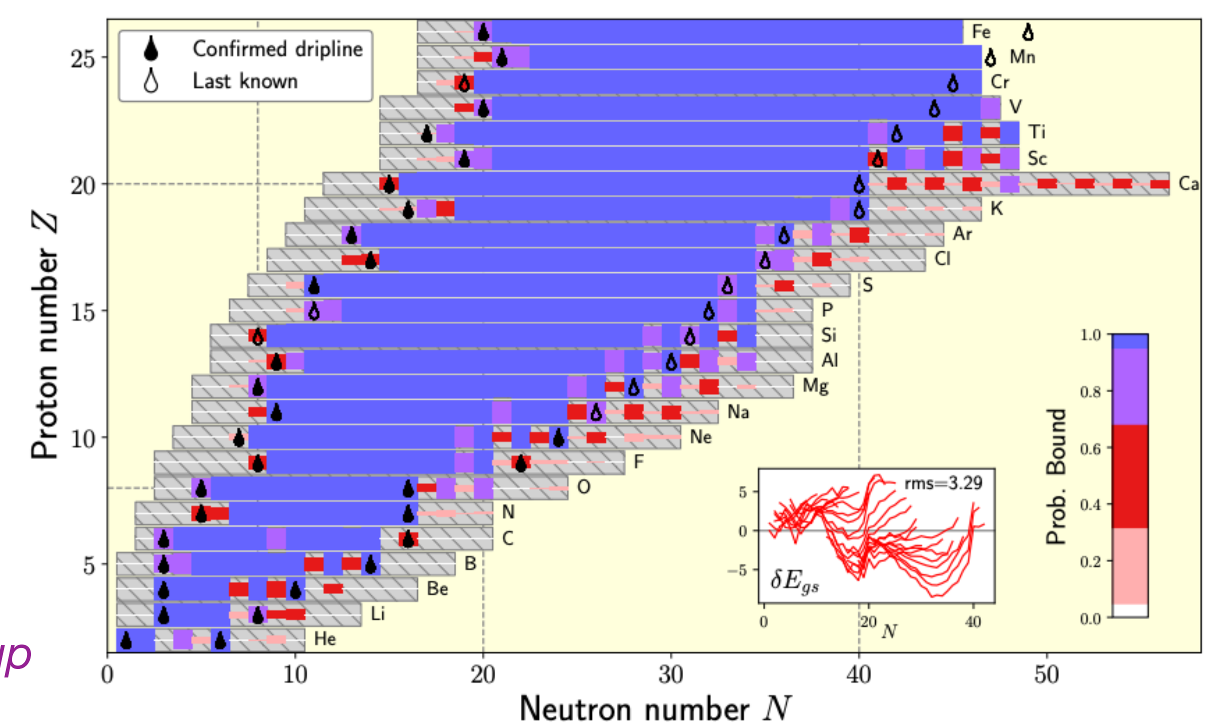
✳ *Ab initio limits of atomic nuclei,*
Stroberg, Holt, Schwenk, Simonis, PRL 126, 022501 (2021)

✳ *In-medium similarity renormalization group with three-body operators*
Heinz, Tichai, Hoppe, Hebeler, Schwenk, arXiv:2102.11172 (2021)

to improve precision of calculations

✳ *Importance truncation for the in-medium similarity renormalization group*
Hoppe, Tichai, Heinz, Hebeler, Schwenk, arXiv:2110.09390 (2021)

to extend the reach of calculations



Calculated probabilities for given isotopes to be bound with respect to one- or two-neutron/proton removal.

Optimization of the single-particle basis

✳ *In a perturbative framework*

Natural orbitals for ab initio no-core shell model calculations; Tichai, Müller, Vobig, Roth PRC 99, 034321 (2019)

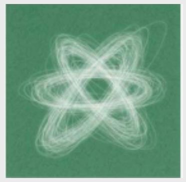
Natural orbitals for many-body expansion methods; Hoppe, Tichai, Heinz, Hebeler, Schwenk, PRC 103, 014321 (2021)

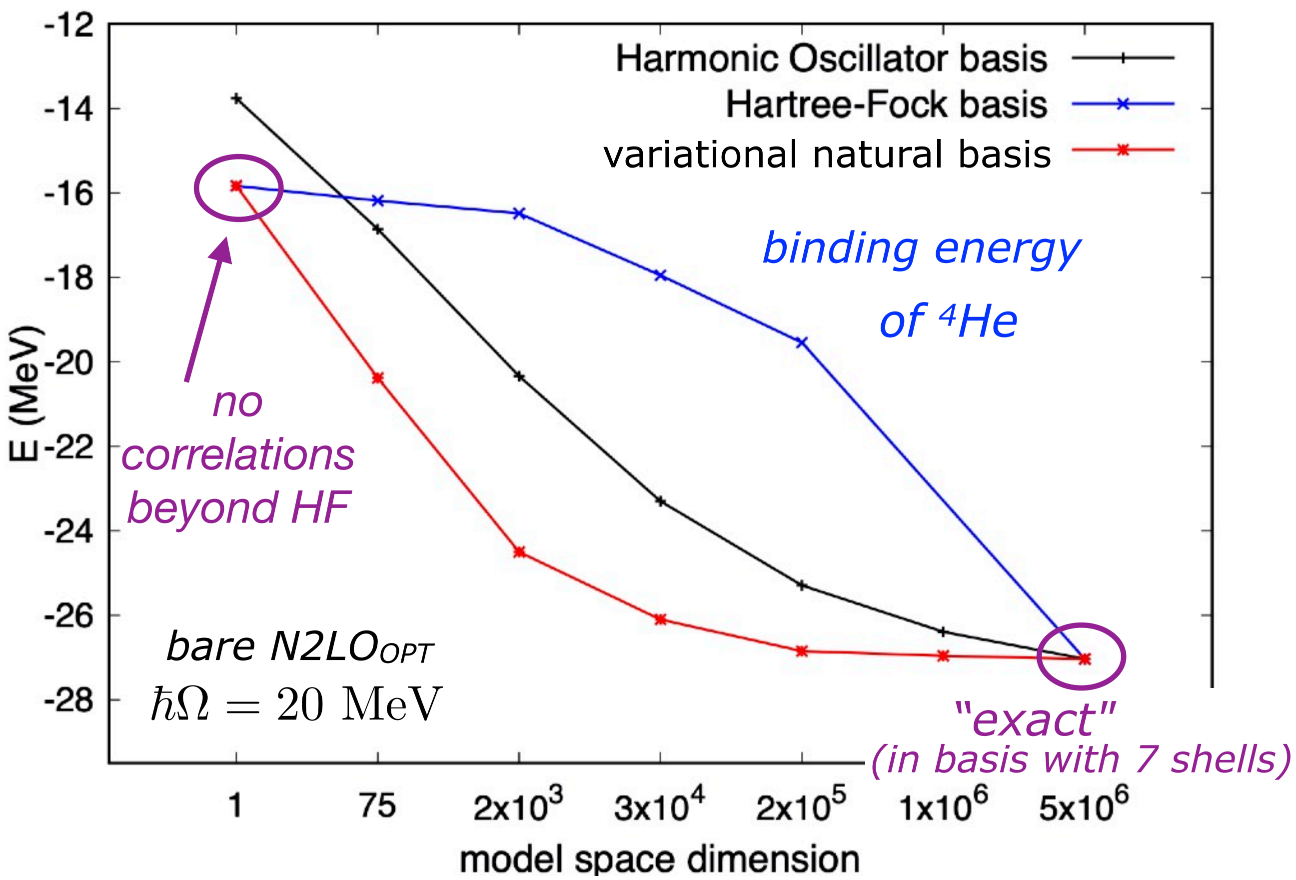
✳ *From a variational principle* *CR et al., PRC 93, 024302 (2016) & PRC 95, 044315 (2017)*

$$\left[\hat{h}(\gamma), \hat{\gamma}\right] = \hat{G}(\sigma)$$

general mean field — *One-nucleon density* — *Source term σ = two-nucleon correlation matrix*

⇒ “variational natural orbitals” (VNAT)



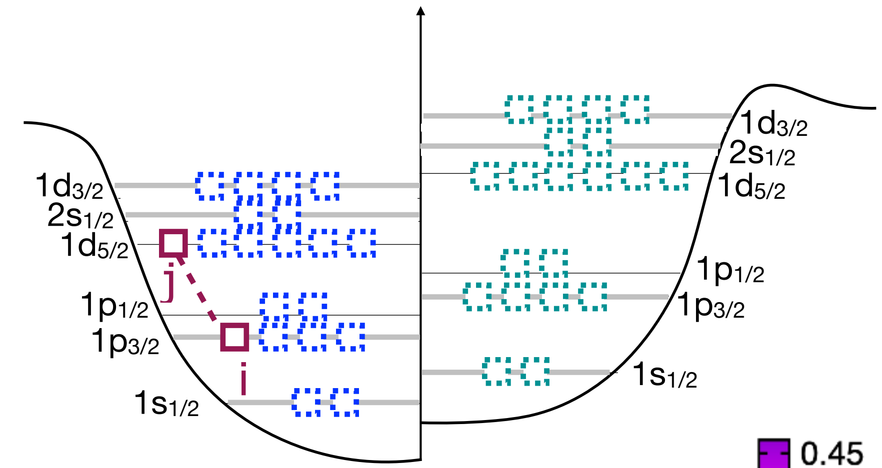


Recently studied from the point of view of entanglement:

Entanglement rearrangement in self-consistent nuclear structure calculations
CR, Savage, Pillet, PRC 103, 034325 (2021), arXiv:2007.09157 (2020)

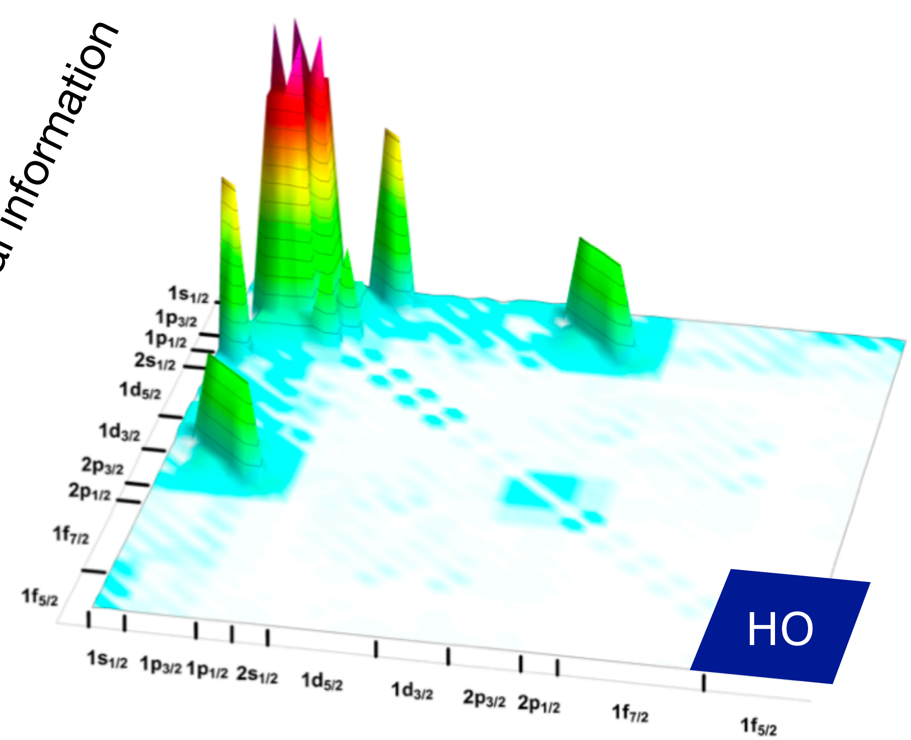
- Mutual information:

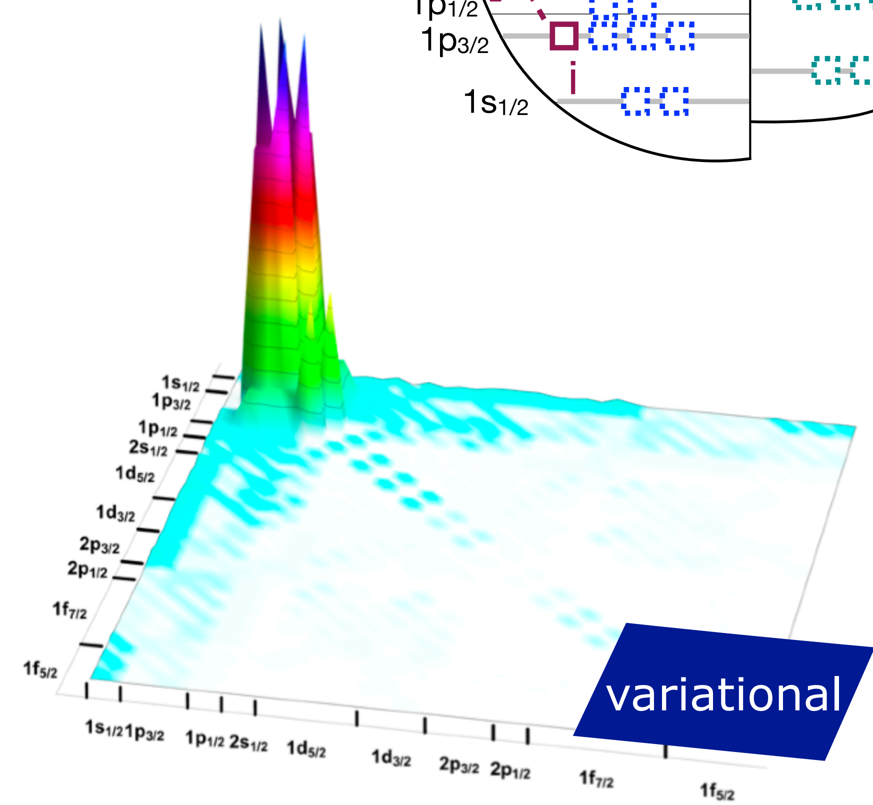
  = correlations between two orbitals embedded in the system

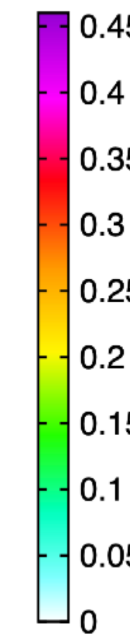


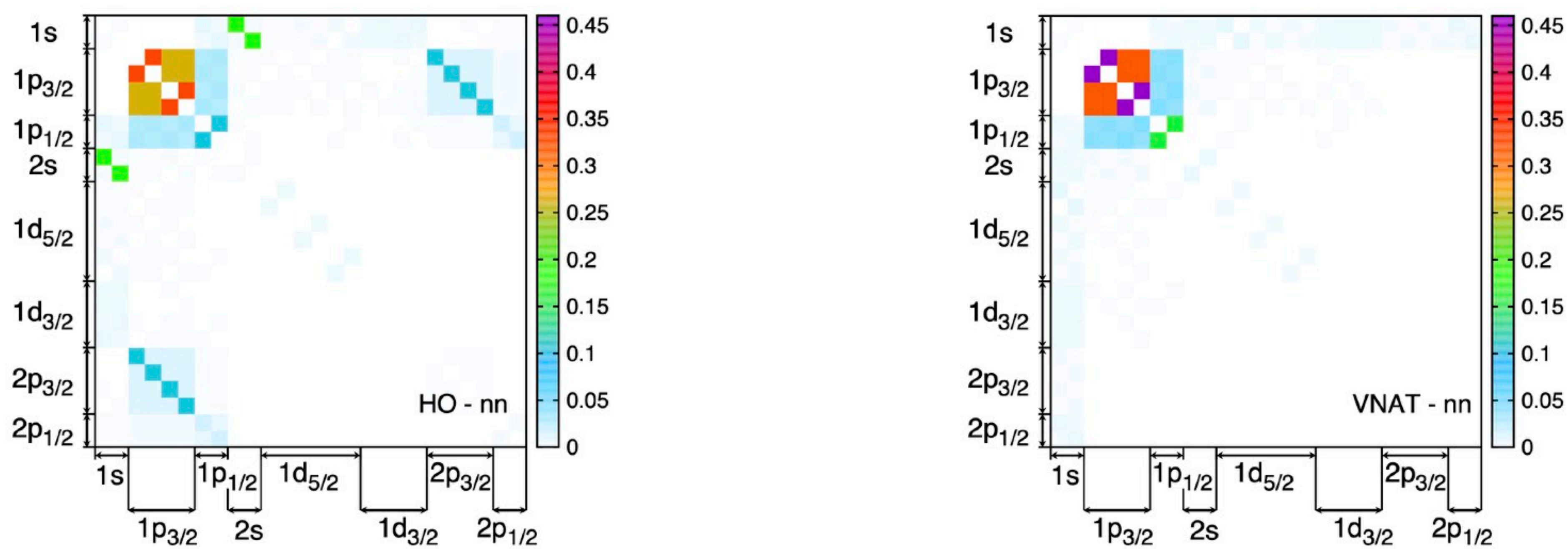
^6He

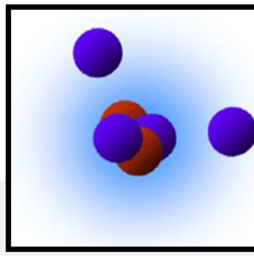
Neutron-neutron mutual information







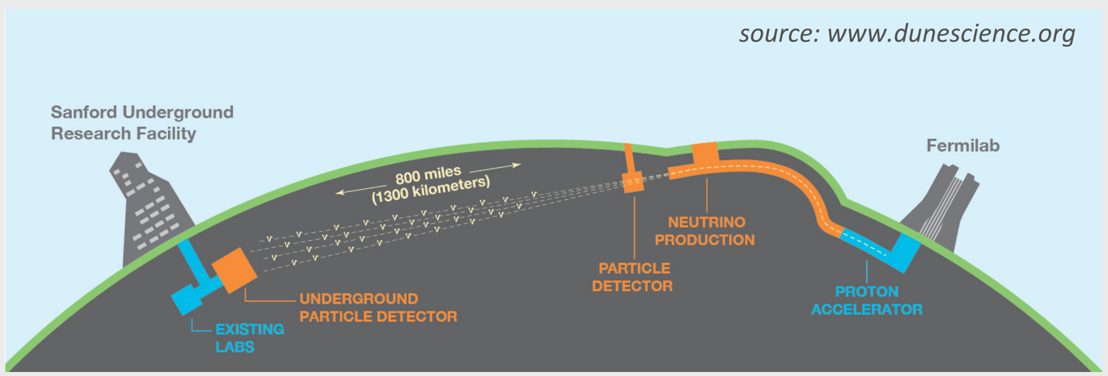




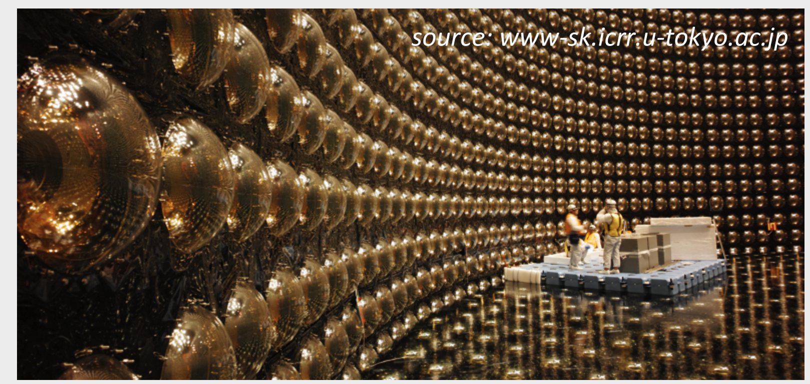
- *HO orbitals: entanglement distributed over the basis*
- *variational orbitals: decoupling of the 1p shell ⇒ emergence of ^4He-core + nn-valence structure*

$$R(\omega,\boldsymbol{q}) = \sum\!\!\!\!\!\!\int_f \left|\langle\Psi_f|O(\boldsymbol{q},\omega)|\Psi_i\rangle\right|^2 \delta(E_f - E_i - \omega)$$

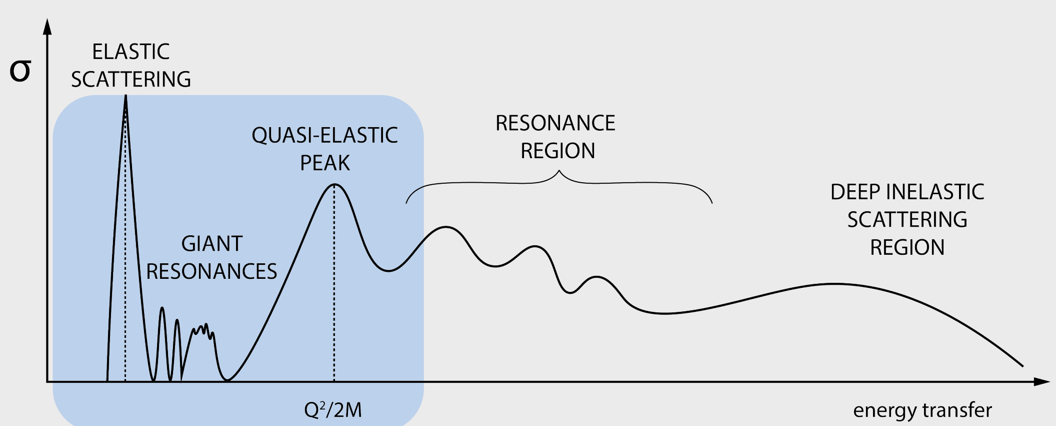
Nuclear theory for neutrino oscillations



Neutrino oscillation experiments require knowledge of neutrino-nucleus cross section for the energy transfers ~hundreds MeV—GeV



Most important nuclei for DUNE and T2HK: ^{12}C, ^{16}O, ^{40}Ar



Possible guidance from *ab initio* nuclear theory

First step: benchmarking with electron data

$$\left.\frac{d\sigma}{d\omega dq}\right|_{\nu/\bar{\nu}} = \sigma_0\left(v_{CC}R_{CC} + v_{CL}R_{CL} + v_{LL}R_{LL} + v_T R_T \pm v_{T'}R_{T'}\right)$$

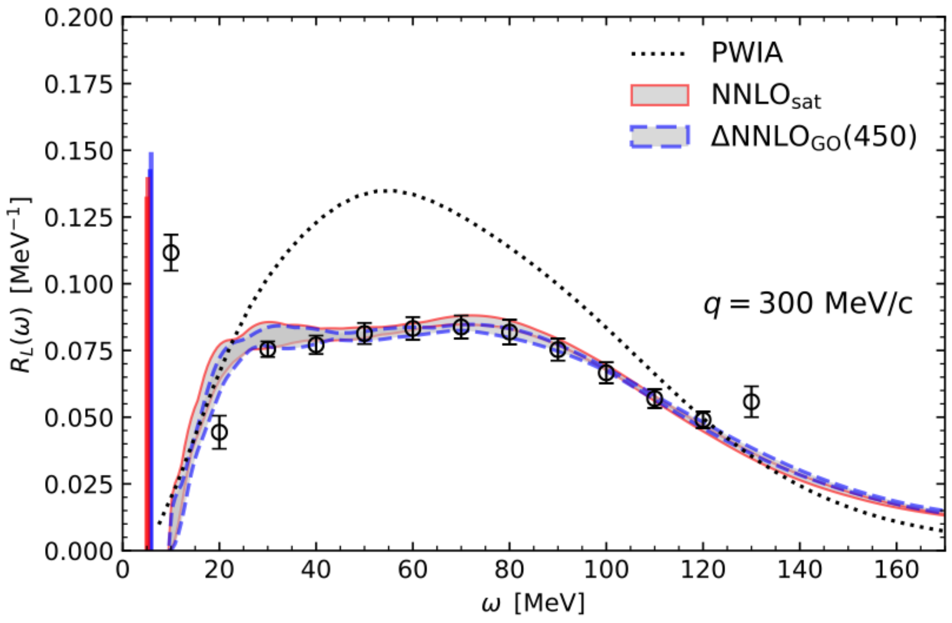
$$\left.\frac{d\sigma}{d\omega dq}\right|_{e} = \sigma_M\left(v_L R_L + v_T R_T\right)$$

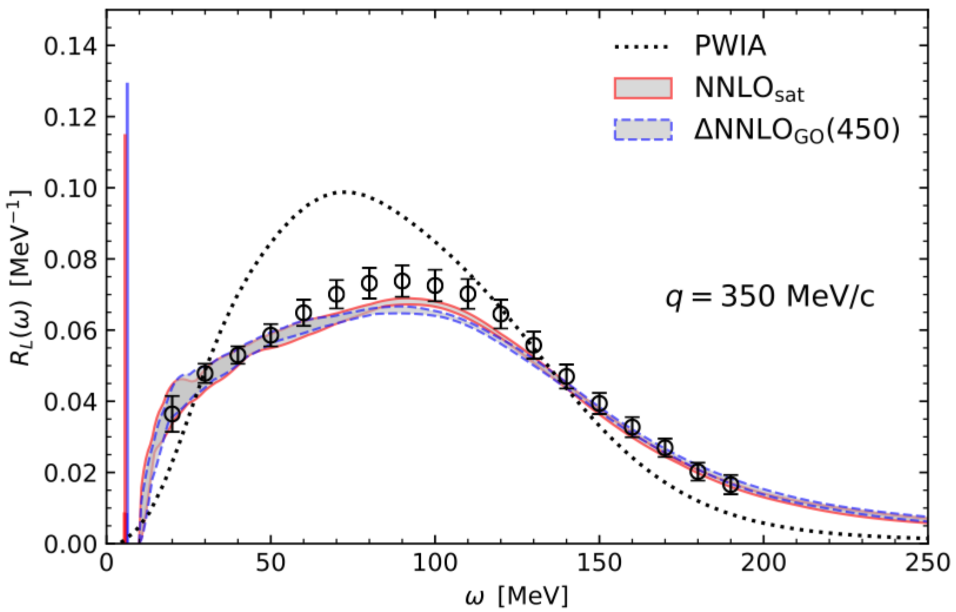
Courtesy of Sonia Bacca (Mainz)

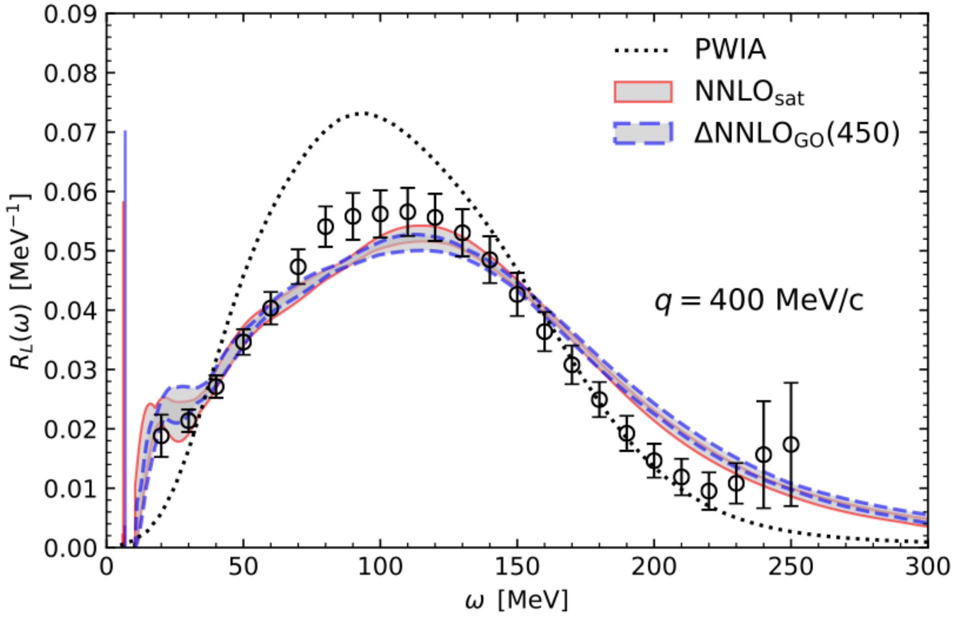
First ab initio results for ^{40}Ca

- Lorentz integral transform combined with coupled cluster method
- Consistent treatment of initial and final-state interactions

*Physical Review Letters **127** (2021) 7, 072501*



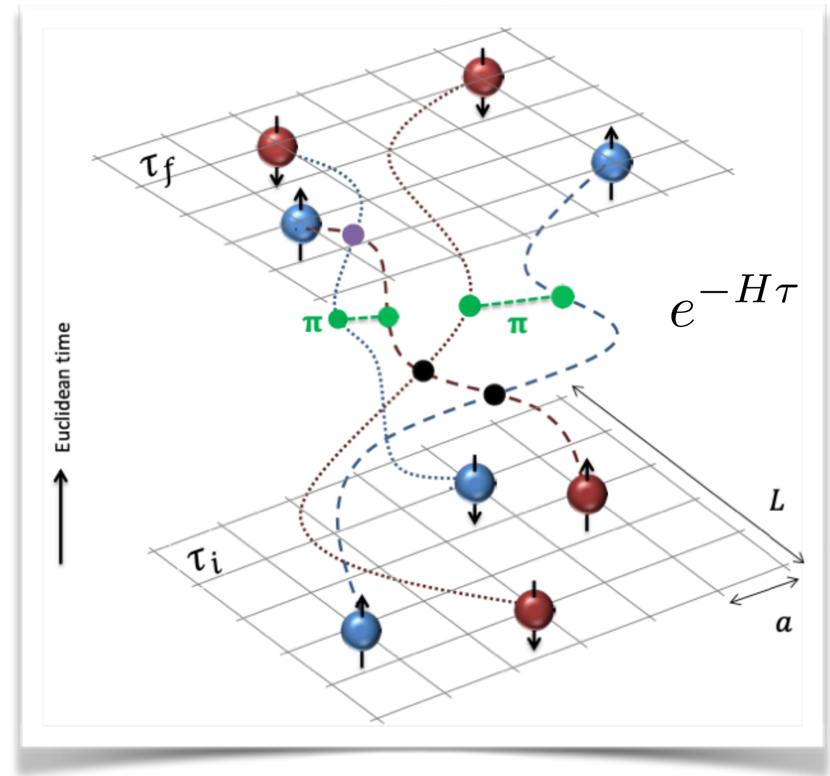




Courtesy of Sonia Bacca (Mainz)

Nuclear Lattice Effective Field Theory (NLEFT)

- Combines chiral EFT and lattice methods
- nucleons on lattice sites interact via chiral EFT forces



☞ *description of cluster states*

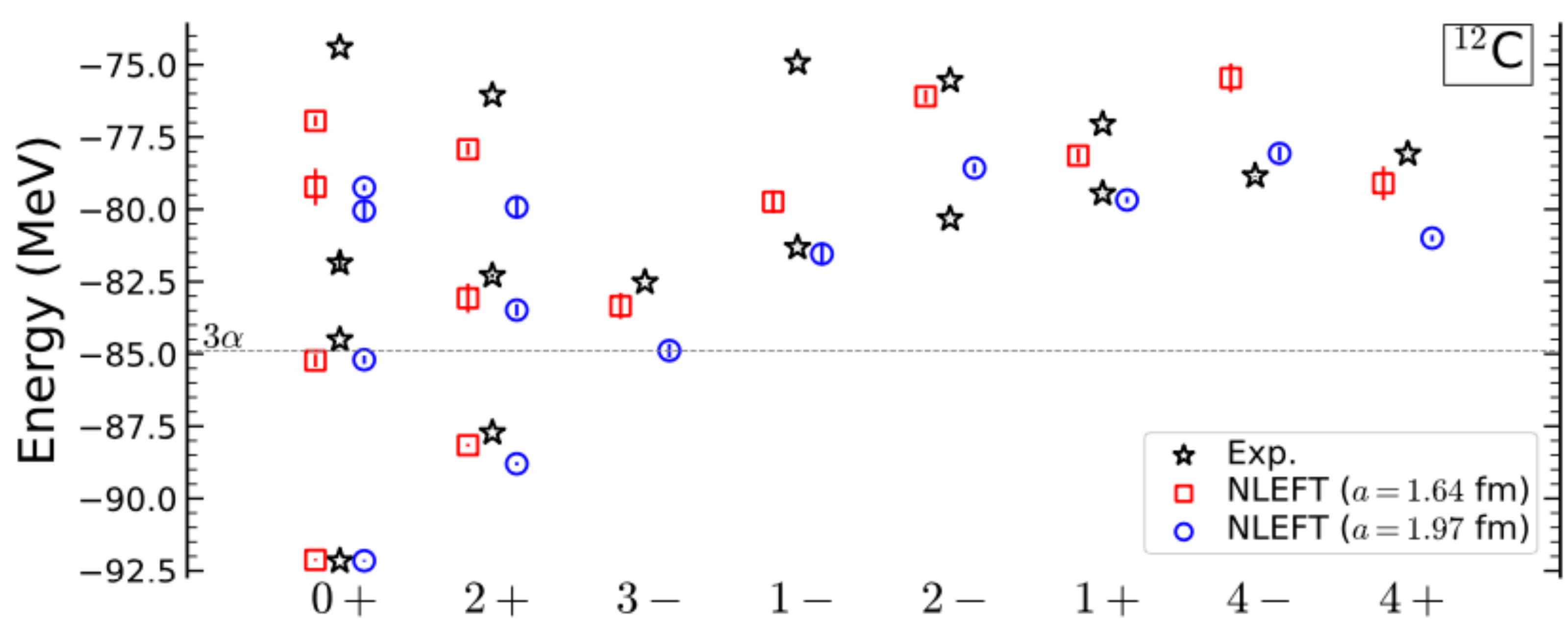
✳ *Ab initio calculation of the Hoyle state,* Epelbaum, Krebs, Lee, Meißner, PRL 106, 192501 (2011)

✳ ***Wigner SU(4) symmetry, clustering, and the spectrum of*** ^{12}***C****,* *Shen, Lähde, Lee, Meißner, EPJA 57, 276 (2021)*

→ good description of the spectrum up to ~15 MeV using

- spin- and isospin-independent NN interaction tuned to ground-state energies of ^{4}He and ^{12}C
- 3-α cluster states and HO particle-hole states as initial states

⇒ either spin-orbit interactions are weak in ^{12}C, or the effects of α clustering are diminishing their influence.



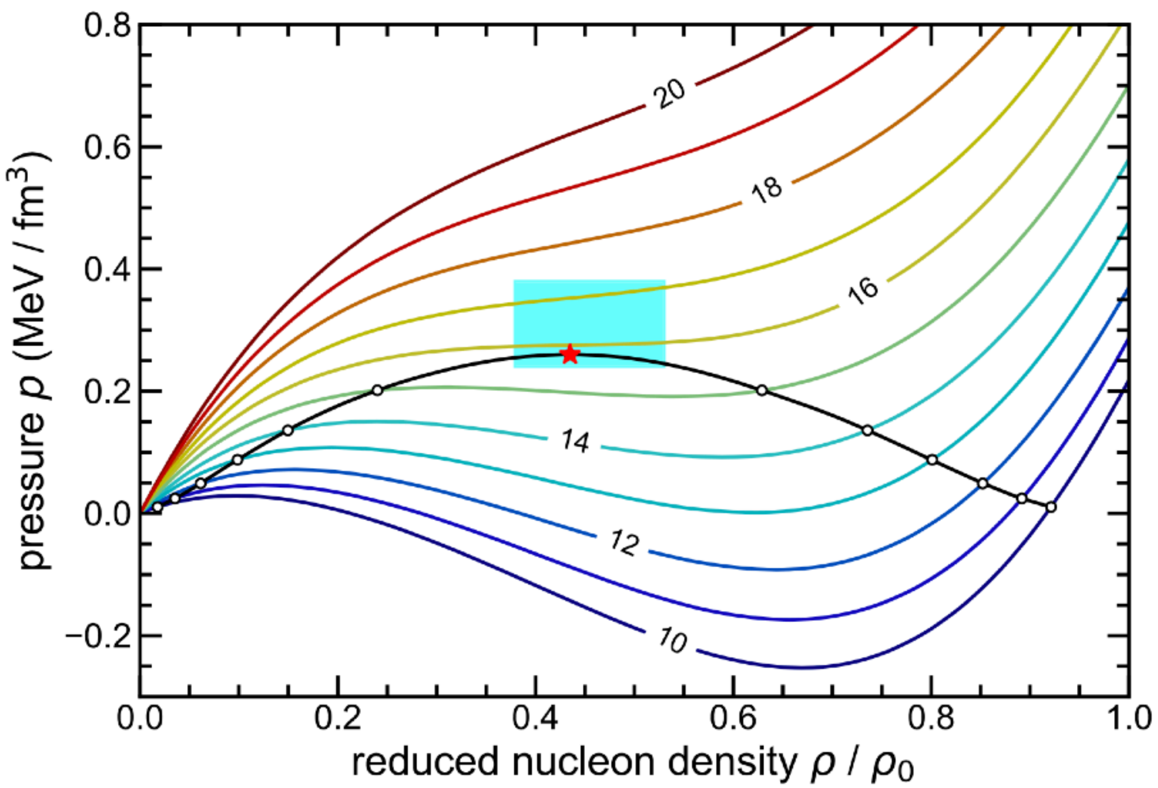
☞ non-zero temperature systems

ab initio calculation of the EoS of nuclear matter with the pinhole trace algorithm

Ab-initio Nuclear Thermodynamics; Lu, Li, Elhatisari, Lee, Drut, Lähde, Epelbaum, Meißner, PRL 125, 192502 (2020)

✳ cost savings = V/A
speedup factor ~ 1000

✳ good parameter-free description of the liquid-vapor phase transition with leading-order pionless EFT (NN and NNN forces)

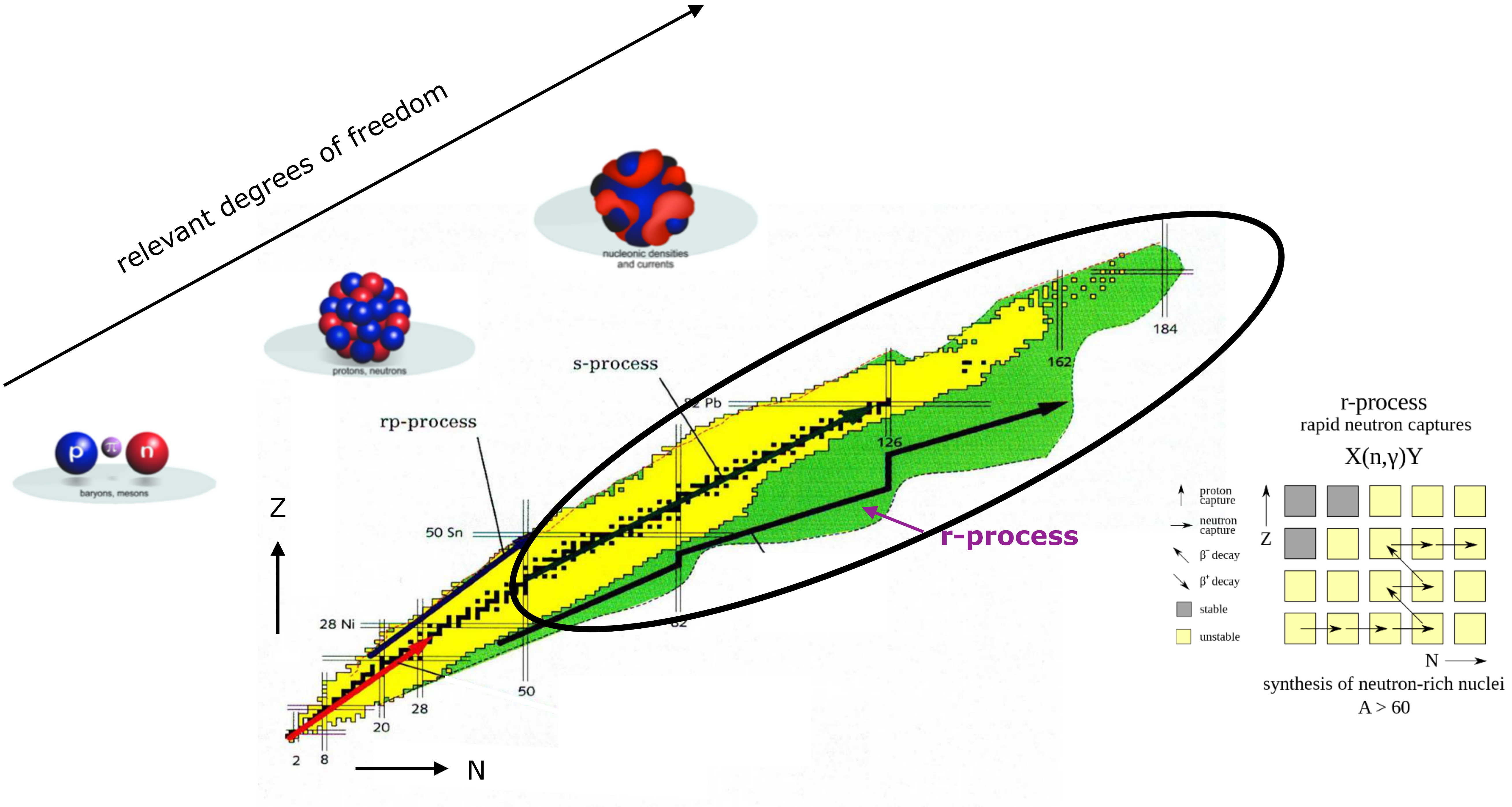


the p-ρ isotherms of symmetric nuclear matter are shown for $L^3 = 6^3$. The black line denotes the liquid-vapor coexistence line, and the red star marks the calculated critical point. The cyan rectangle marks the empirical critical point extracted from heavy-ion collisions [54].

☞ reactions

Ab initio alpha-alpha scattering, Elhatisari, Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, *Nature,* 528**,** 111 (2015)

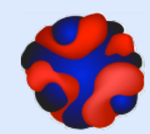
Many-body methods for heavy nuclei



Relativistic Nuclear Field Theory (RNFT)

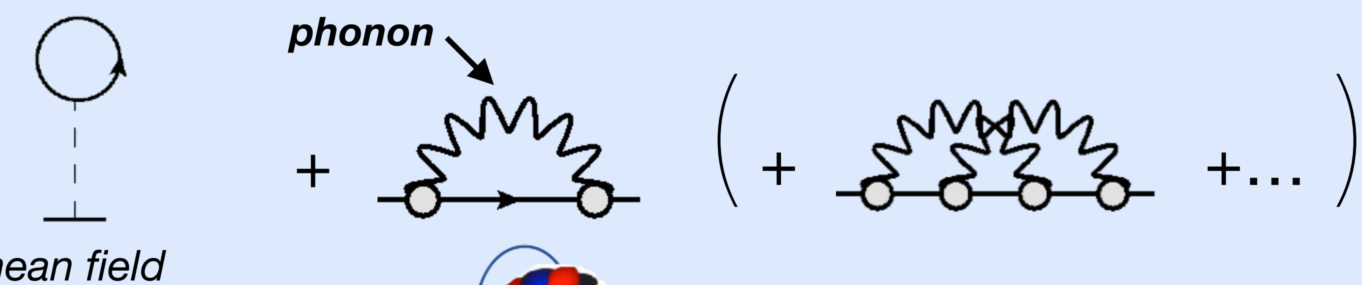
Degrees of freedom in RNFT:

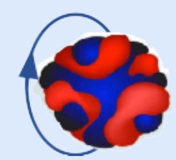
 =

- ✳ relativistic effective mesons π σ ω ρ (m ~ 140-800 MeV) *quantum hadrodynamics*
- ✳ relativistic nucleons p n (S_n ~ 10 MeV)
- ✳ phonons (collective vibrations of the nucleus)  (E ~ few MeV)

systematic expansion in the PVC vertex

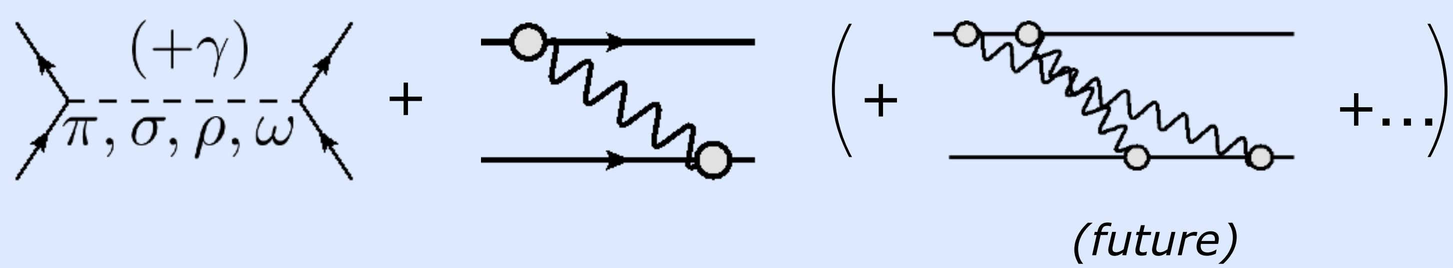
Nucleonic motion =





particle-vibration coupling (PVC)

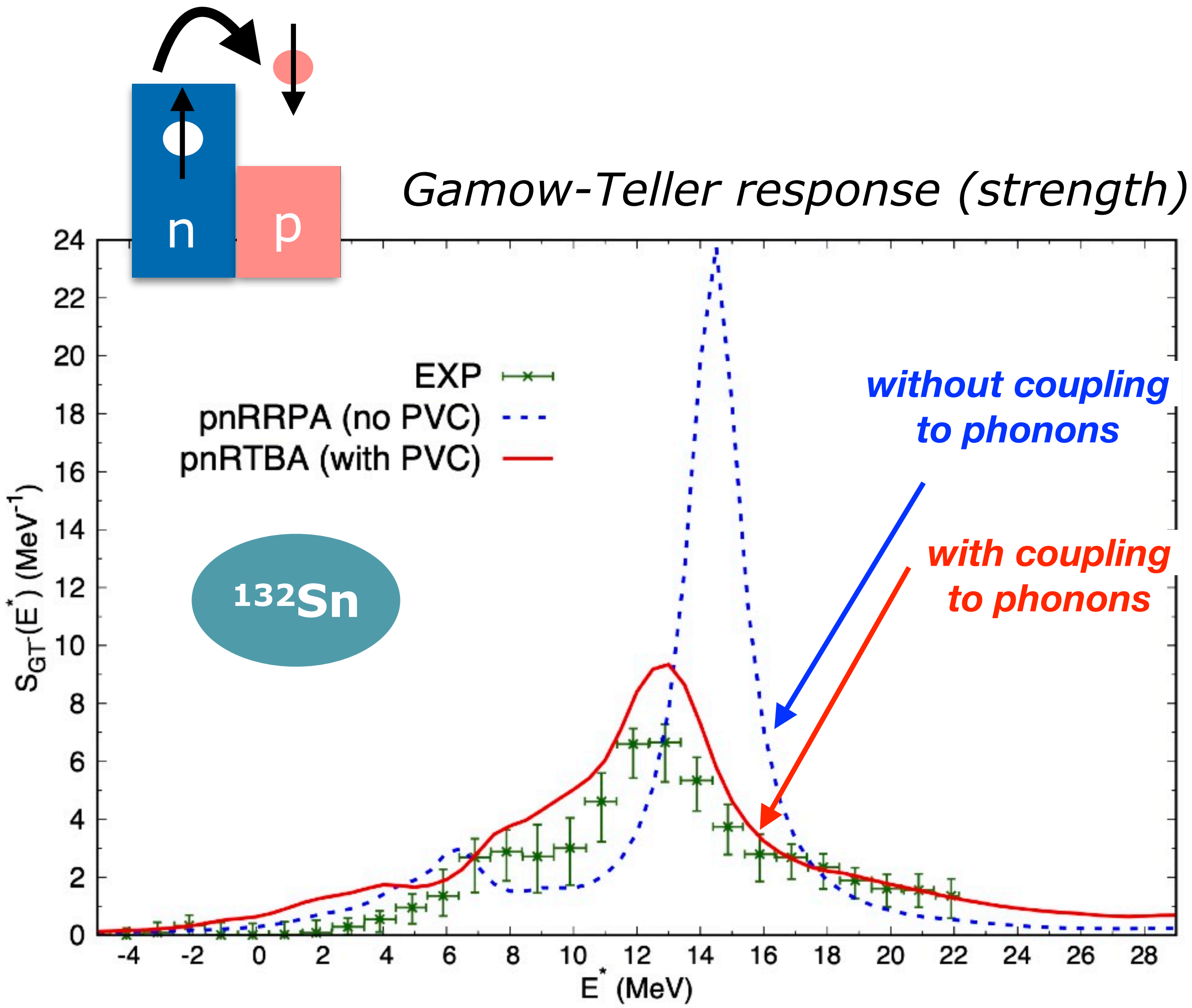
Effective NN interaction =

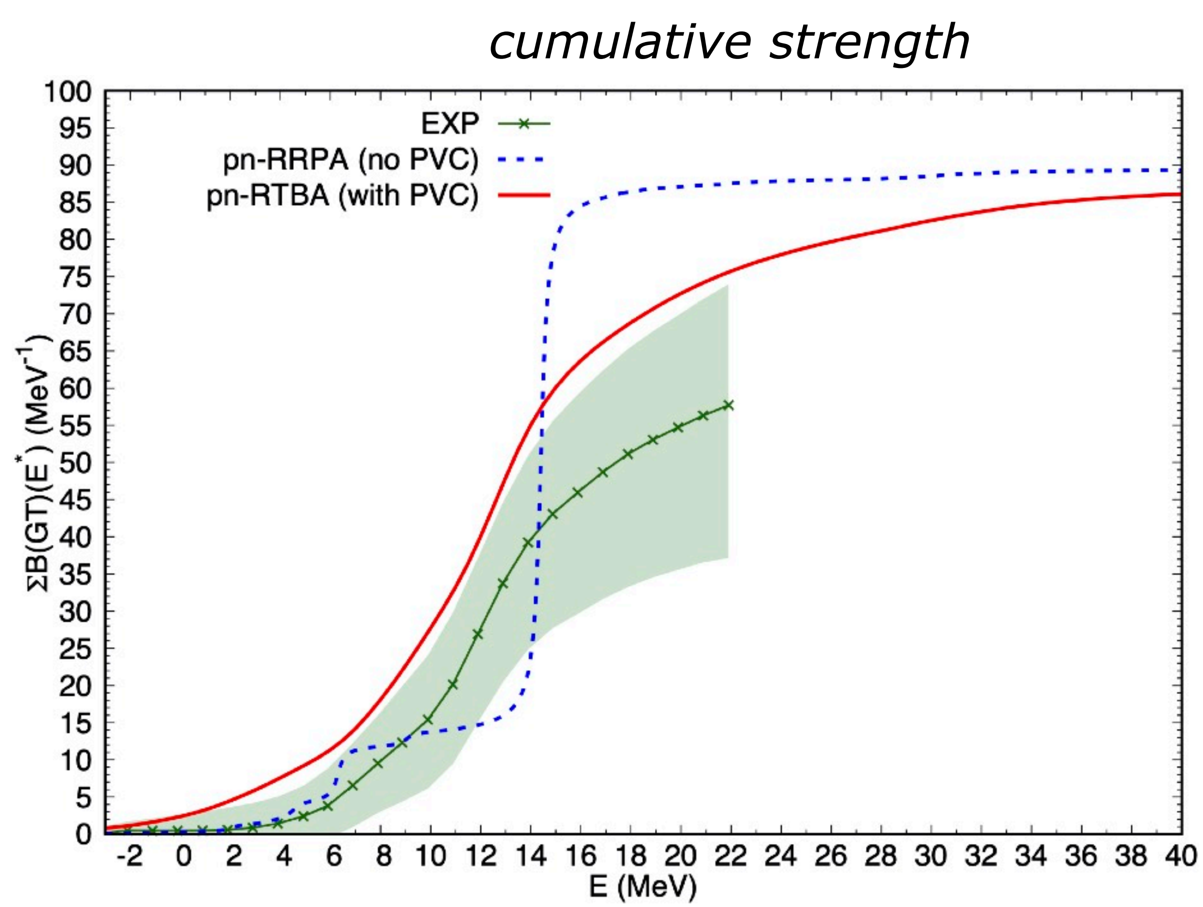


- ✦ *Applicability up to heavy/superheavy masses to be useful for astrophysical applications*
- ✦ *while allowing for a precise description of nuclear phenomena*
- ✦ *not ab-initio but no new parameters are introduced when going beyond mean field*

Gamow-Teller response and β-decay half-lives of r-process nuclei

CR, Litvinova PRC 98, 051301 (2018).

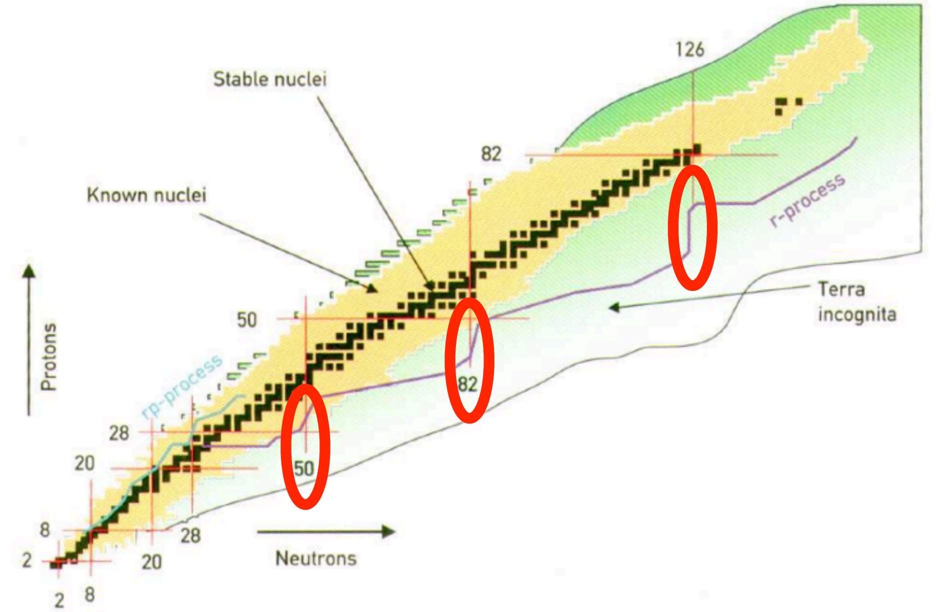


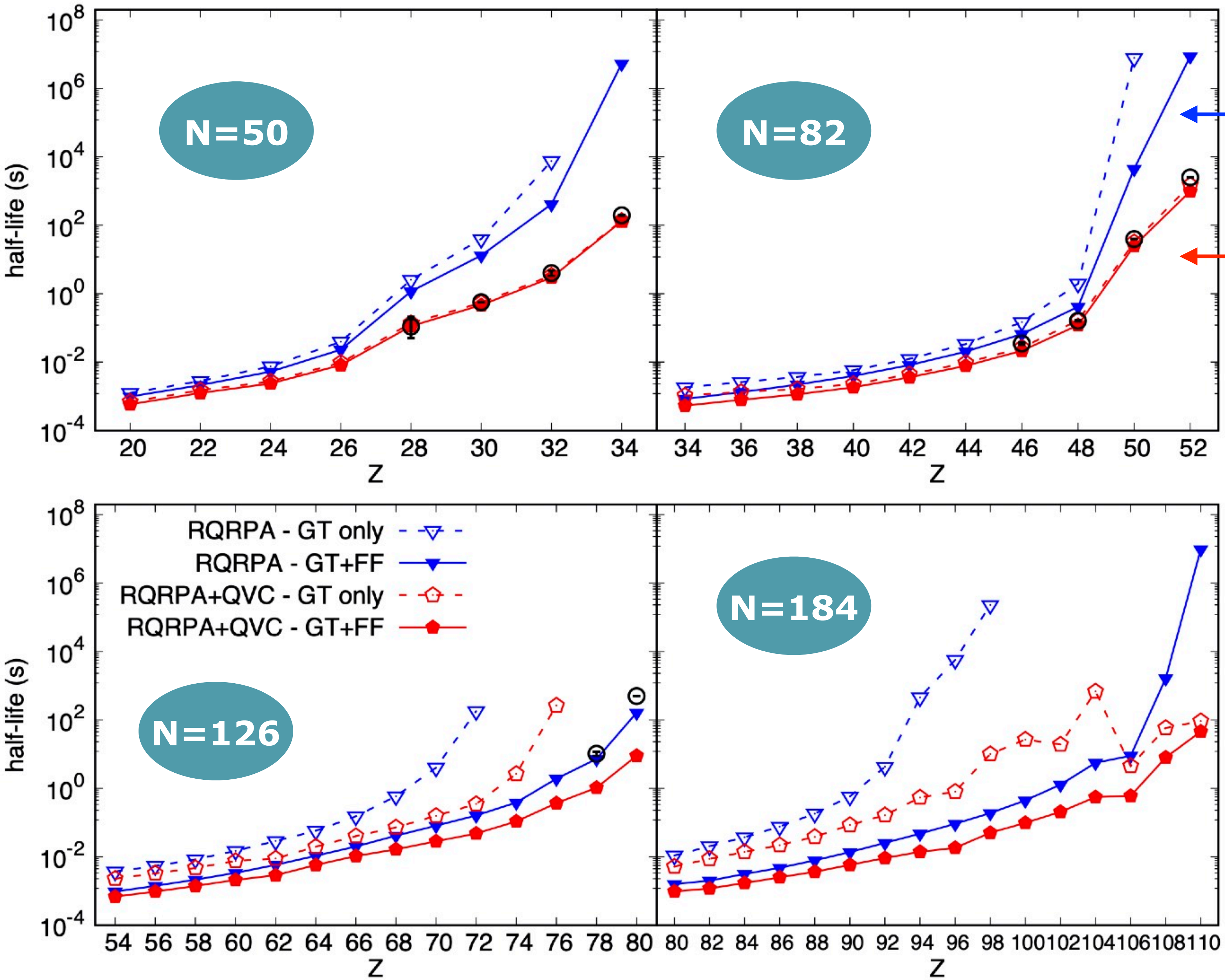


The particle-vibration coupling provides a natural "quenching mechanism"

β-decay half-lives of r-process nuclei including first-forbidden transitions

CR, Litvinova, Martínez-Pinedo, NIC-XVI proceedings, arXiv:2111.14841 (2021)
CR, Martínez-Pinedo, Litvinova, in preparation





without coupling to phonons

with coupling to phonons

no quenching of GT or FF operators
(g_A=-1.276)

- large improvement of the half-lives for N=50,82 without extra parameter
- large impact of the FF modes in N=126,184 chains

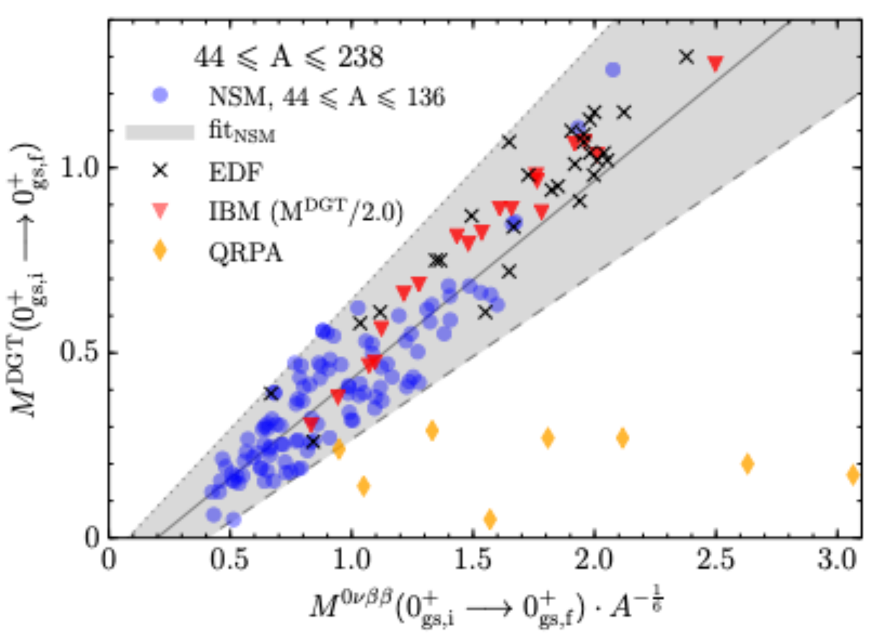
EFT for heavy nuclei

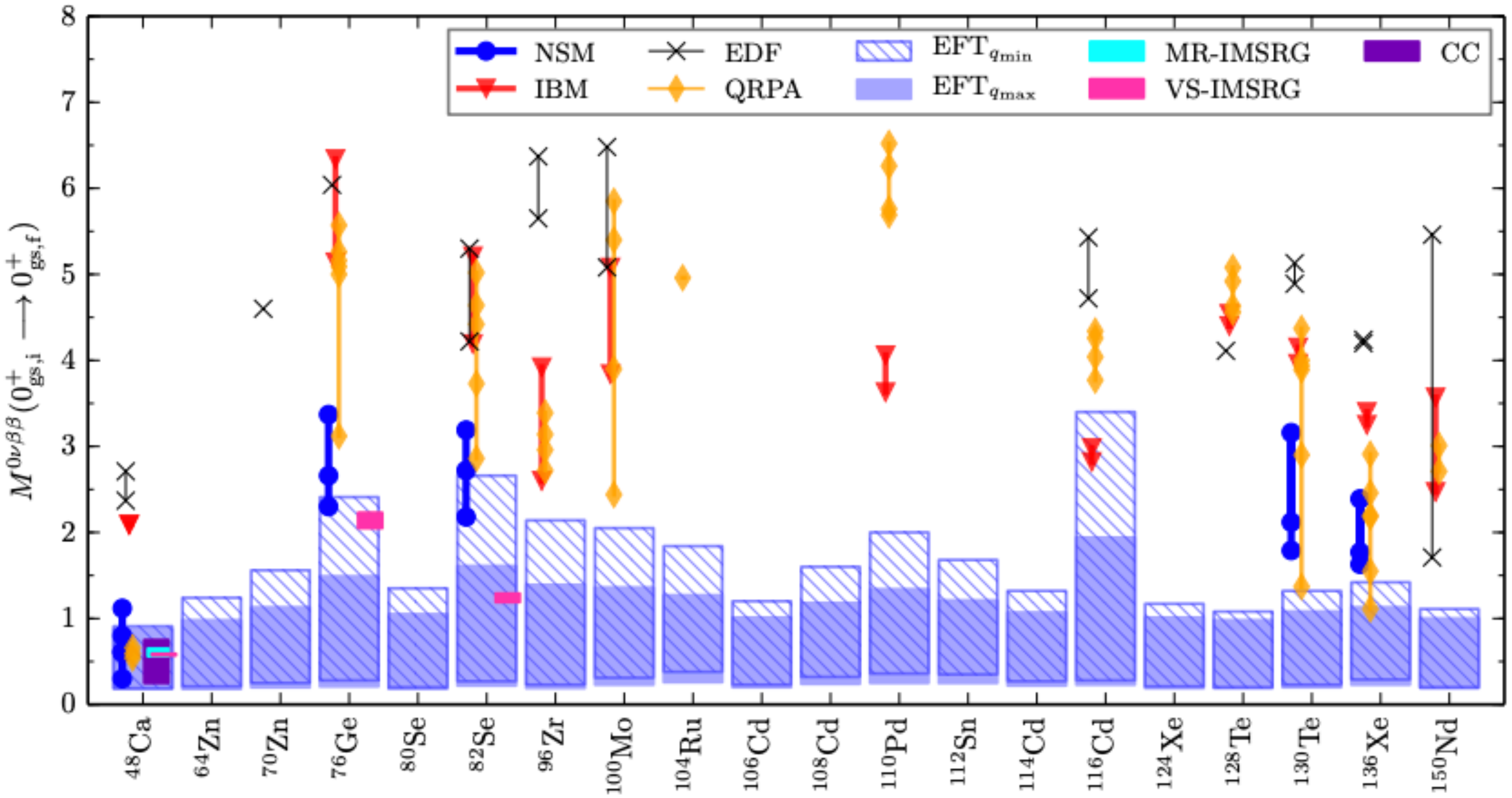
- EFT with collective quadrupole phonons (d) coupled to nucleons (p,n)
- Effective Gamow-Teller (GT) operator with low-energy constants fitted to GT data

$$\hat{O}_{GT} = C_\beta (\tilde{p} \otimes \tilde{n})^{(1)} + \sum_\ell C_{\beta\ell} \left[\left(d^\dagger + \tilde{d} \right) \otimes (\tilde{p} \otimes \tilde{n})^{(\ell)} \right]^{(1)} + \sum_{L\ell} C_{\beta L\ell} \left[\left(d^\dagger \otimes d^\dagger + \tilde{d} \otimes \tilde{d} \right)^{(L)} \otimes (\tilde{p} \otimes \tilde{n})^{(\ell)} \right]^{(1)}$$

Neutrinoless double-beta decay from an effective field theory for heavy nuclei,
C. Brase, J. Menéndez, E. A. Coello Pérez, and A. Schwenk, arXiv:2108.11805 (2021)

- used established correlations between double GT and 0νββ decay to predict 0νββ matrix element with uncertainty estimate





Conclusion, perspectives

Fast progress of *ab-initio* methods based on chiral EFT forces

and continuous effort to extend the reach and precision of the calculations

✳ theoretical uncertainties

Roth et al. working on a range of methods using concepts from Bayesian statistics as well as Machine Learning techniques to improve uncertainty estimates and model space extrapolations for NCSM and IM-SRG methods (paper coming soon)

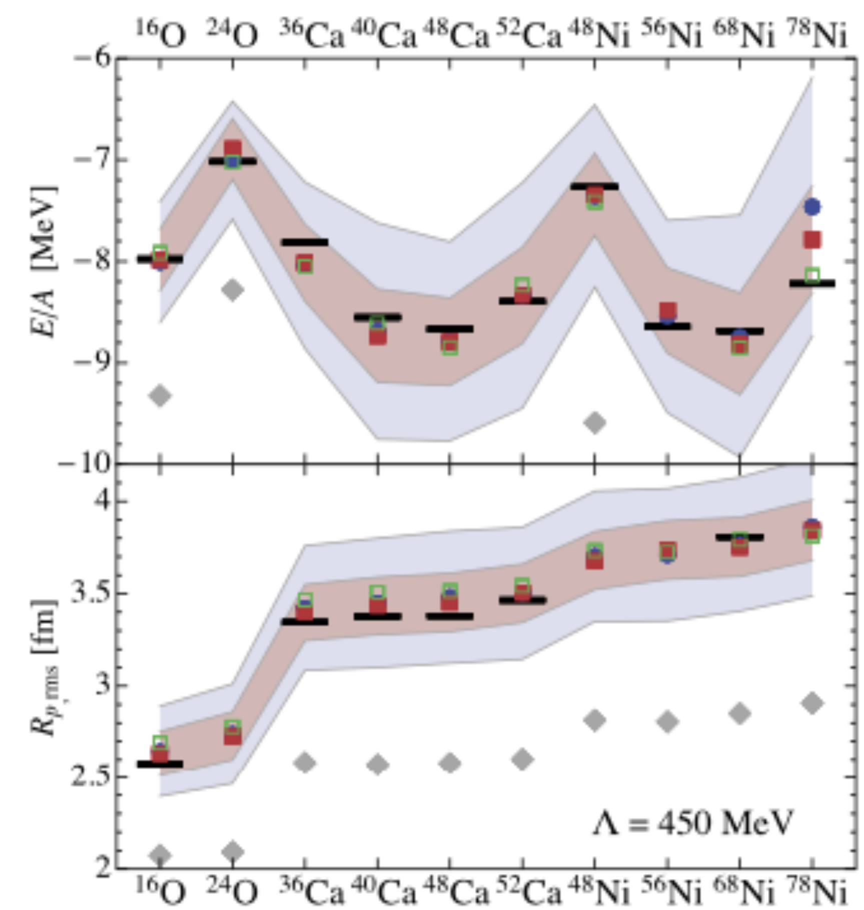
✳ development of chiral interactions

- *Family of chiral two- plus three-nucleon interactions for accurate nuclear structure studies,* *Hüther ,Vobig , Hebeler, Machleidt, Roth, PLB 808, 135651 (2020).*

  → accurate description of masses and radii in mid-mass nuclei, and spectroscopy up to sd-shell

- LENPIC Collaboration working towards a really consistent formulation of chiral two- plus three-body forces from a fundamental level

  Bochum/Bonn/Darmstadt/Jülich: Epelbaum, Krebs, Reinert, Meißner, Hebeler, Hüther, Roth, Vobig, Nogga
  + Iowa, Ohio, Kraków, Japan



Light nuclei with semilocal momentum-space regularized chiral interactions up to third order, PRC 103, 054001 (2021)

Conclusion, perspectives

Heavy nuclei remain out of reach of *ab-initio* methods

✳ urgent need to improve the nuclear physics inputs for ββ-decay experiments and r-process simulations

→ RNFT and EFT for heavy nuclei are possible ways

→ works in pair with experimental progress (radioactive-beam facilities)

✳ in the longer term, would like to link these methods to *ab-initio* concepts

→ RNFT: can one avoid the use of phenomenological functionals?

→ EFT for heavy nuclei: can one derive the parameters?

Conclusion, perspectives

Towards Quantum Computing nuclei

✳ Quantum Computing holds the promise of exact solutions of the (nuclear) many-body problem

✳ Studies of entanglement in nuclei can help design algorithms for near-term devices

- example: The variational natural single-particle basis localizes entanglement

  ⇒ can be useful for designing workflows for hybrid classical-quantum computations of nuclei (weakly vs strongly entangled parts of the Hilbert space)

active space diagonalization ⇄ orbital optimization (full space)

(new orbitals naturally ordered by entanglement)