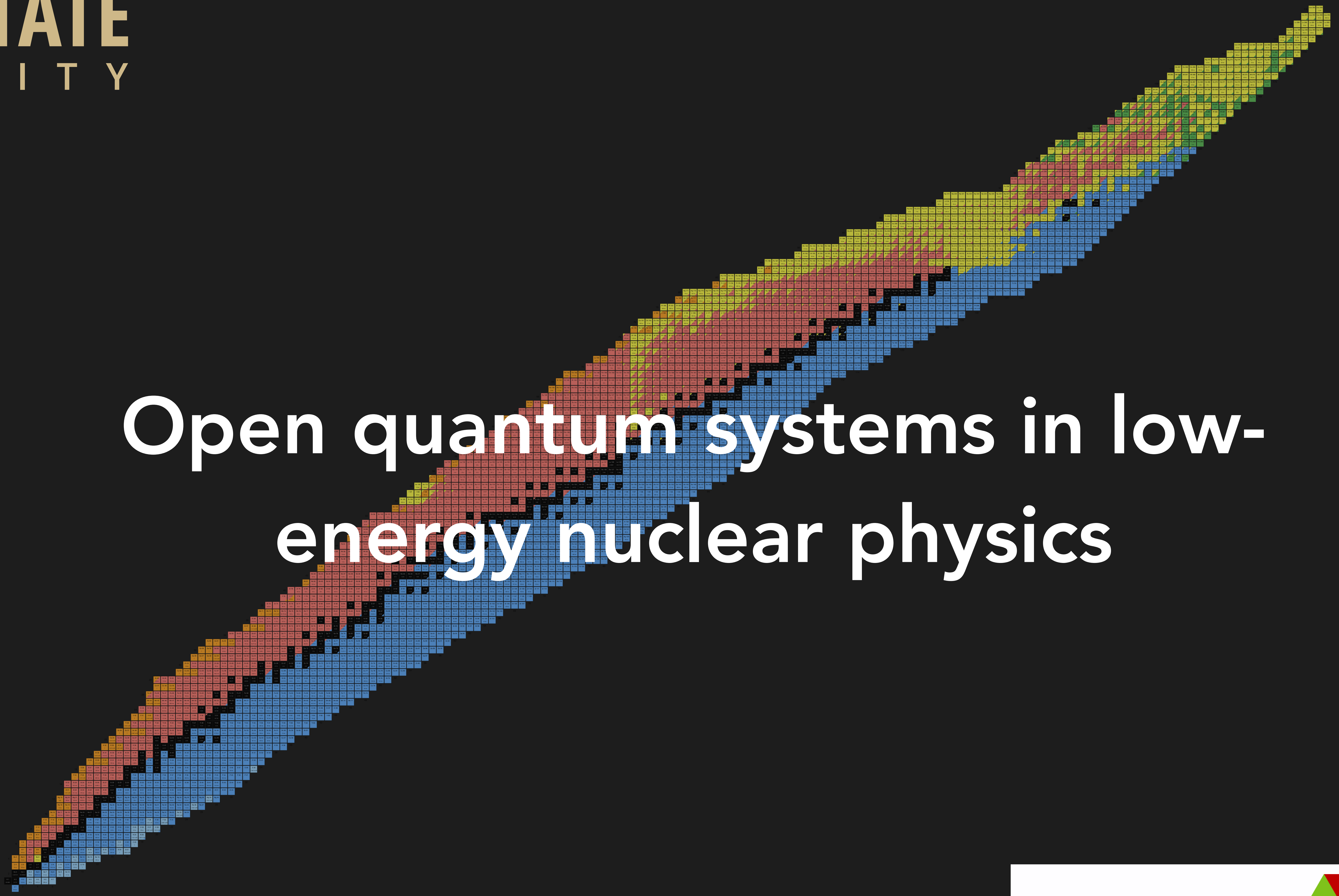
Open quantum systems in low-energy nuclear physics



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Dec. 1, 2025

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NSF: PHY-2238752 (CAREER)
DOE: DE-SC0026198 (STREAMLINE 2, ML/AI)
DOE: DE-SC0013617 (Office of Nuclear Physics, FRIB Theory Alliance)

NSF FRIB U.S. DEPARTMENT OF ENERGY | Office of Science

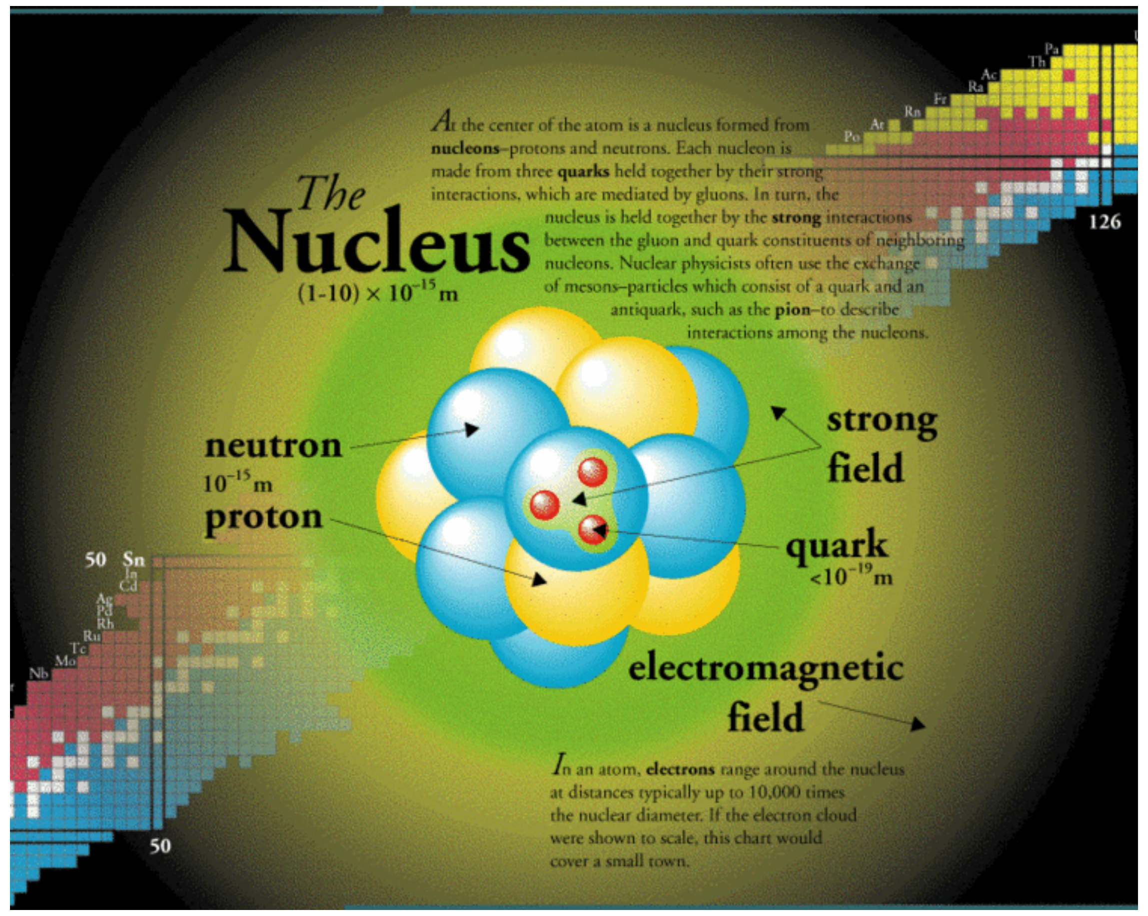
Argonne NATIONAL LABORATORY

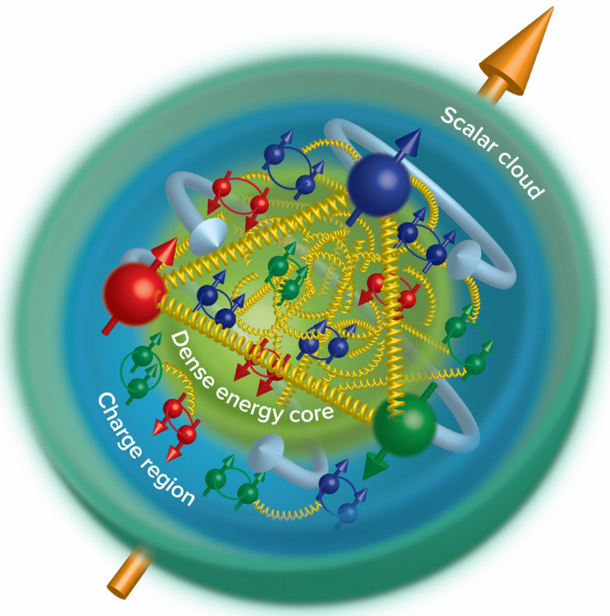
Nuclear physics

- How do quarks and gluons make up protons, neutrons, and, ultimately, atomic nuclei?
- What are the nuclear processes that drive the birth, life, and death of stars?
- How do we use atomic nuclei to uncover physics beyond the Standard Model?
- How do the rich patterns observed in the structure and reactions of nuclei emerge from the interactions between neutrons and protons?

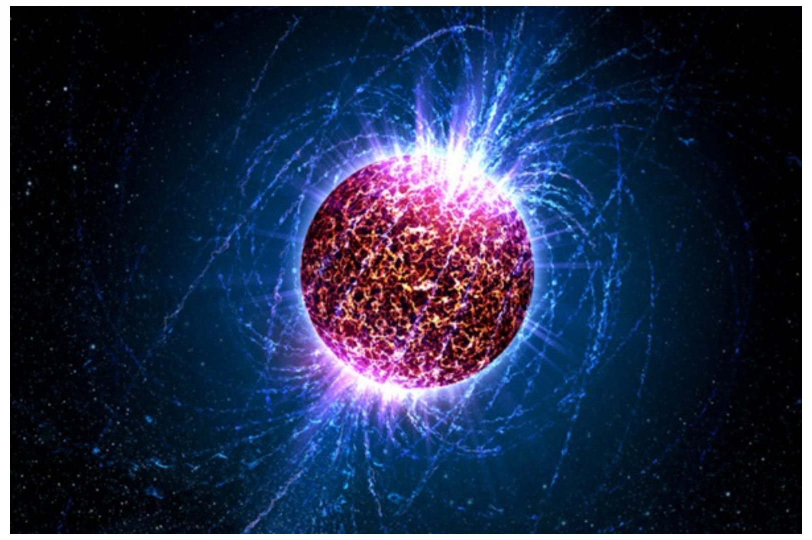
↓

My focus: low-energy structure and reactions.

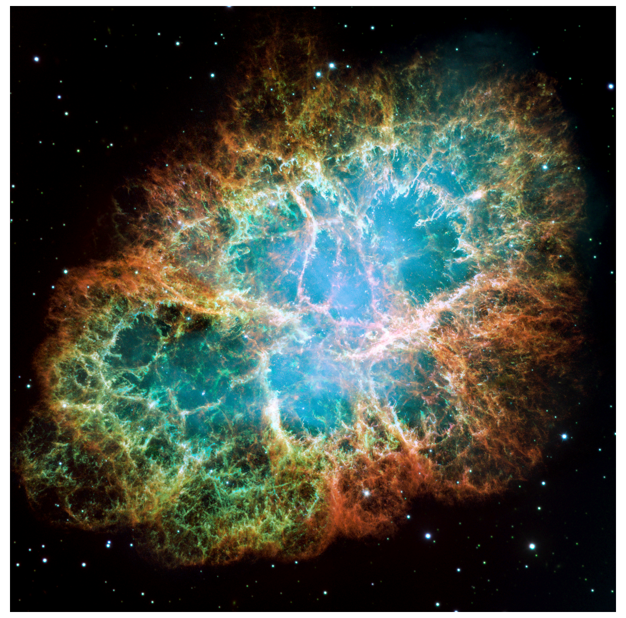




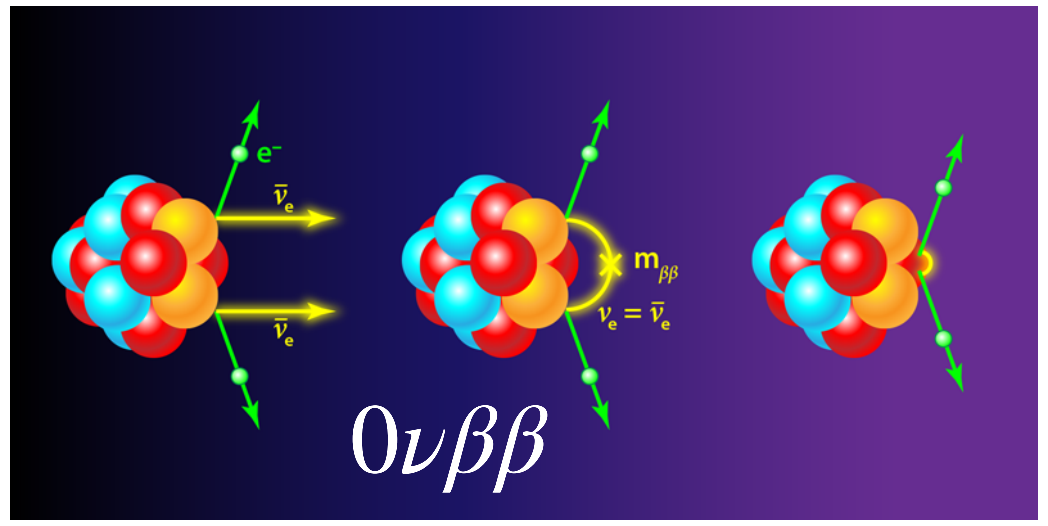
QCD, hadron physics



Nuclear astrophysics

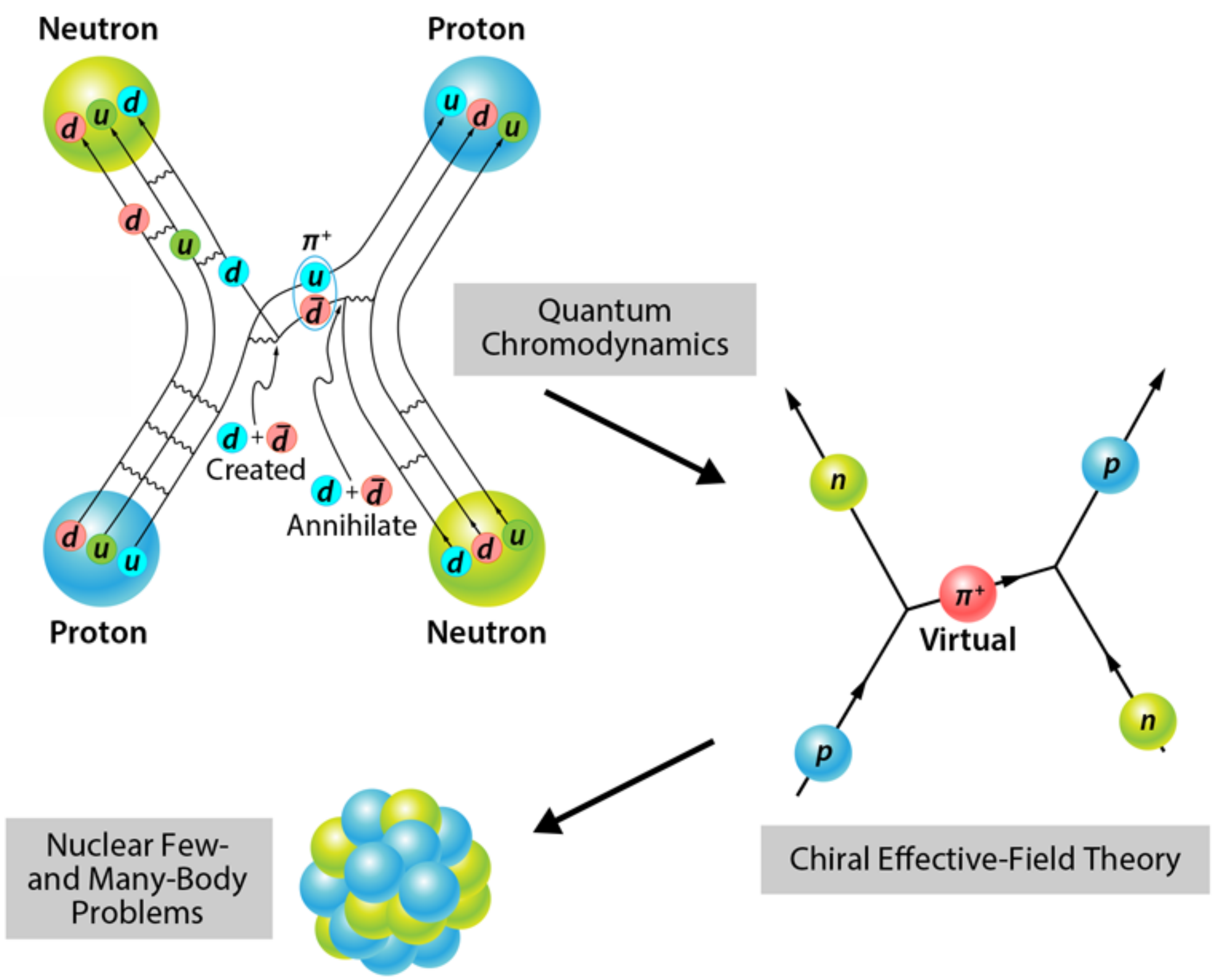


Low-energy tests of the SM, neutrino physics

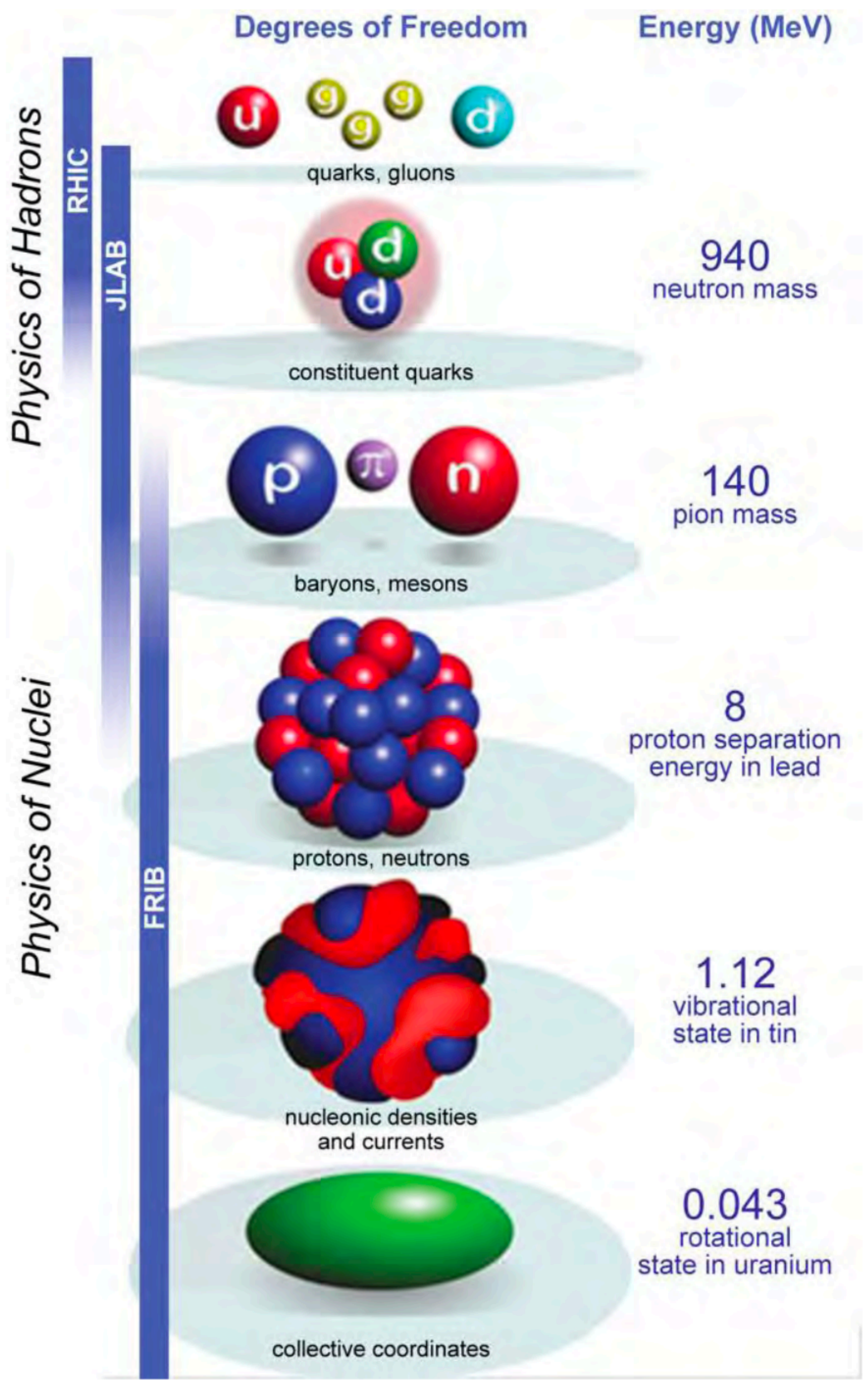


Low-energy nuclear physics

At low energy (< M_{QCD} ~1 GeV): nucleons as degrees of freedom.



Strong residual nucleon-nucleon interaction.

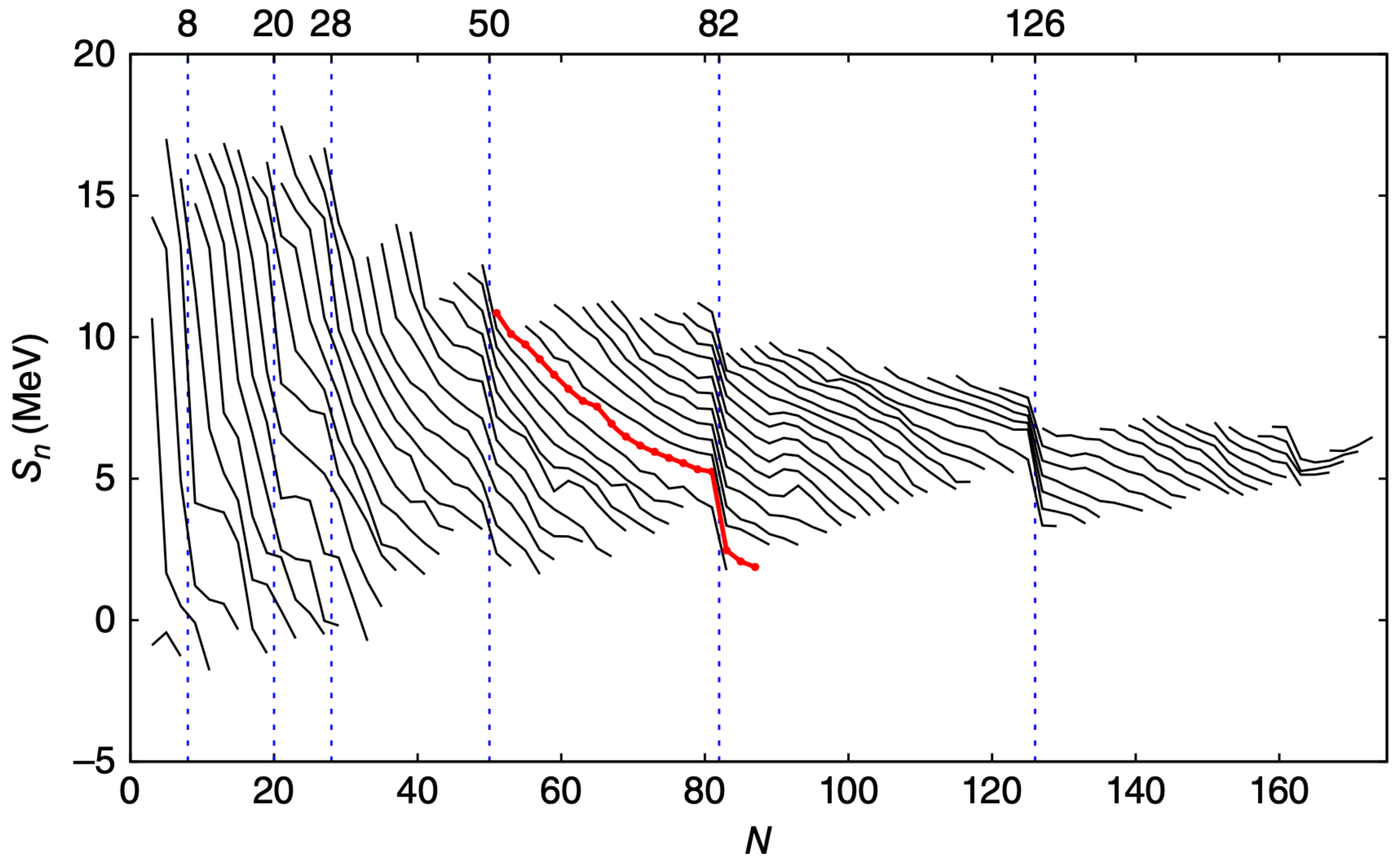


Strongly correlated fermionic quantum many-body problem (for p and n).

Low-energy nuclear physics

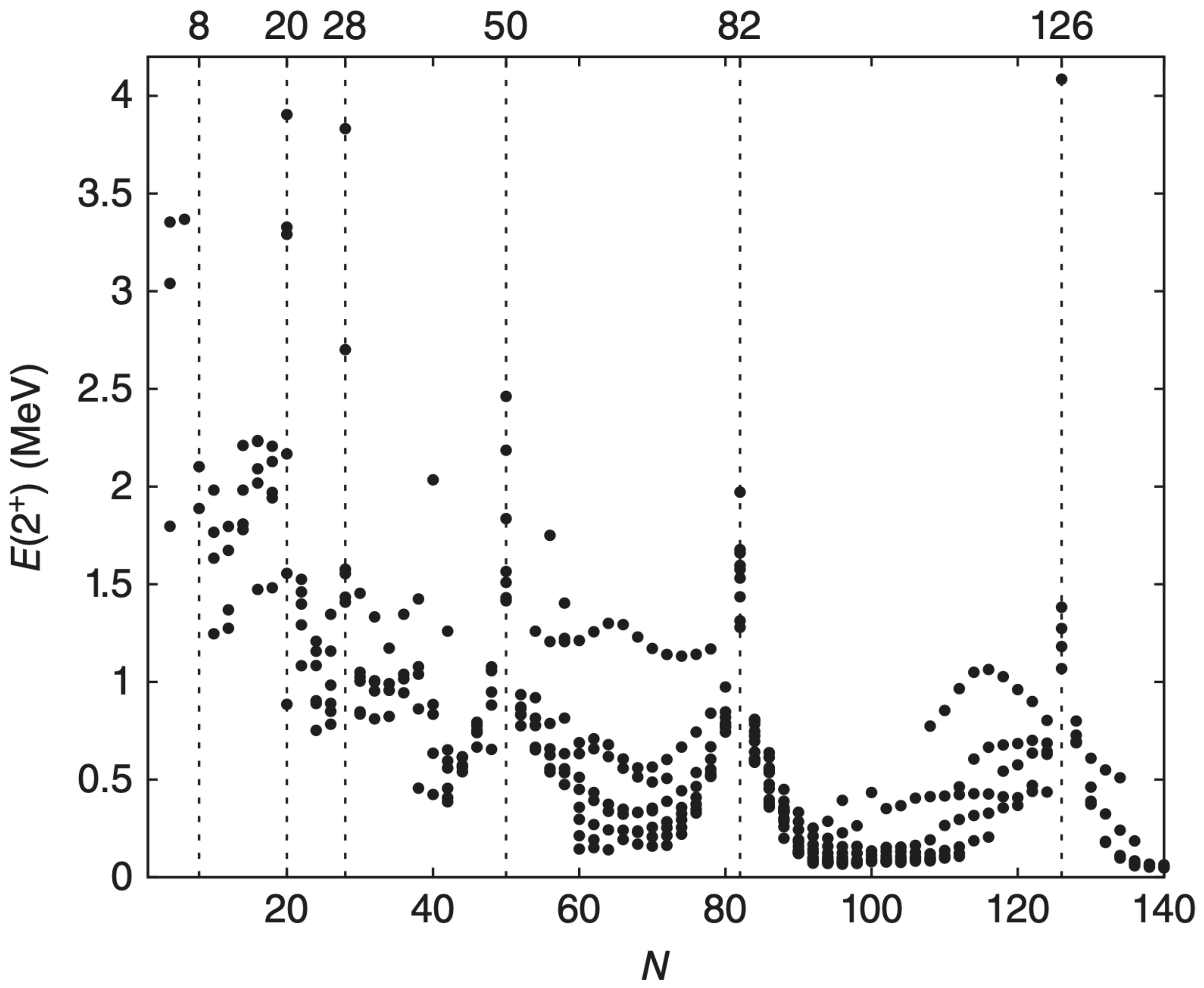
Emergent phenomena at similar scales, complex many-body physics.

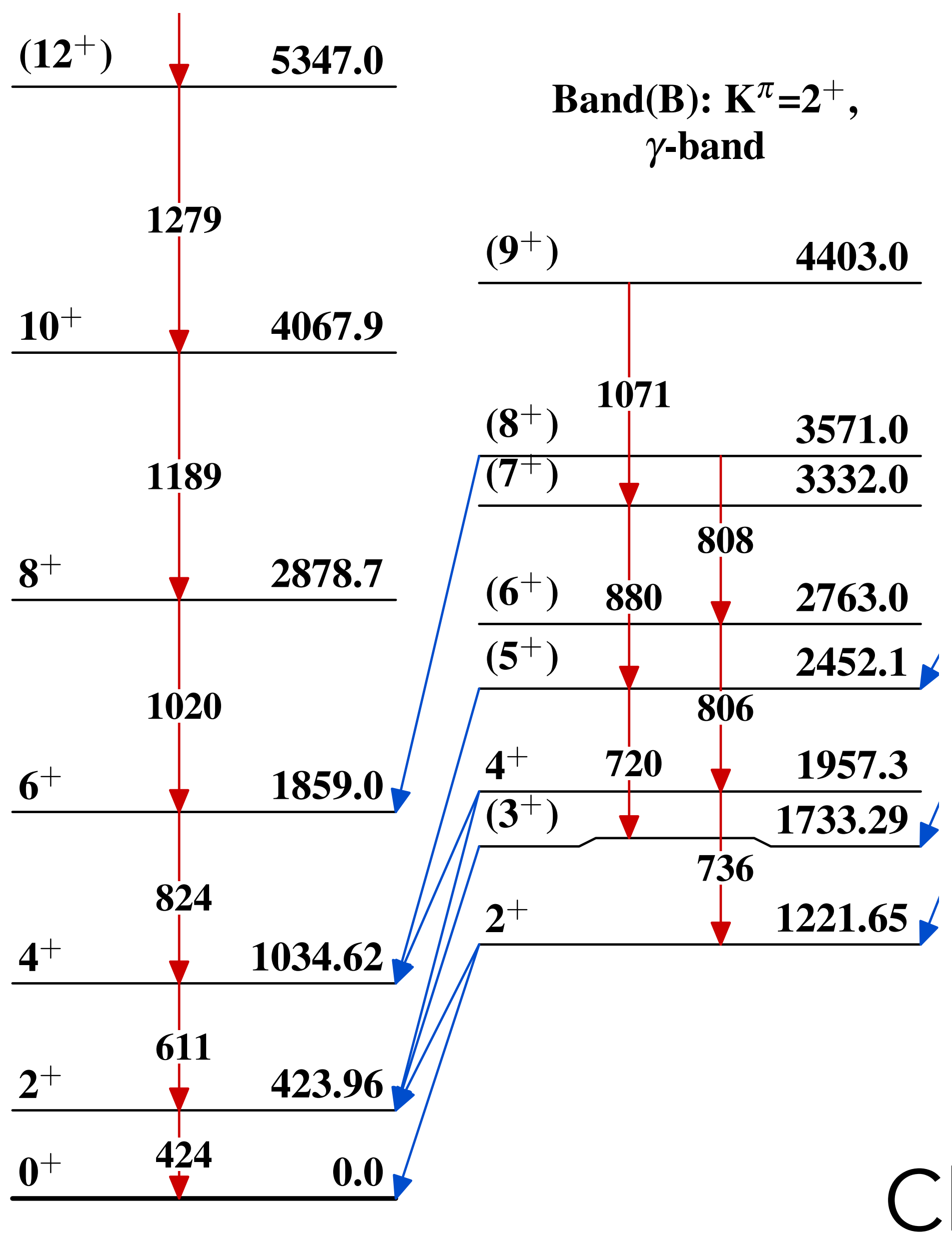
V. Zelevinsky & A. Volya, *Physics of Atomic Nuclei*



Self-consistent shell structure

Pairing superfluidity

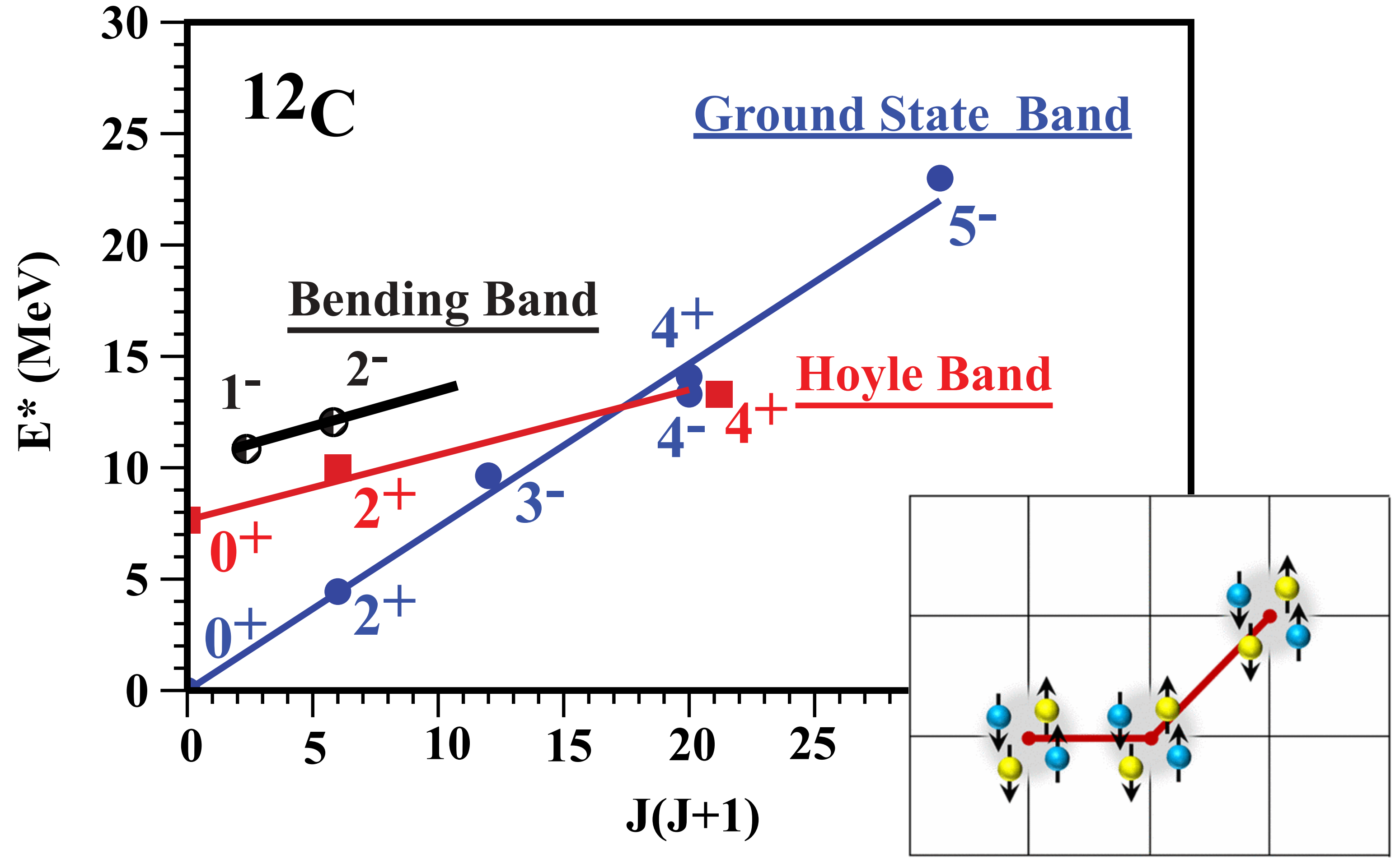




Spontaneous deformation, collective motion

Clustering

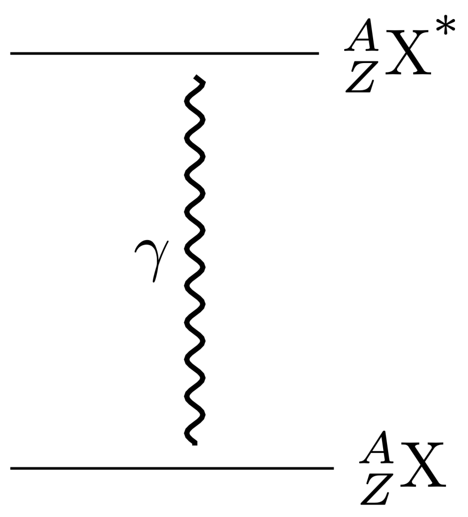
D. J. Marín-Lámbarri *et al.*, PRL **113**, 012502 (2014)



E. Epelbaum *et al.*, PRL **109**, 252501 (2012)

Decay modes of atomic nuclei

Several possible decay modes with vastly different, overlapping timescales.
Competition between modes can happen.

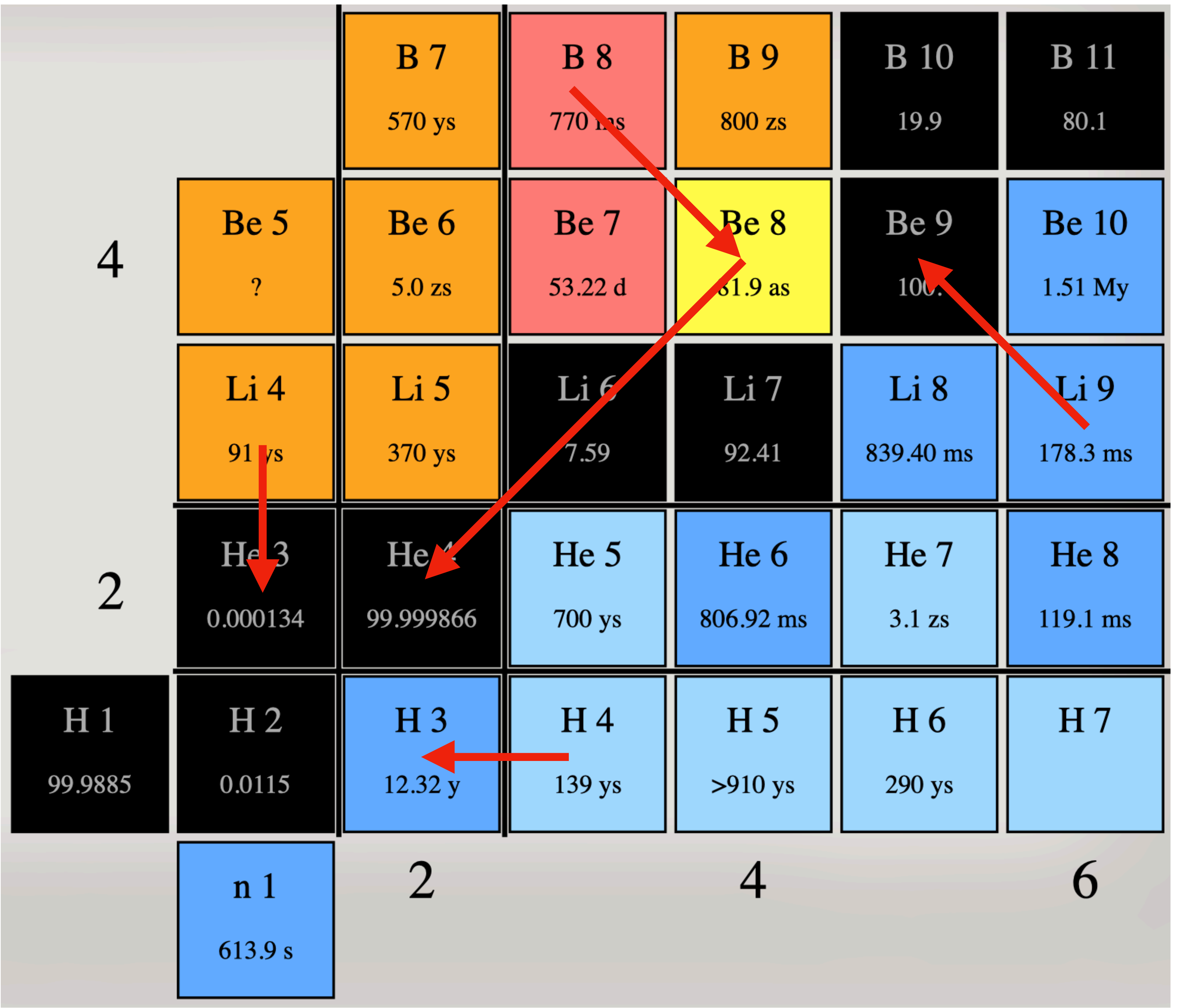


γ-decay
(EM force)

+ exotic decay modes!

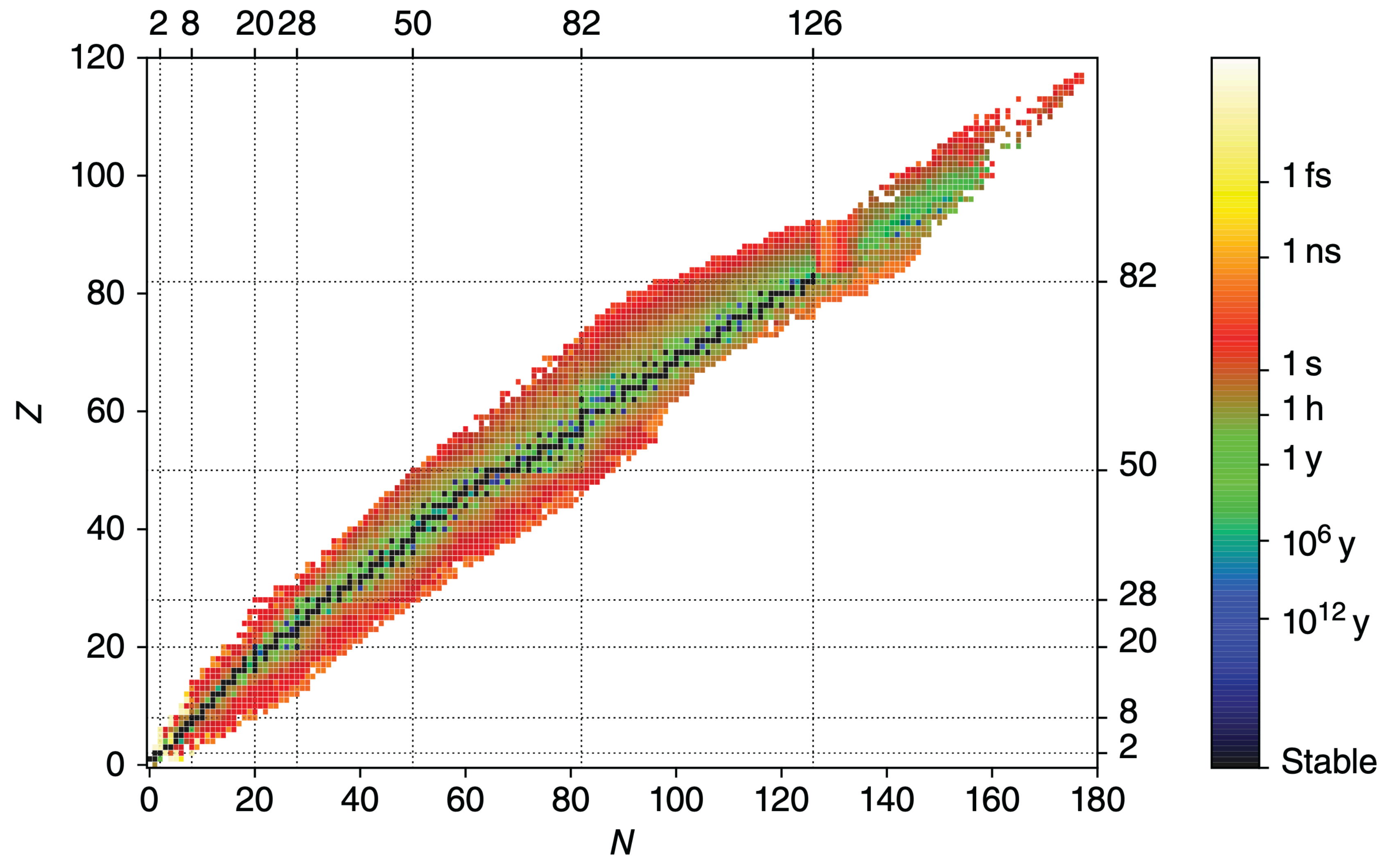
p-decay
(tunneling+Coulomb)

α-decay
(tunneling)

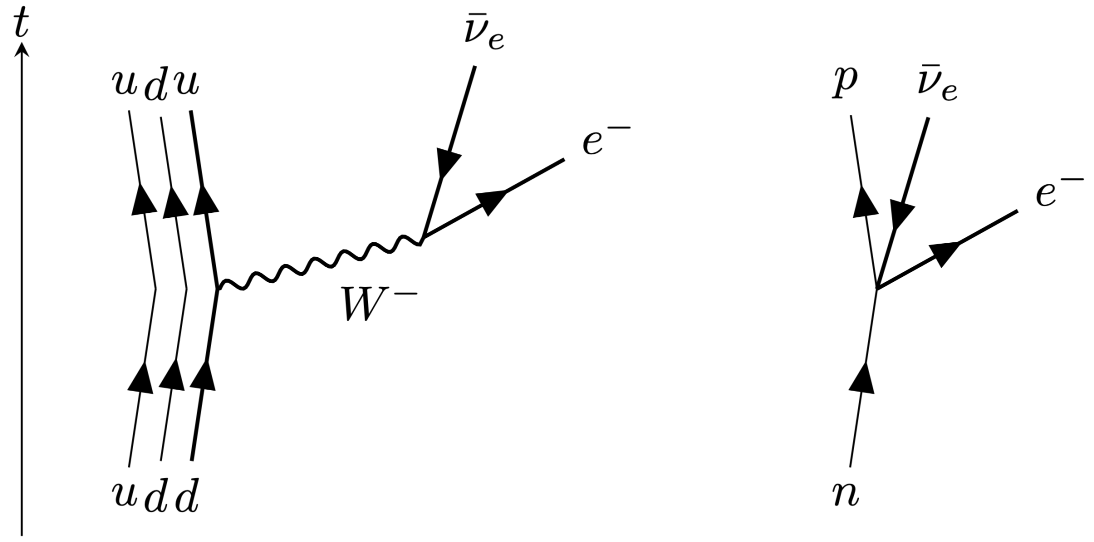


β-decay
(weak force)

n-decay
(tunneling)



V. Zelevinsky & A. Volya, *Physics of Atomic Nuclei*



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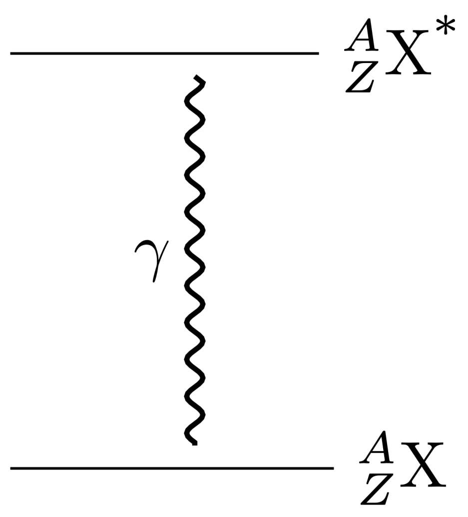

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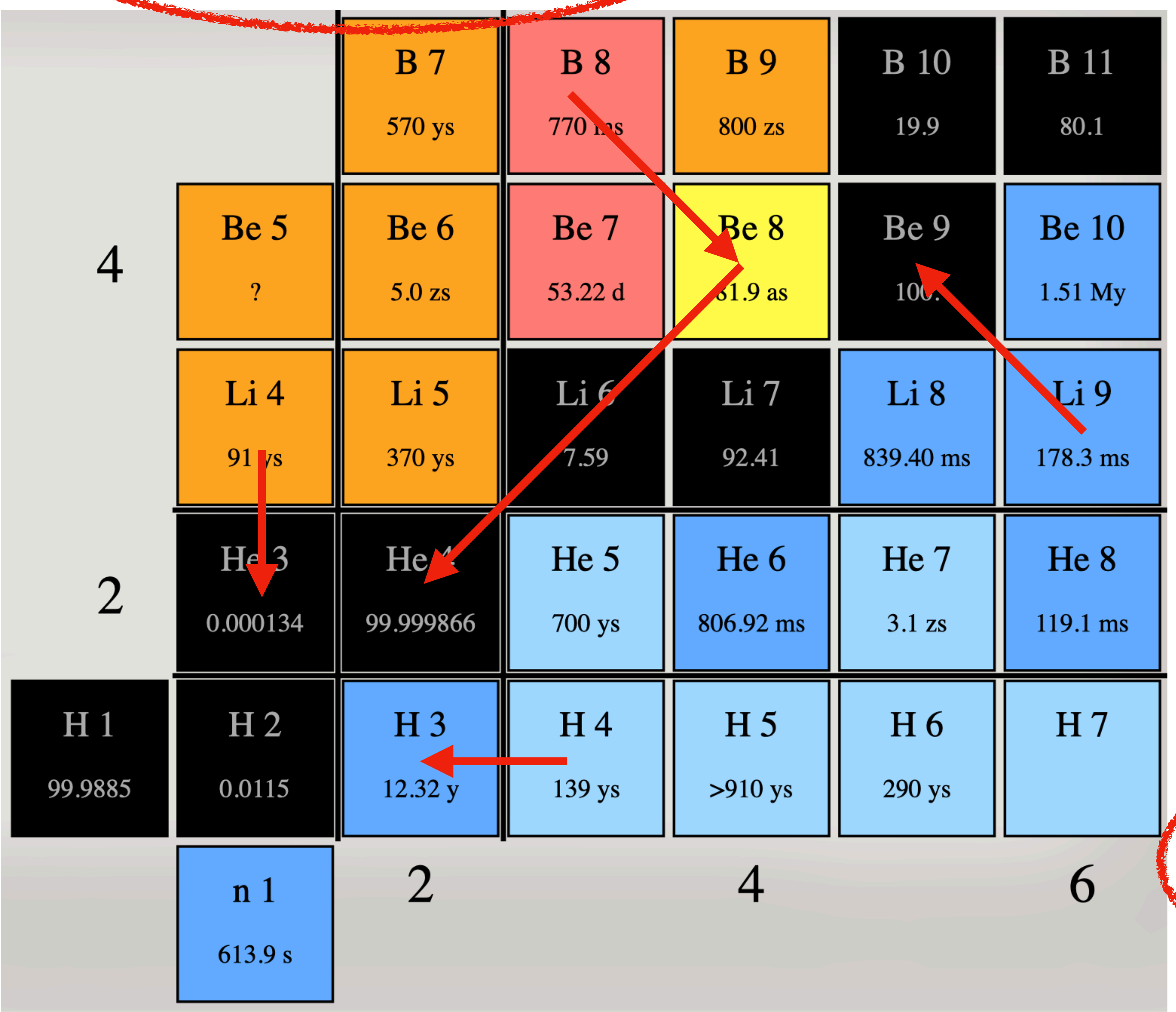

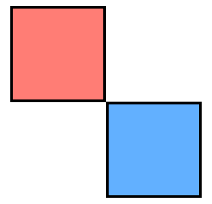

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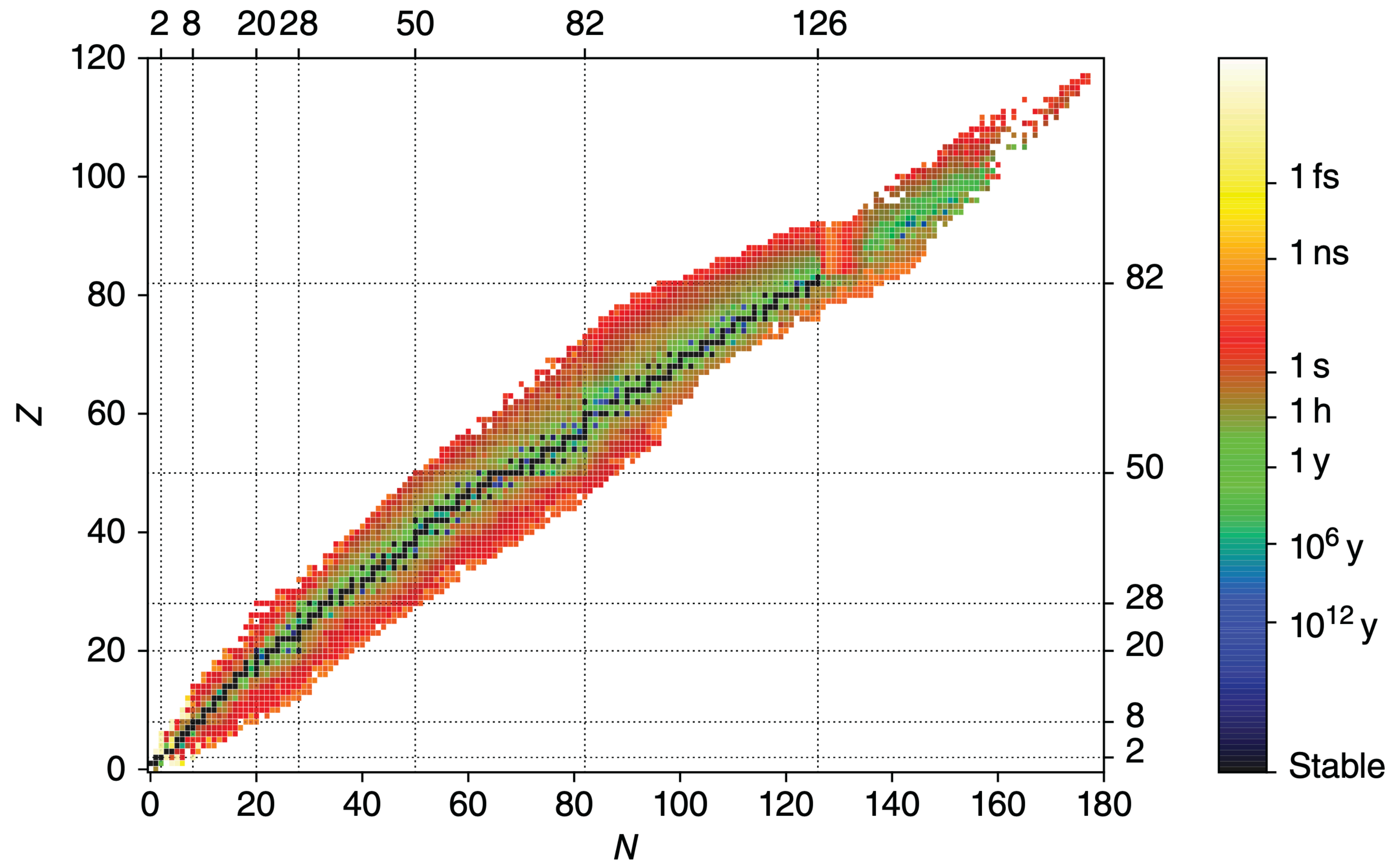
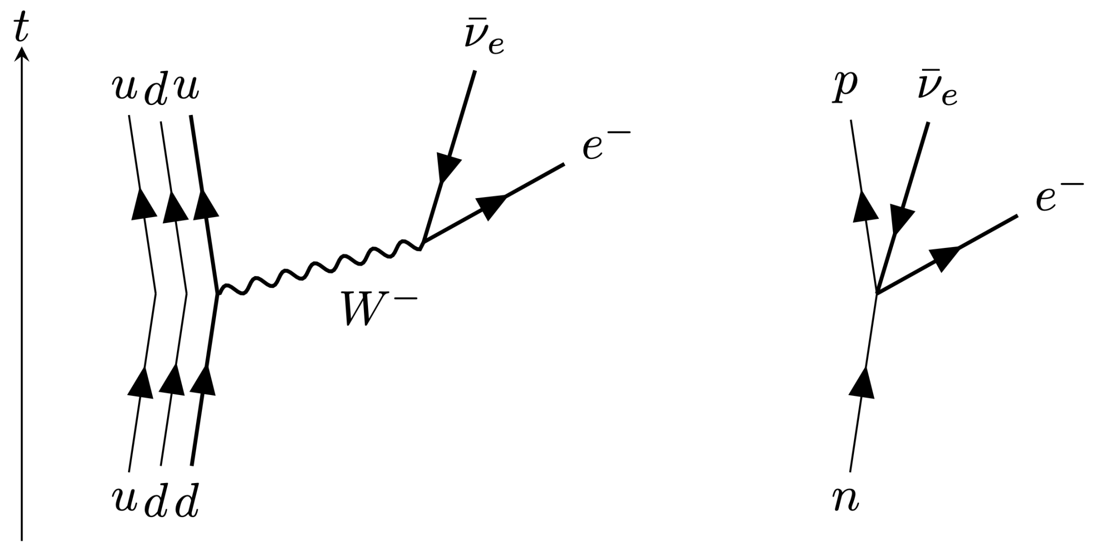


V. Zelevinsky & A. Volya, *Physics of Atomic Nuclei*

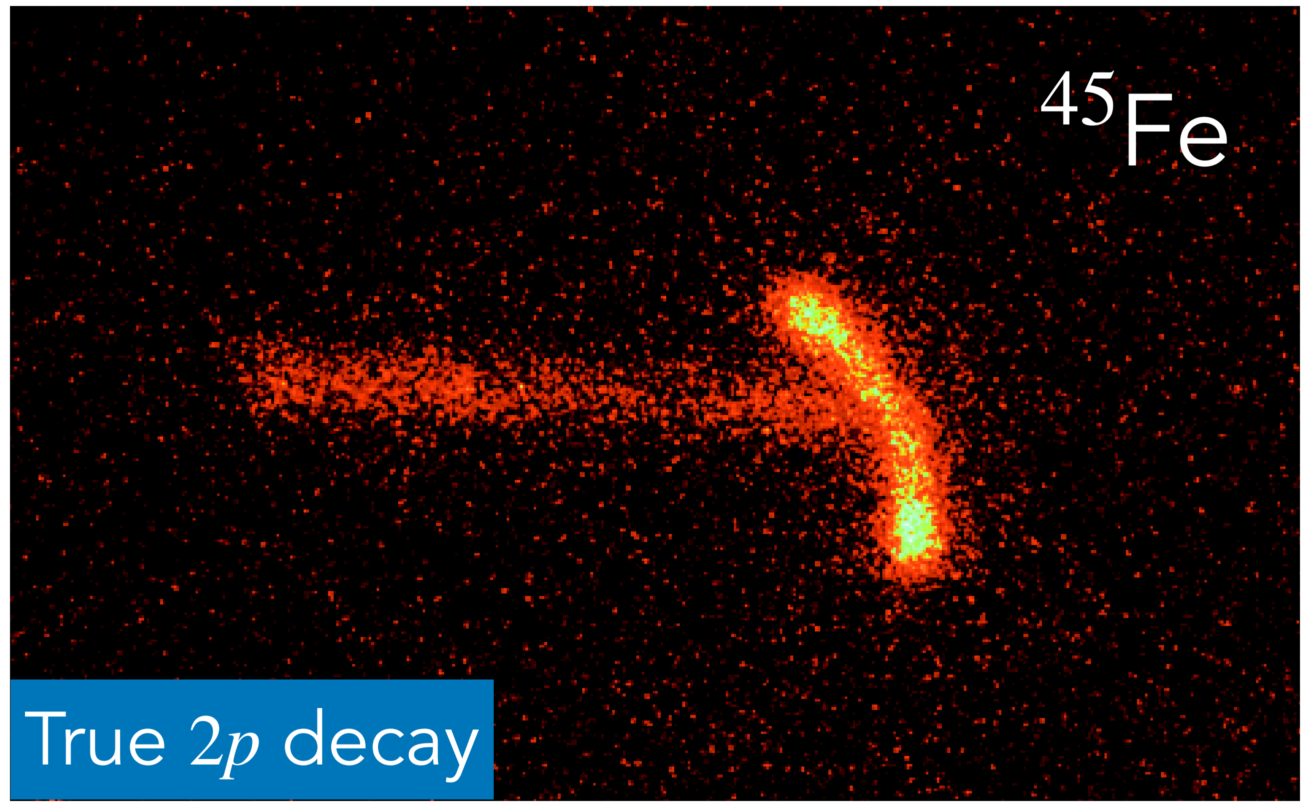


Specifically: $\tau \gtrsim 10^{-22}$ s $\sim \tau_{NN}$
(stability w.r.t. NN forces)

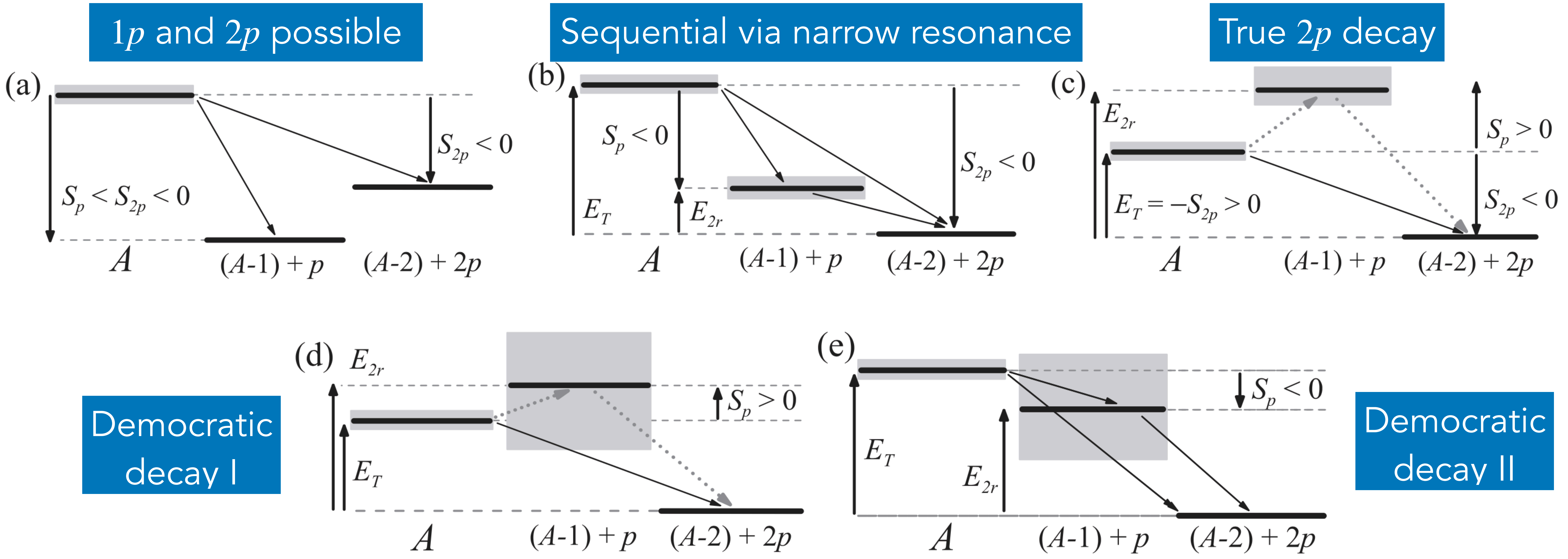
Exotic decay modes

New types of radioactivity discovered in exotic nuclei. Example: $2p$ decay.

M. Pfützner *et al.*, Rev. Mod. Phys. **84**, 567 (2012)



K. Miernik *et al.*, Phys. Rev. Lett. **99**, 192501 (2007)



Decay dynamic depends on relative energies and widths, *i.e.* the structure.

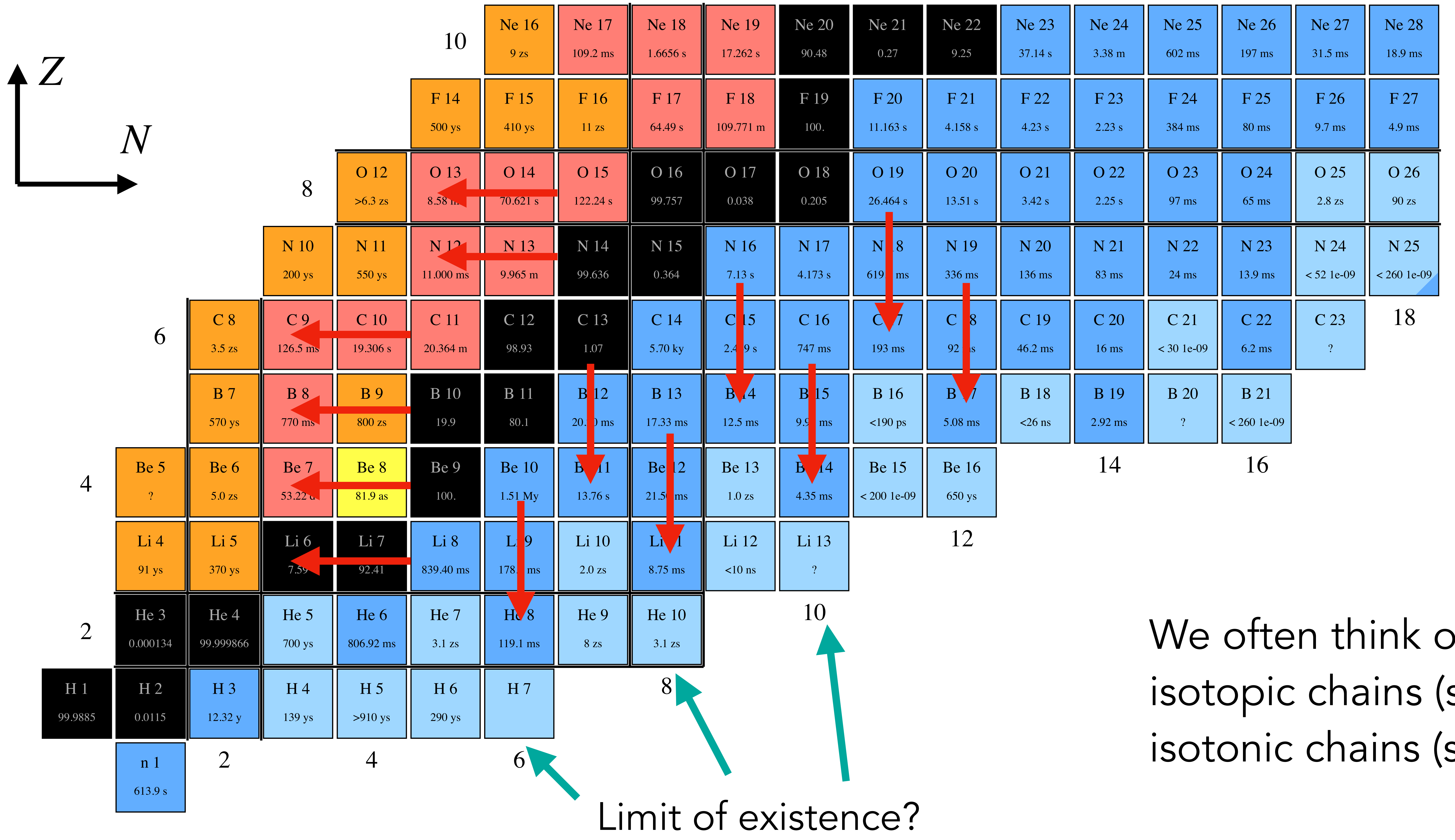
↕

Structure depends on nearby decay thresholds (open & closed) and continuum.

→ **structure-continuum couplings**

Nuclear existence vs. stability

Limits of existence ($T_{1/2} \gtrsim 10^{-22}$ s) **vs.** limits of stability with respect to n and p emission, or drip lines.



Accepted definition: the limits where S_n or S_p cross zero.

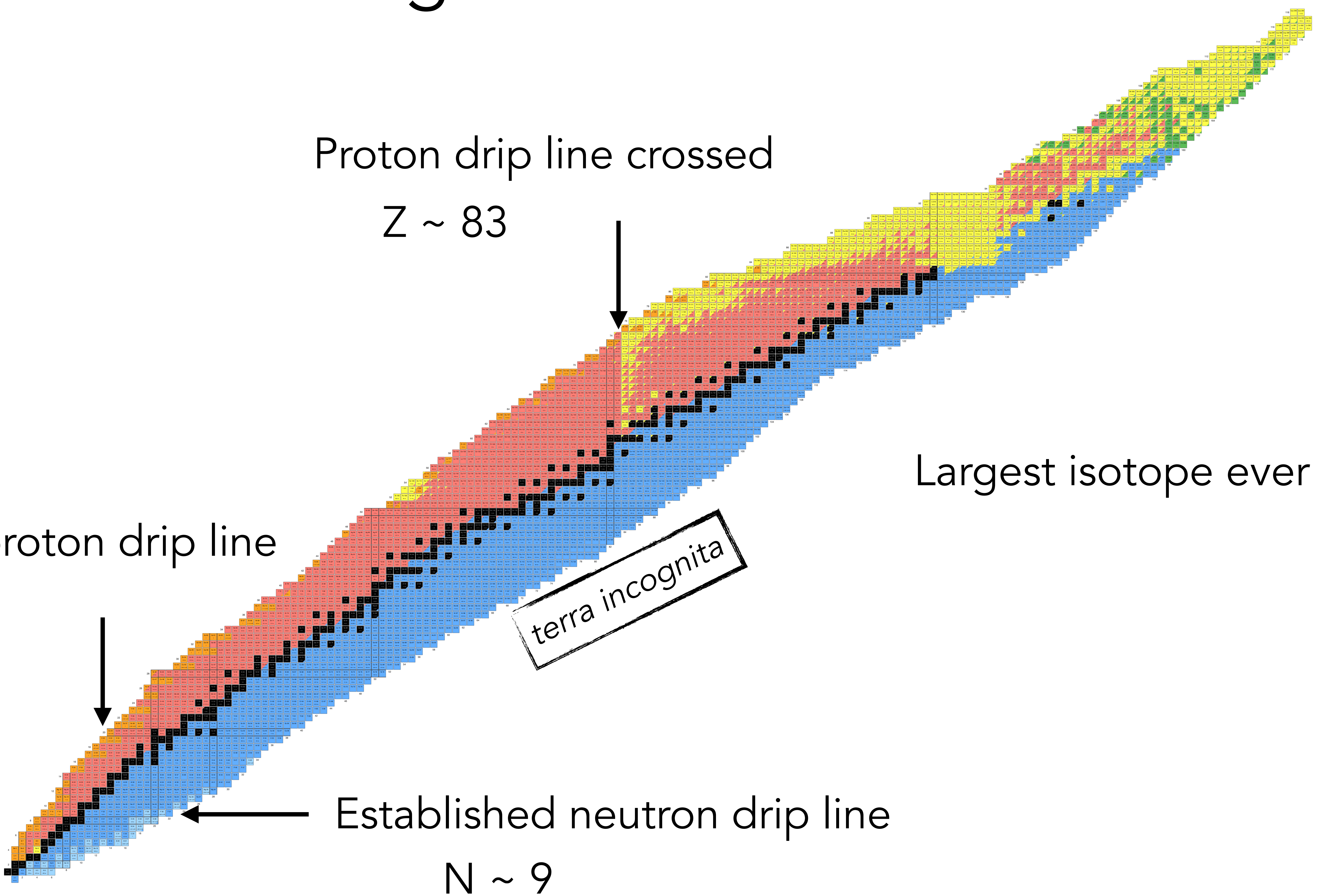
M. Thoennessen, Rep. Prog. Phys. **67**, 1187 (2004)

We often think of the neutron drip line along isotopic chains (same Z), but we should look at isotonic chains (same N).

State of our knowledge

Proton drip line crossed

Z ~ 83



Largest isotope ever made: $^{294}_{118}\mathrm{Og}$

Established proton drip line

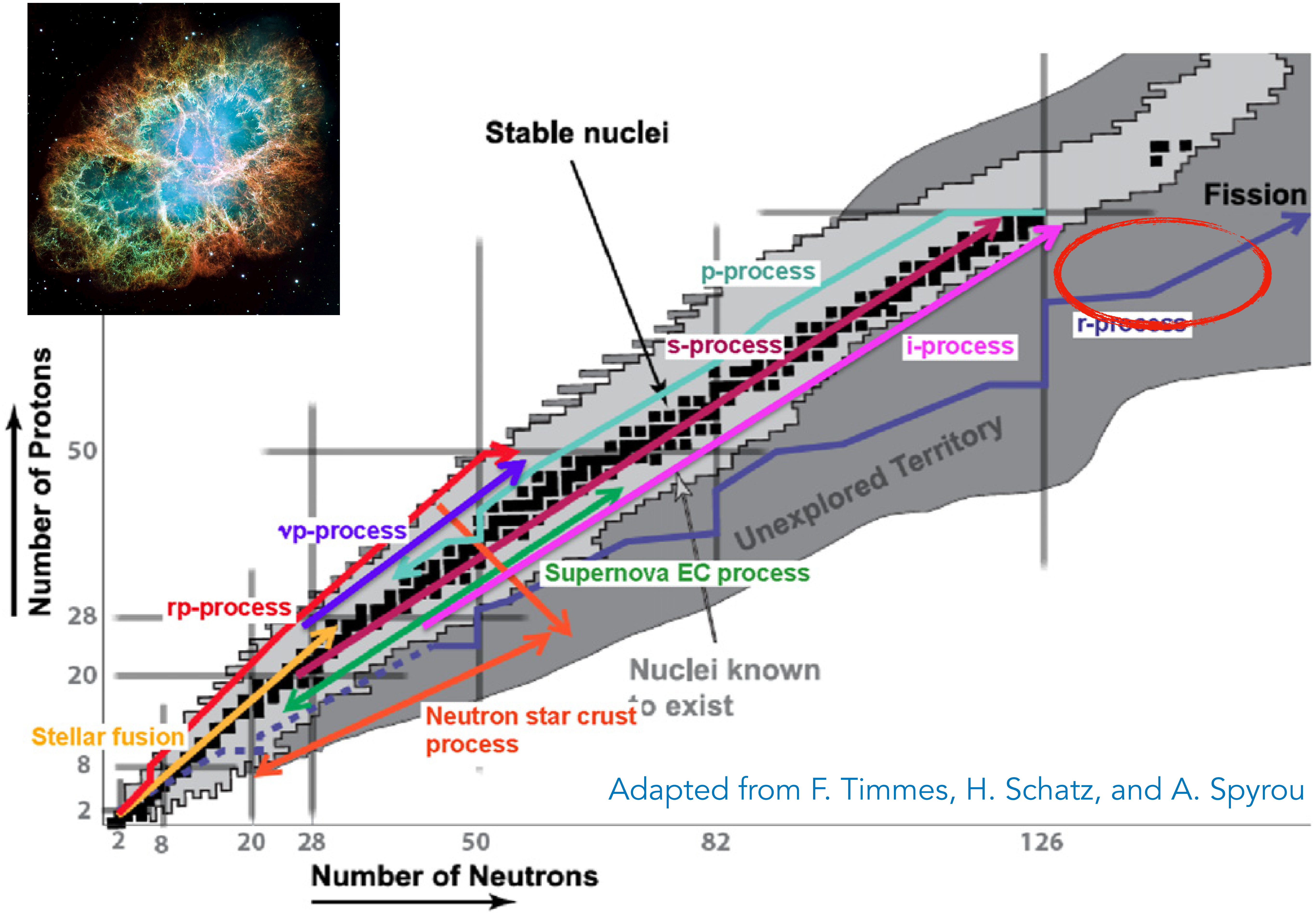
Z ~ 13

Established neutron drip line

N ~ 9

Relevance for astrophysics

Rapid neutron capture (r process) is right in the *terra incognita*.



Adapted from F. Timmes, H. Schatz, and A. Spyrou

The abundances along an isotopic chain in $(n,\gamma) \rightleftarrows (\gamma,n)$equilibrium are set by the temperature, neutron abundance, and the ***neutron separation energies*** [...].

M. R. Mumpower *et al.*,
Prog. Part. Nucl. Phys. **86**, 86 (2016)

And much more…

C. A. Bertulani and A. Gade,
Phys. Rep. **485**, 195 (2010)

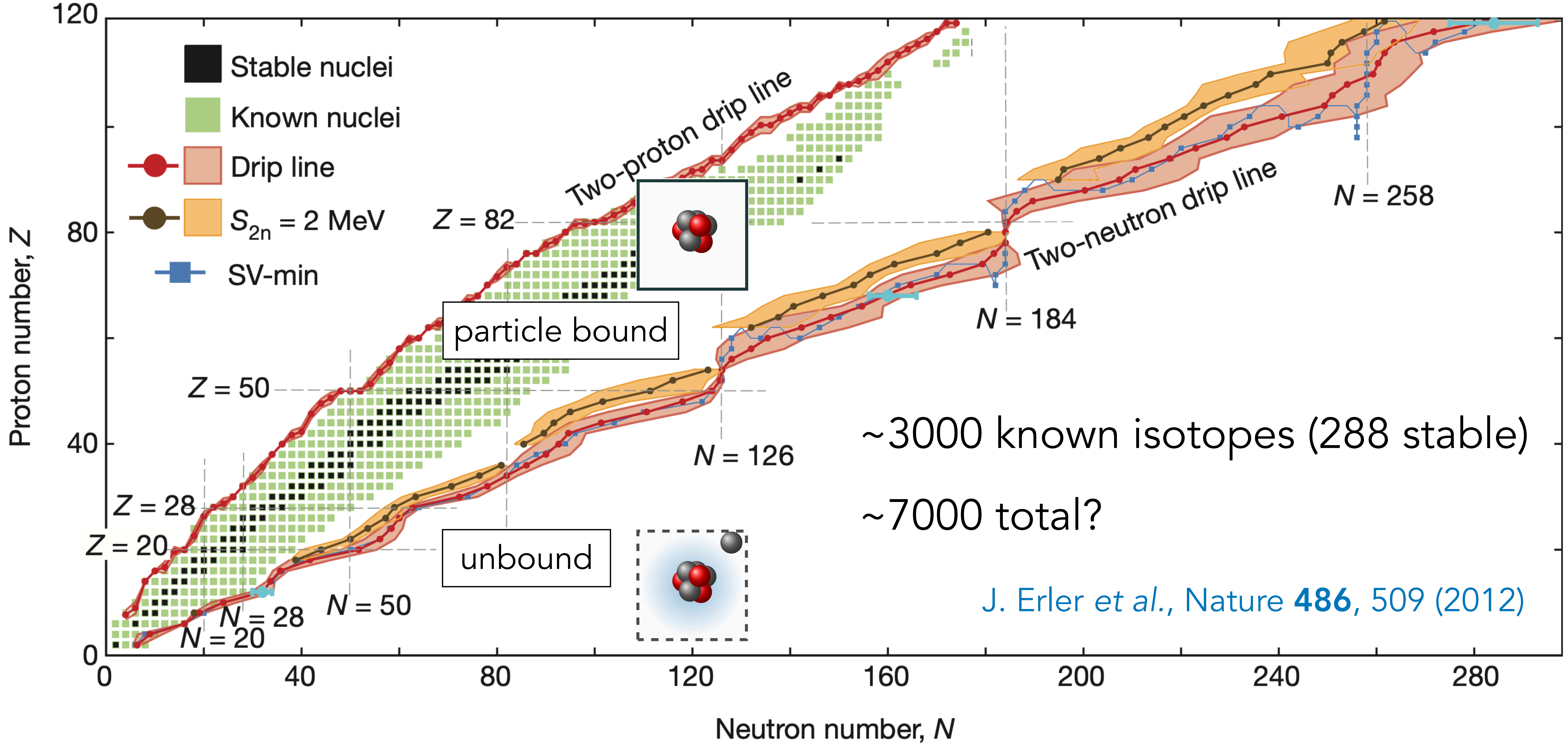
H. Grawe *et al.*, Rep. Prog. Phys. **70**, 1525 (2007)

A. Aprahamian *et al.*,
Prog. Part. Nucl. Phys. **54**, 535 (2005)

And neutron stars…

Exploration of the drip lines

Limits of nuclear stability: Which (N, Z) combinations are stable?



Considerable potential for discovery:

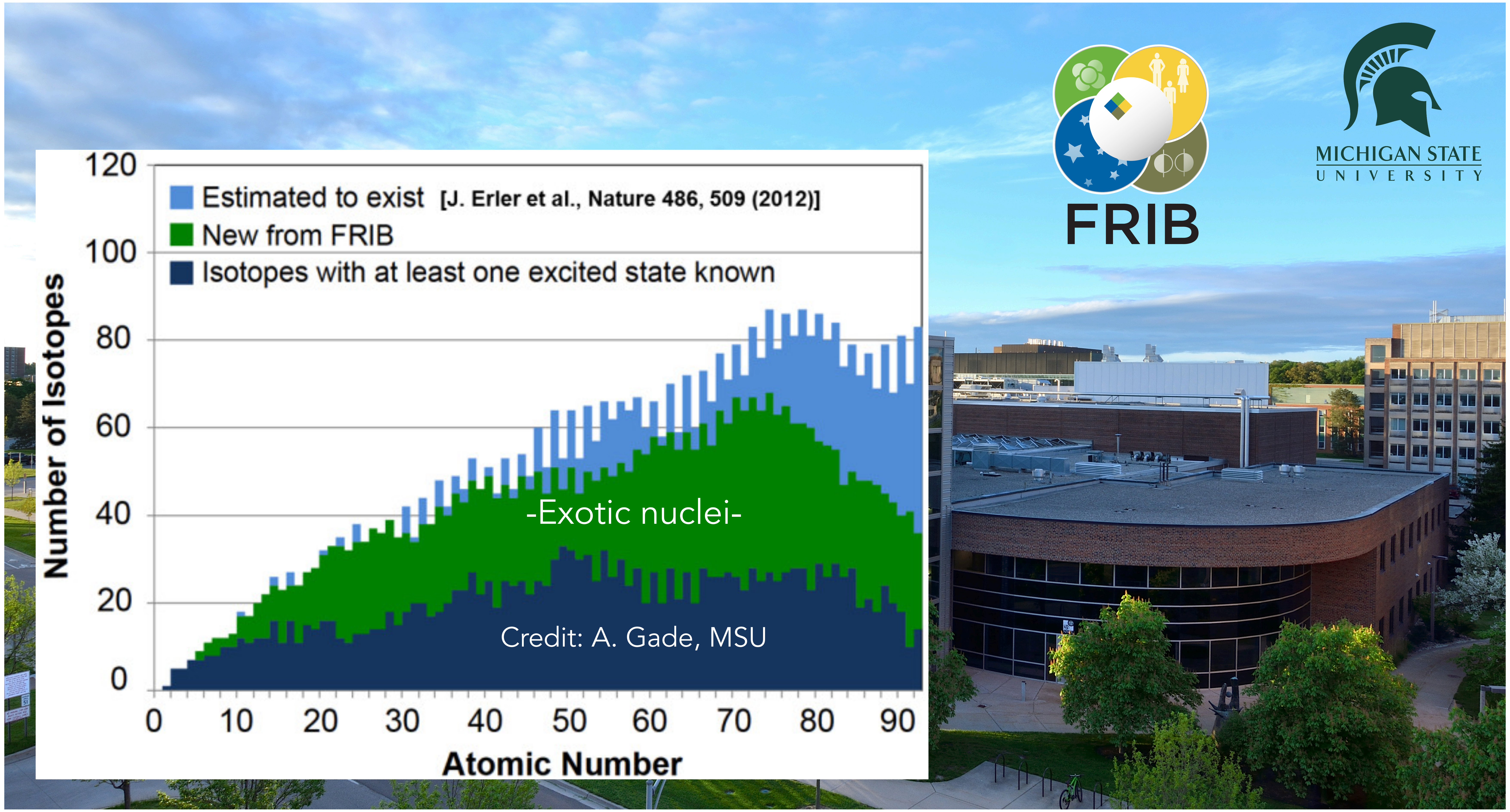
1. Nuclear structure in extreme N/Z conditions.
2. Possible new emergent phenomena.

Facility for Rare Isotope Beams (FRIB)

- Nuclear structure
- Nuclear astrophysics
- Test of fundamental symmetries
- Applications

Theory community:
FRIB Theory Alliance.

Facility for Rare Isotope Beams (FRIB)



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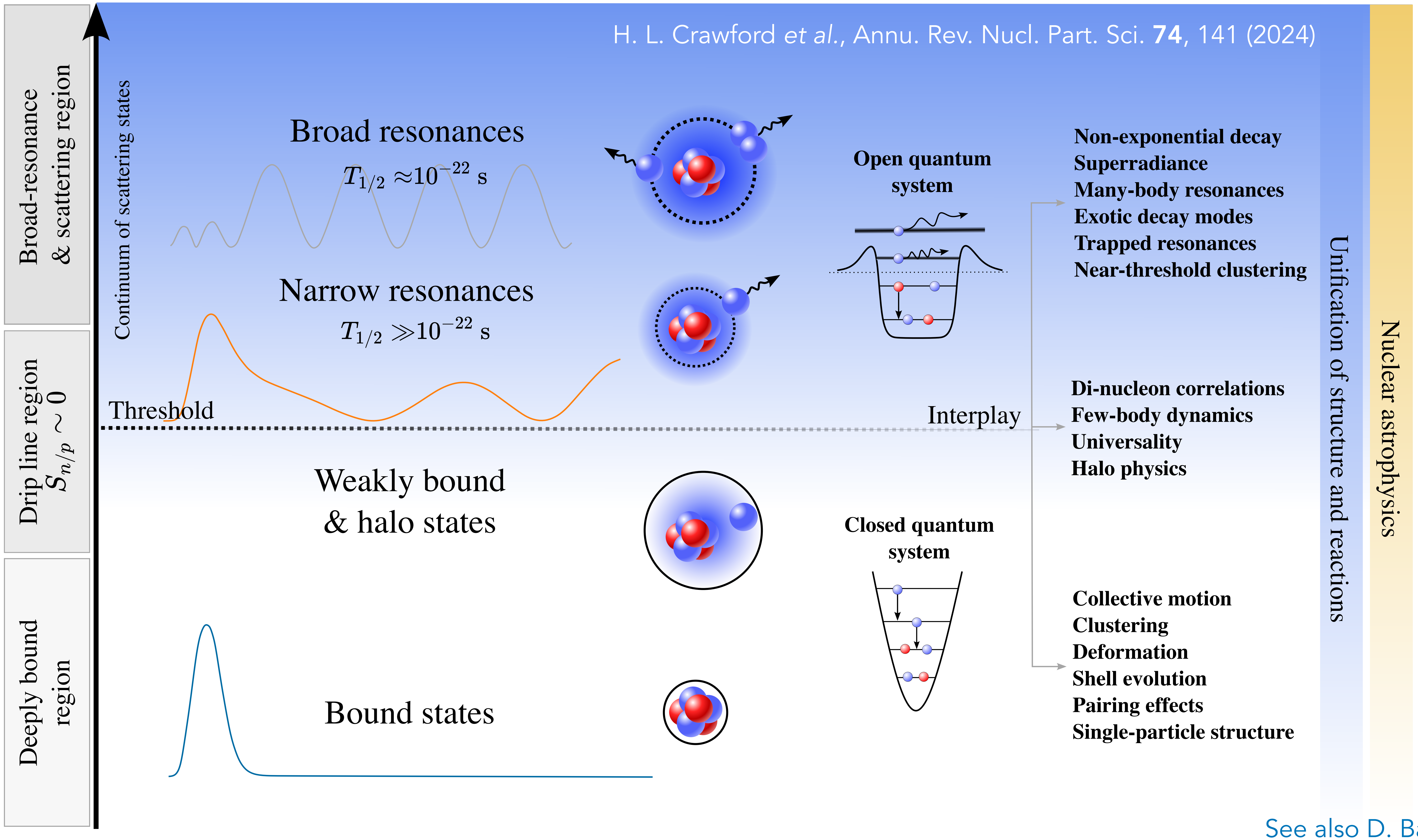
Physics of exotic nuclei



Nuclei as open quantum systems.

Interplay between NN forces, many-body effects, and weak bind/decay.

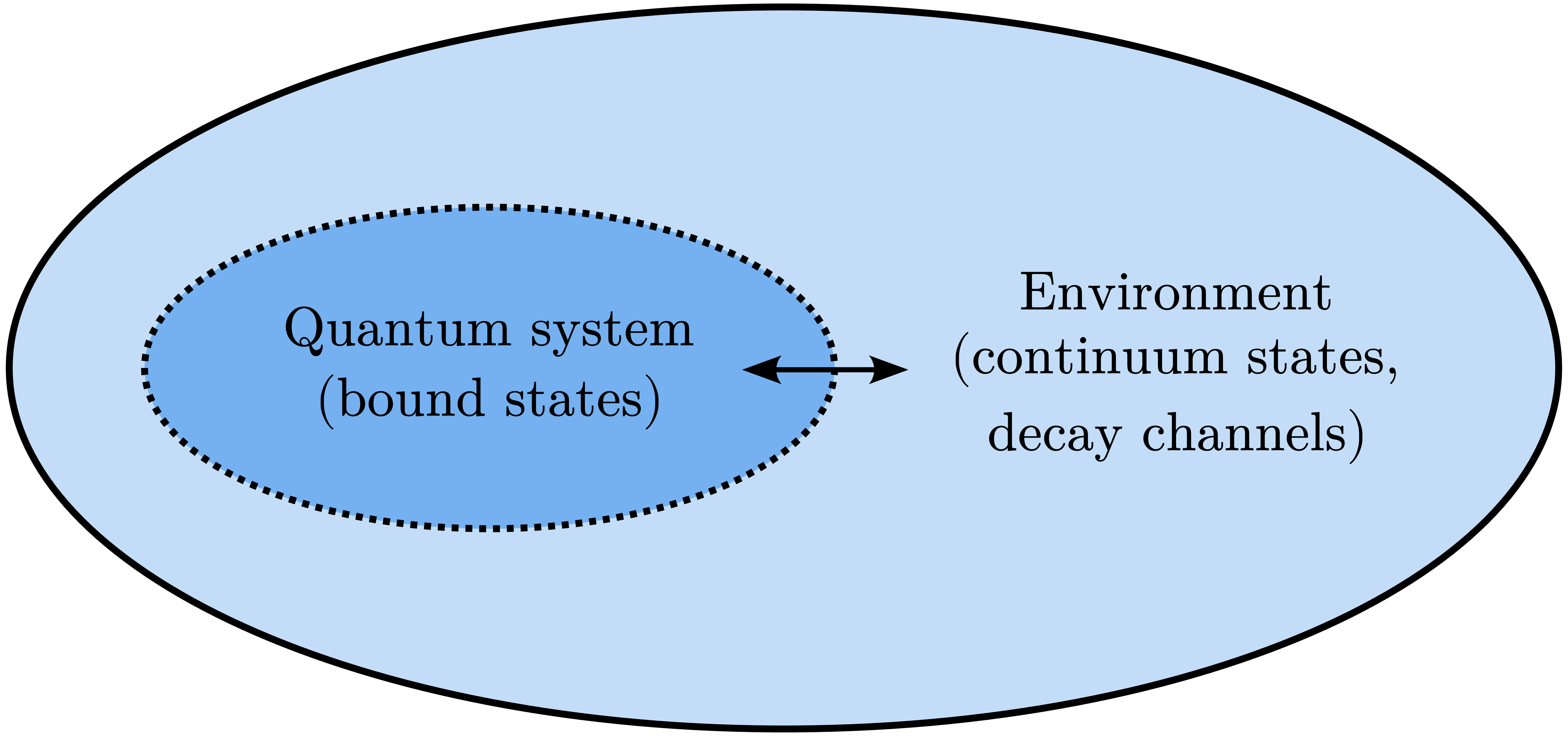
Structure and reactions must be described simultaneously.

See also D. Bazin *et al.*, Few-Body Syst. **64**, 25 (2023)

C. W. Johnson *et al.*, J. Phys. G **47**, 123001 (2020)

Nuclei as open quantum systems (OQSs)

Quantum systems coupled to an environment.



Quantum/quantum coupling:

$$\mathcal{H} = \mathcal{H}_{\text{system}} \otimes \mathcal{H}_{\text{evironment}}$$

Narrow resonances: weak couplings
→ Possibly Markovian, but usually not.

Broad resonances: strong couplings
→ Highly non-Markovian

Non-Hermitian description of the system, but unitary evolution of system+environment.

Fermionic, many-body, strongly correlated…

Theoretical approaches for nuclear OQSs

Historically: Feshbach projection formalism.

$$\hat{P} + \hat{Q} = \hat{1}$$

discrete states — Continuum states

$$\hat{H} = \hat{P}\hat{H}\hat{P} + \hat{P}\hat{H}\hat{Q} + \hat{Q}\hat{H}\hat{P} + \hat{Q}\hat{H}\hat{Q}$$

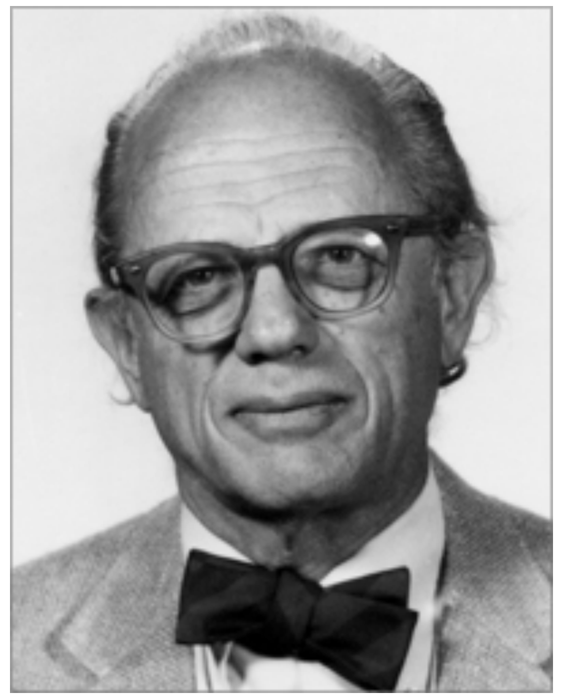
$$\mathcal{H} = \mathcal{H}_{\text{bound}} \otimes \mathcal{H}_{\text{cont}}$$

Derive an energy-dependent Hamiltonian:

$$\hat{H}(E) = \hat{H}_{QP}(\hat{H}_{PP} - E)^{-1}\hat{H}_{PQ} \rightarrow \hat{H}_{QQ} + \hat{\Delta}(E) - \frac{i}{2}\hat{W}(E)$$

Complex energies!

energy shift — decay



H. Feshbach

``Structure into the continuum"

Continuum Shell Model (CSM)

N. Auerbach *et al.*, Rep. Prog. Phys. **74**, 106301 (2011)

Shell Model Embedded in the Continuum (SMEC)

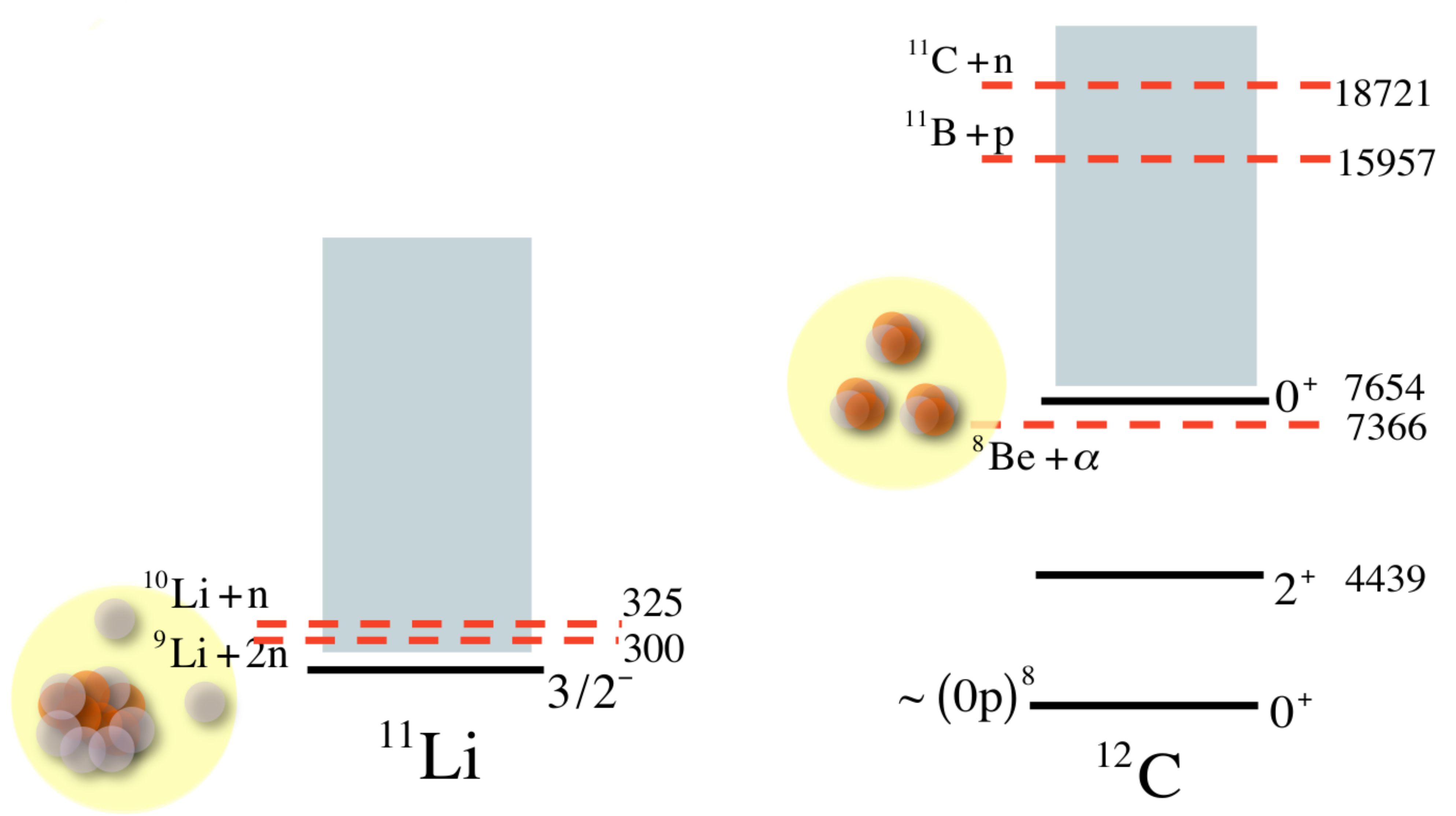
J. Okołowicz *et al.*, Phys. Rep. **374**, 271 (2003)

Problem: cumbersome beyond two-particle decay.

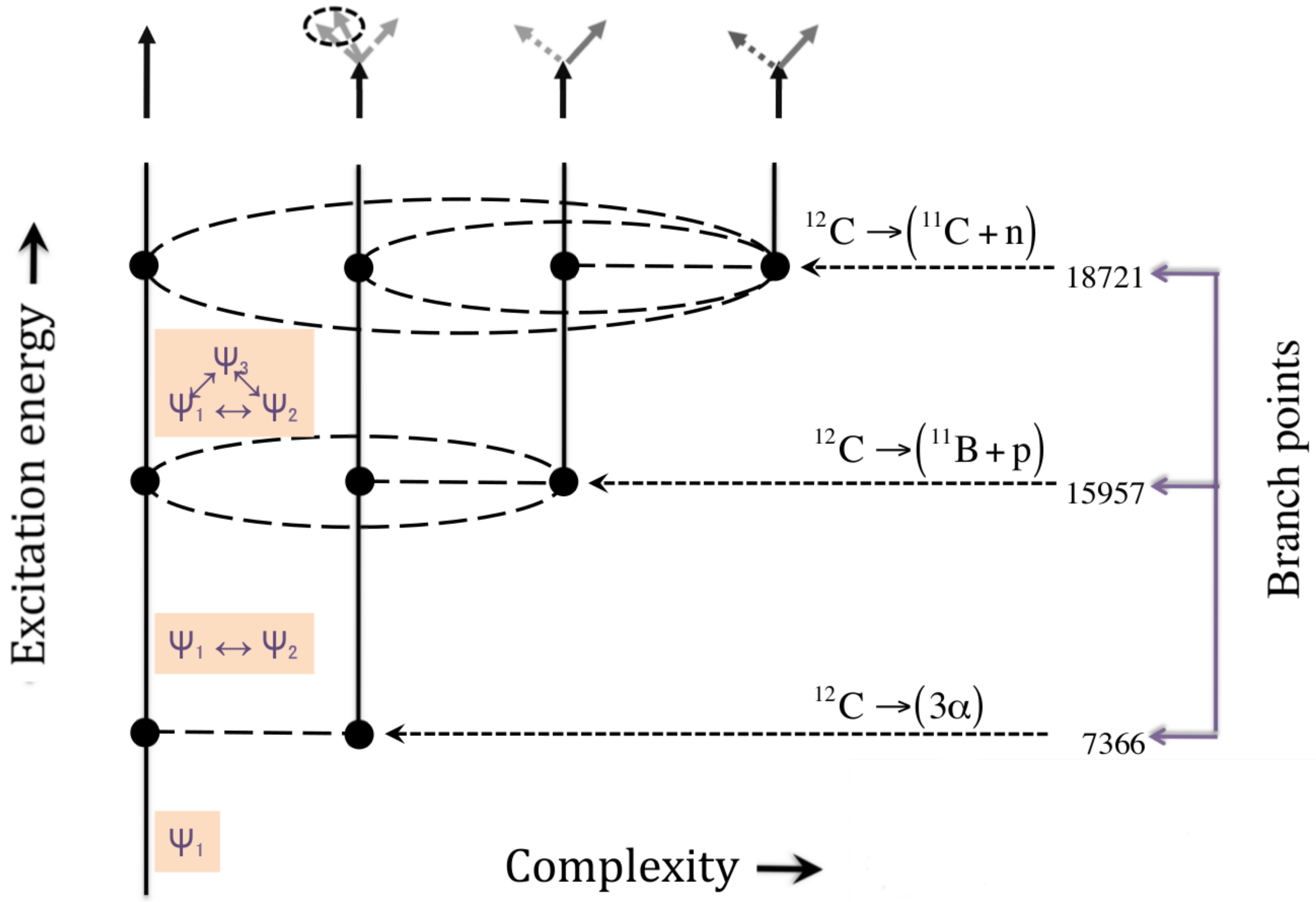
Near-threshold clustering

``Alignment" of the wave function with nearby decay channels.

J. Okołowicz *et al.*, Prog. Theor. Phys. Supp.**196**, 230 (2012)

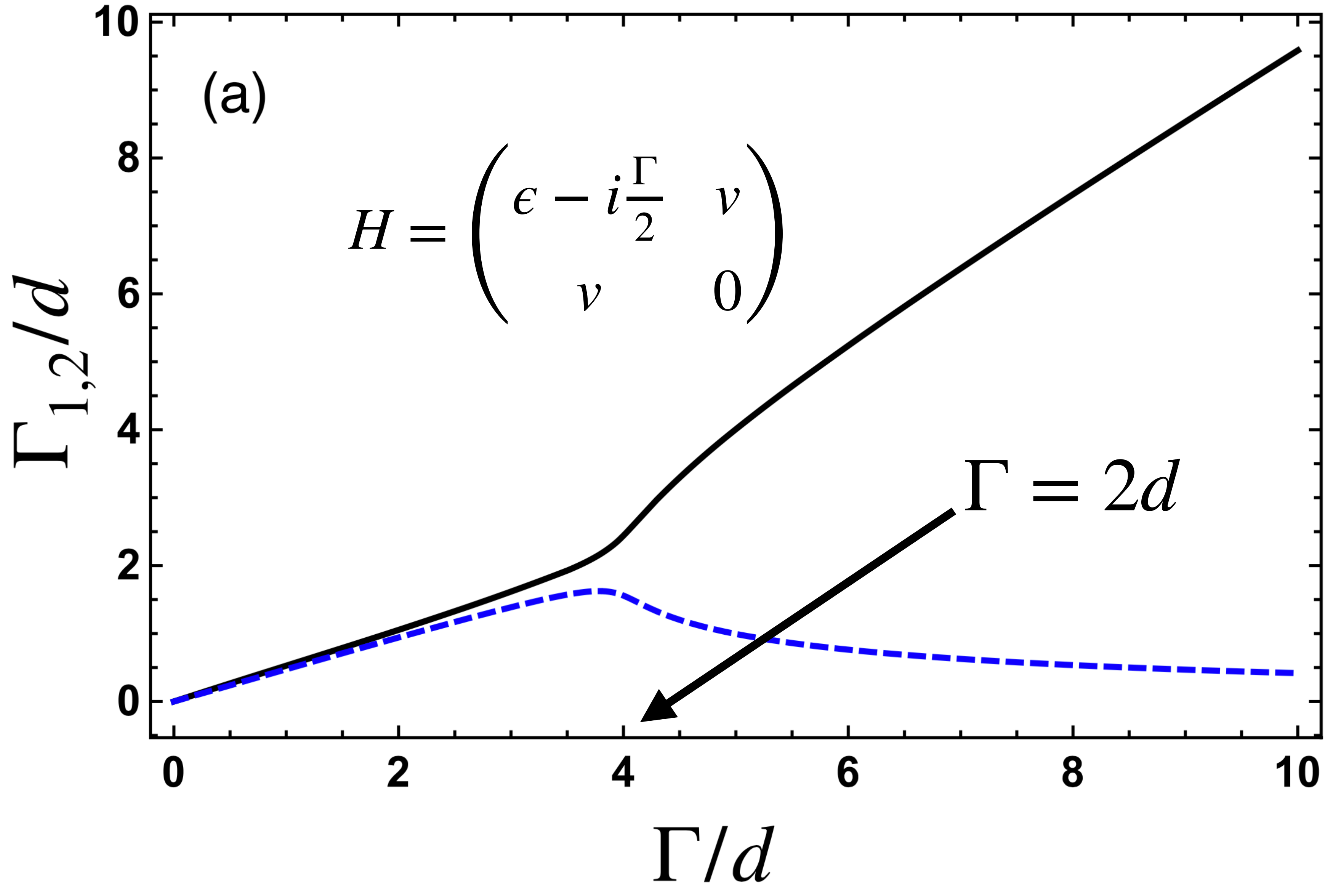


Multichannel network of couplings in ^{12}C



Superradiance

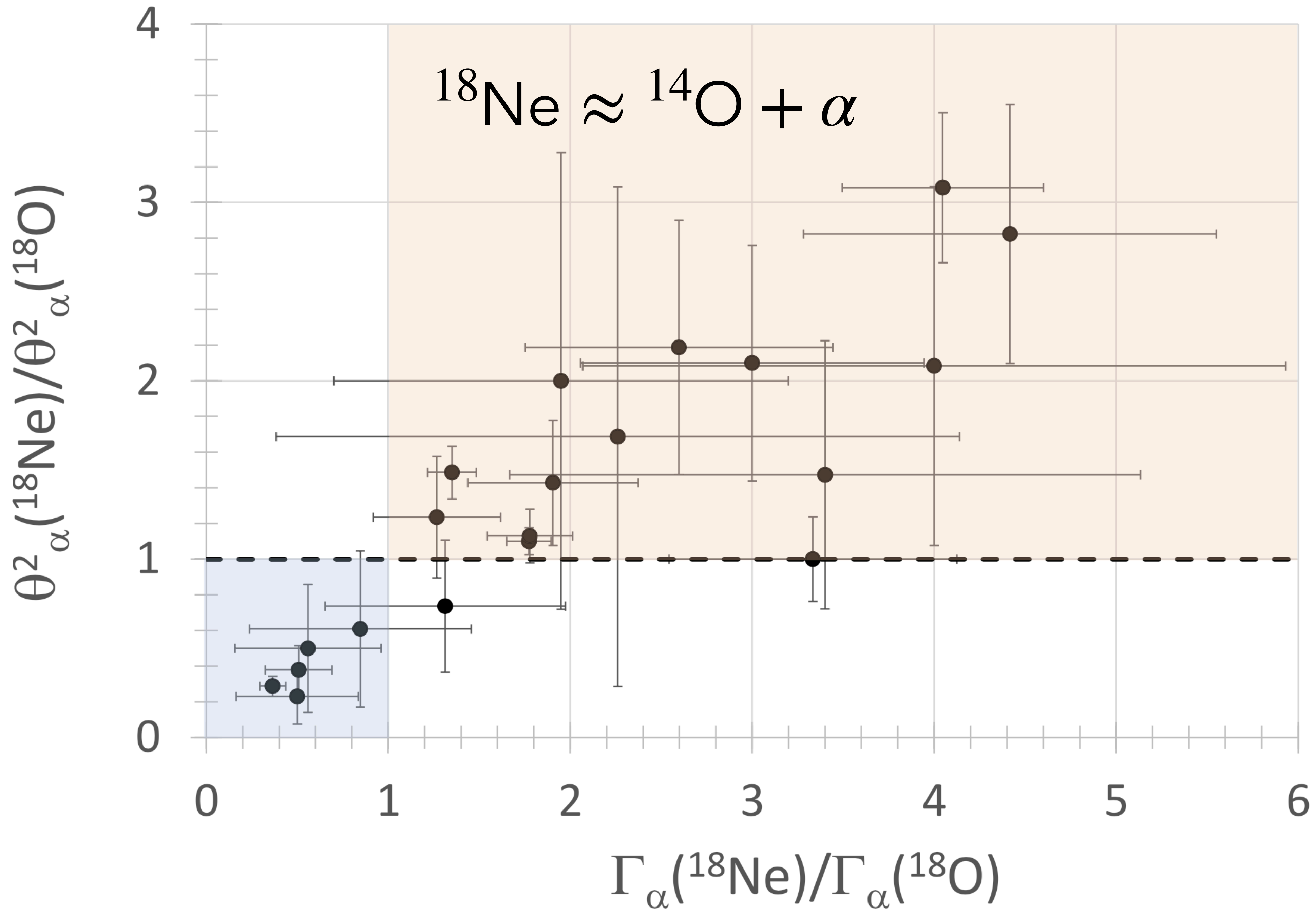
Collectivization of the width in overlapping resonances



$$d = \sqrt{\epsilon^2 + 4v^2} \qquad \Gamma_{1,2} = -2\Im(E_{1,2})$$

$$E_{1,2} = \frac{1}{2}\left(\epsilon - i\frac{\Gamma}{2} \pm \sqrt{\left(\epsilon - i\frac{\Gamma}{2}\right)^2 + 4v^2}\right)$$

A. Volya *et al.* *Commun Phys* **5**, 322 (2022)



As one state ``absorbs'' all the $\alpha$-decay width, its wave function ``aligns'' with the corresponding threshold.

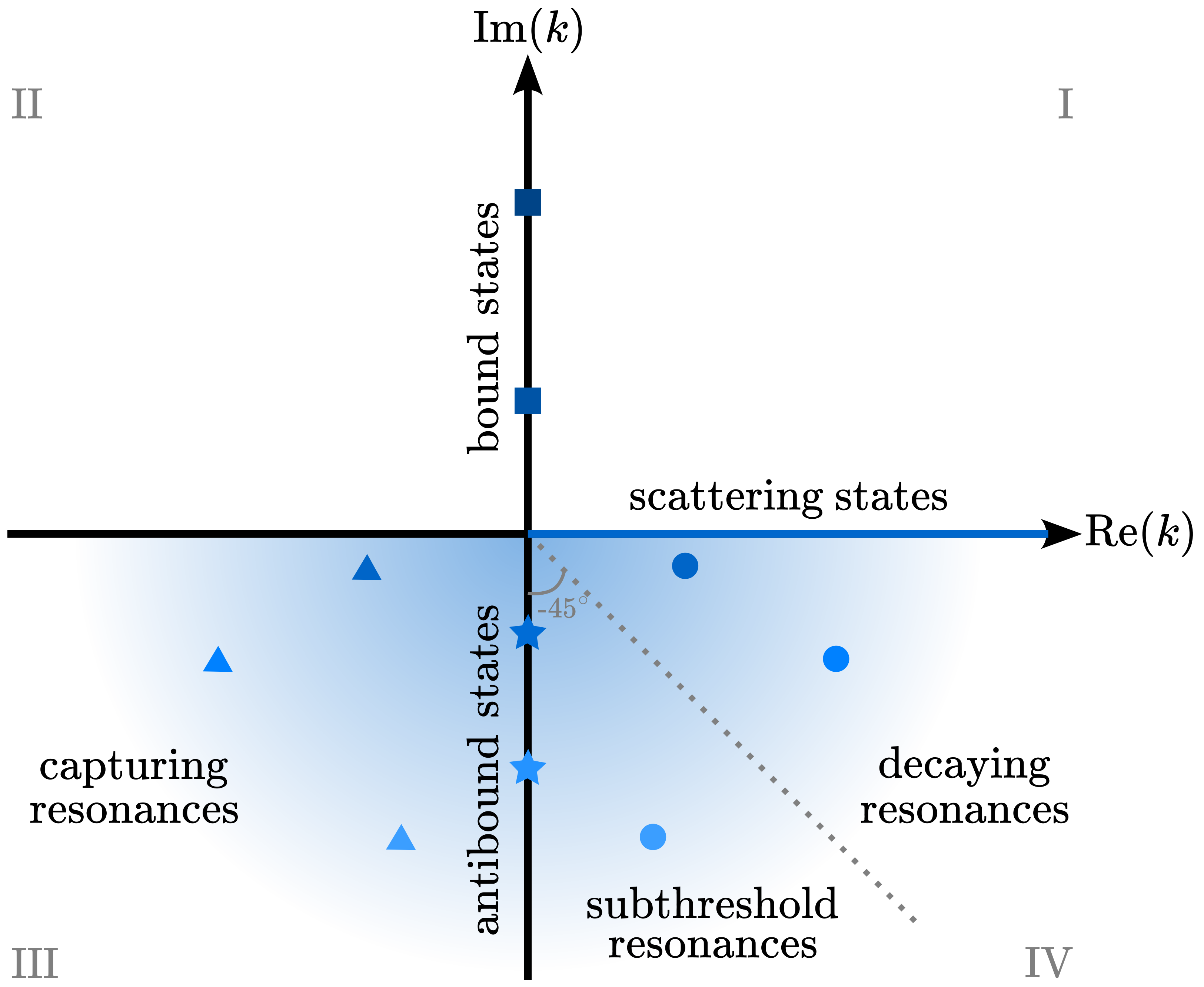
Theoretical approaches for nuclear OQSs

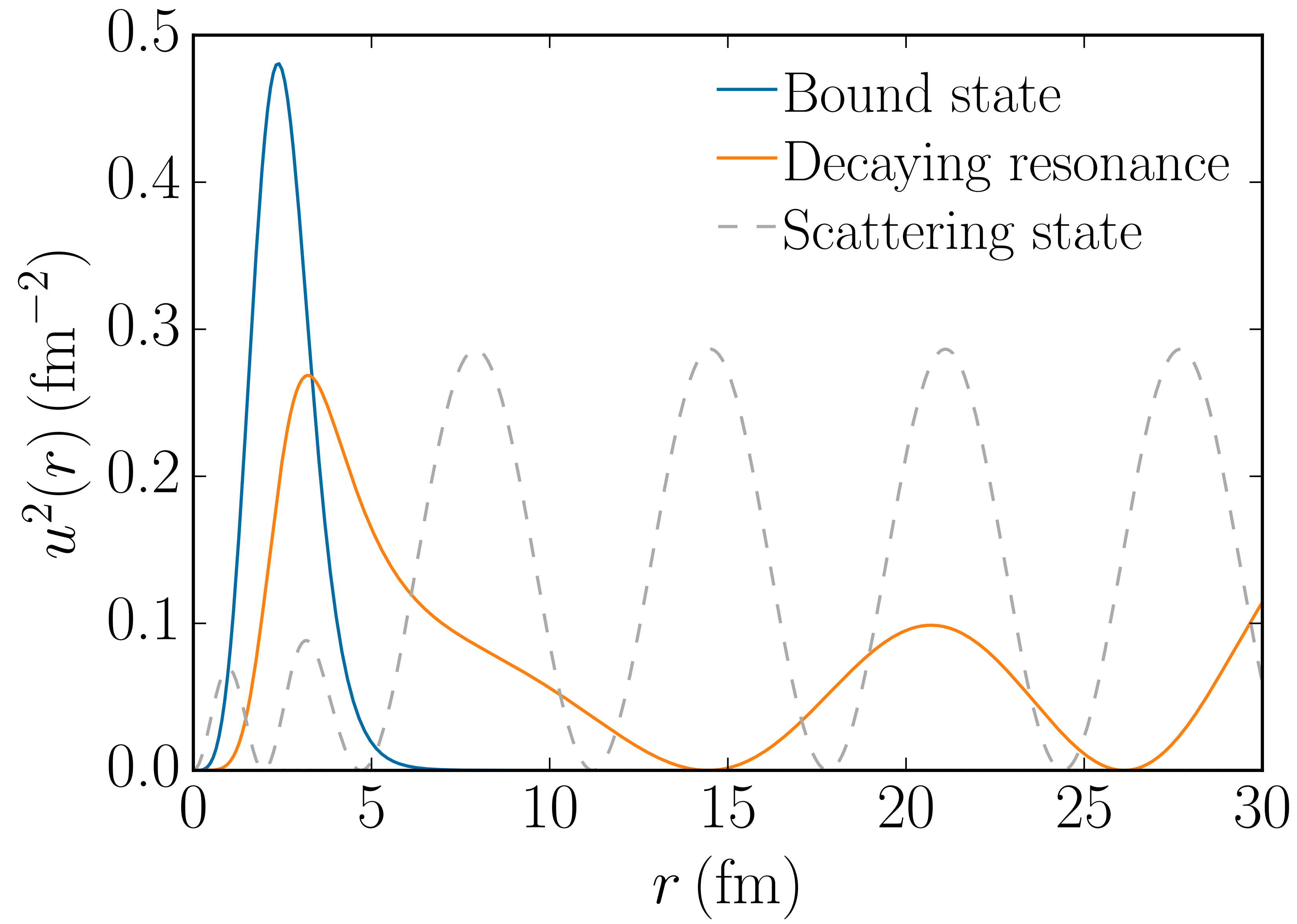
Quasi-stationary formalism. $\mathcal{H} = \mathcal{H}_{\text{discrete}} \otimes \mathcal{H}_{\text{scatt}}$

J.J. Thomson, Proc. London Math. Society, 197 (1884)

G. Gamow, Z. Physik **51**, 204 (1928), A. F. J. Siegert, Phys. Rev. **56**, 750 (1939)

Resonances as generalized eigenstates of non-Hermitian Hamiltonians associated with poles of the S-matrix.





G. Gamow

Gamow/Siegert states: stationary solutions with outgoing boundary condition.

$$\tilde{E} = E - i\frac{\Gamma}{2}$$

Rigorous formulation in the rigged Hilbert space (RHS).

Gel'fand, Vilenkin, Maurin, Böhm, etc.

Theoretical approaches for nuclear OQSs

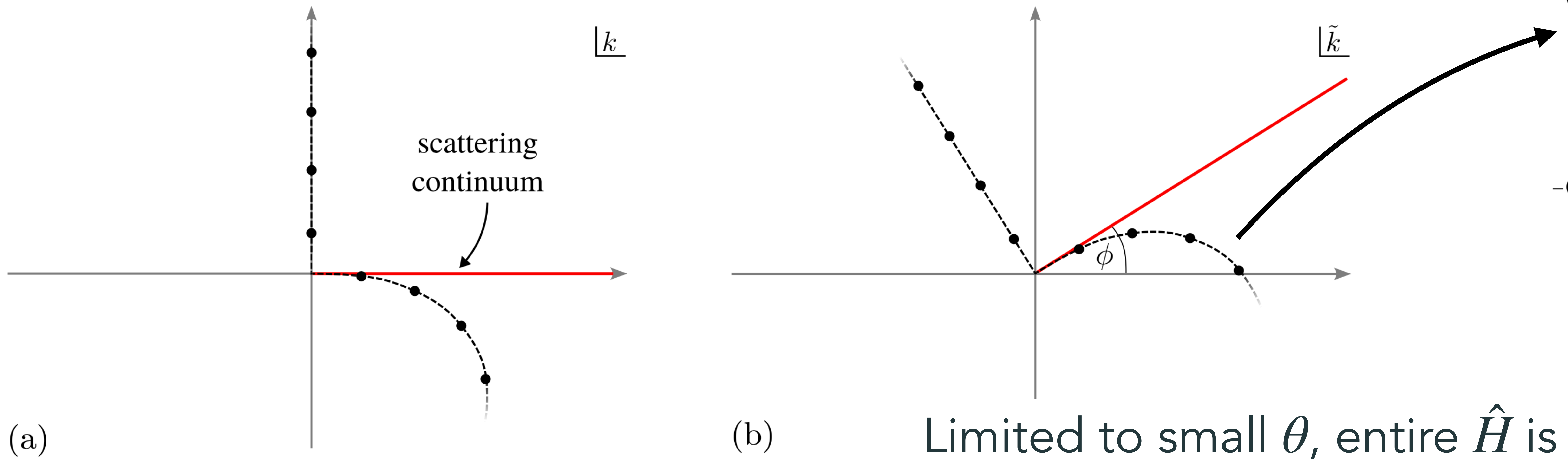
Uniform complex scaling.

N. Moiseyev, *Non-Hermitian Quantum Mechanics* (2011)

Rotate $\hat{H}$ in k-space to ``reveal'' poles in the 4th quadrant.

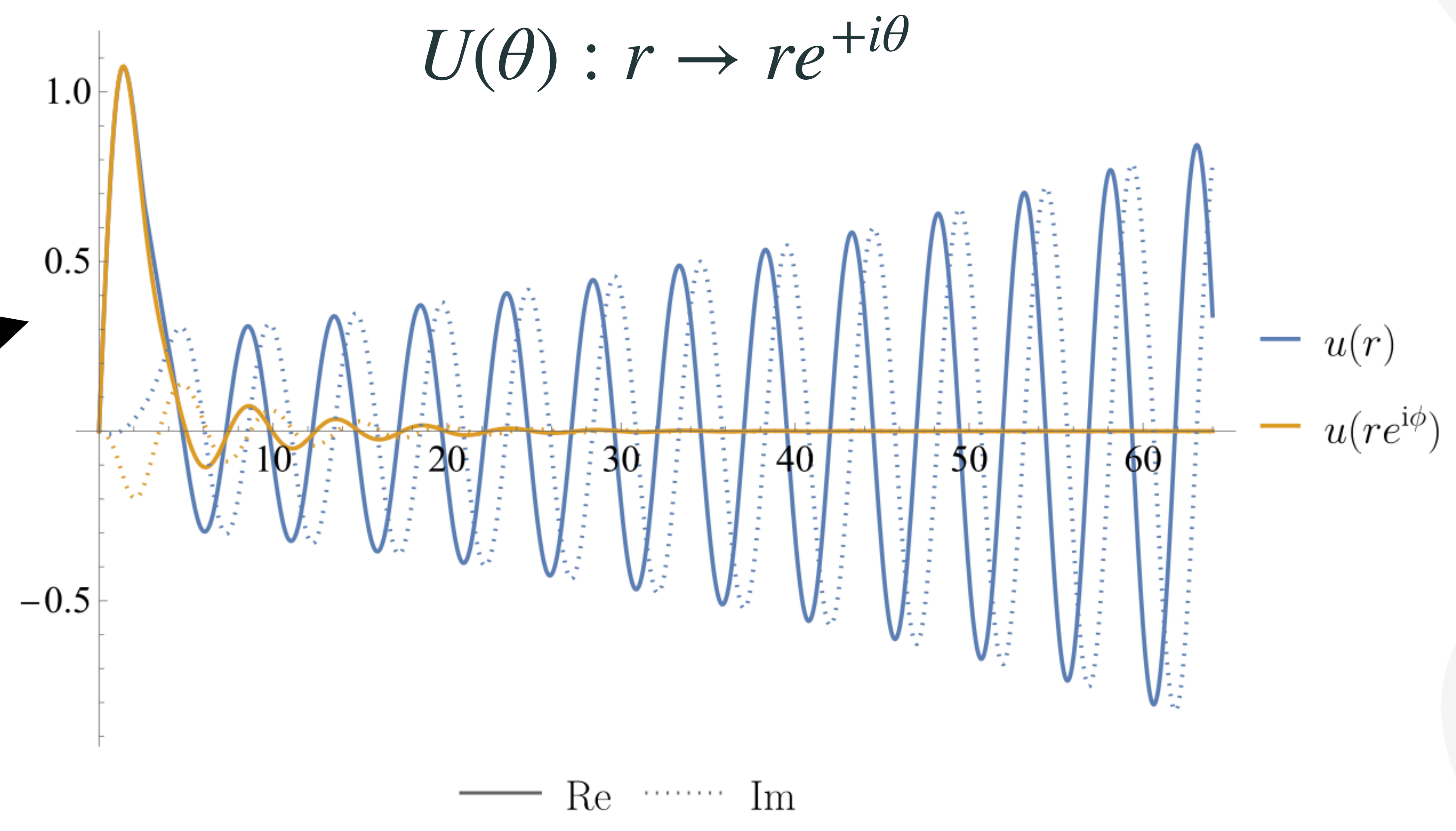
$$U(\theta) : k \rightarrow ke^{-i\theta} \qquad H(\theta) = U(\theta) H U^{-1}(\theta)$$

→ Non-Hermitian $H(\theta)$ matrix. Bound spectrum unchanged.



N. Yapa *et al.*, Phys. Rev. C **107**, 064316 (2023)

Square-integrable wave functions with complex energies.



Limited to small θ, entire $\hat{H}$ is rotated, repeated diagonalizations, but all decay channels automatically included.

Theoretical approaches for nuclear OQSs

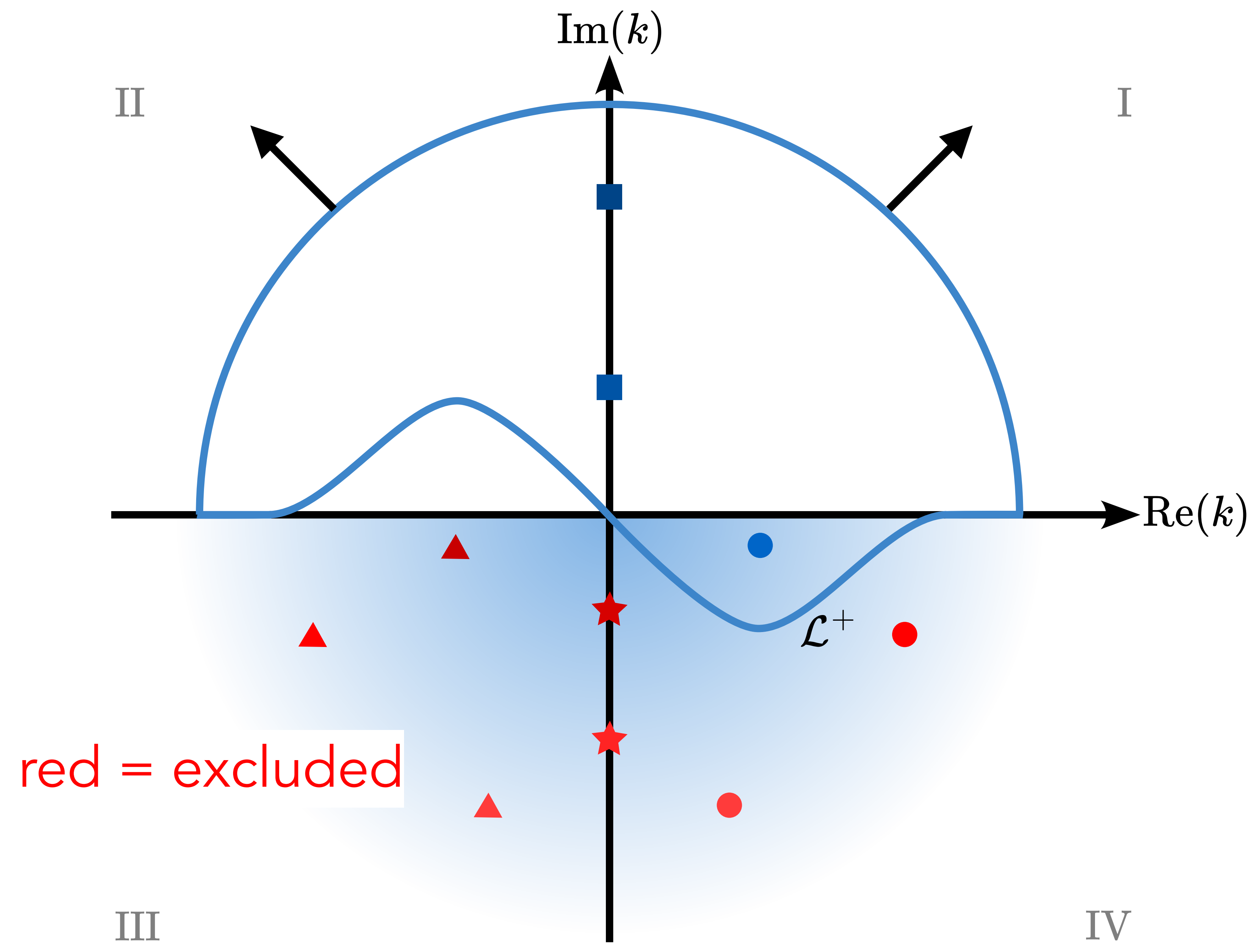
T. Berggren

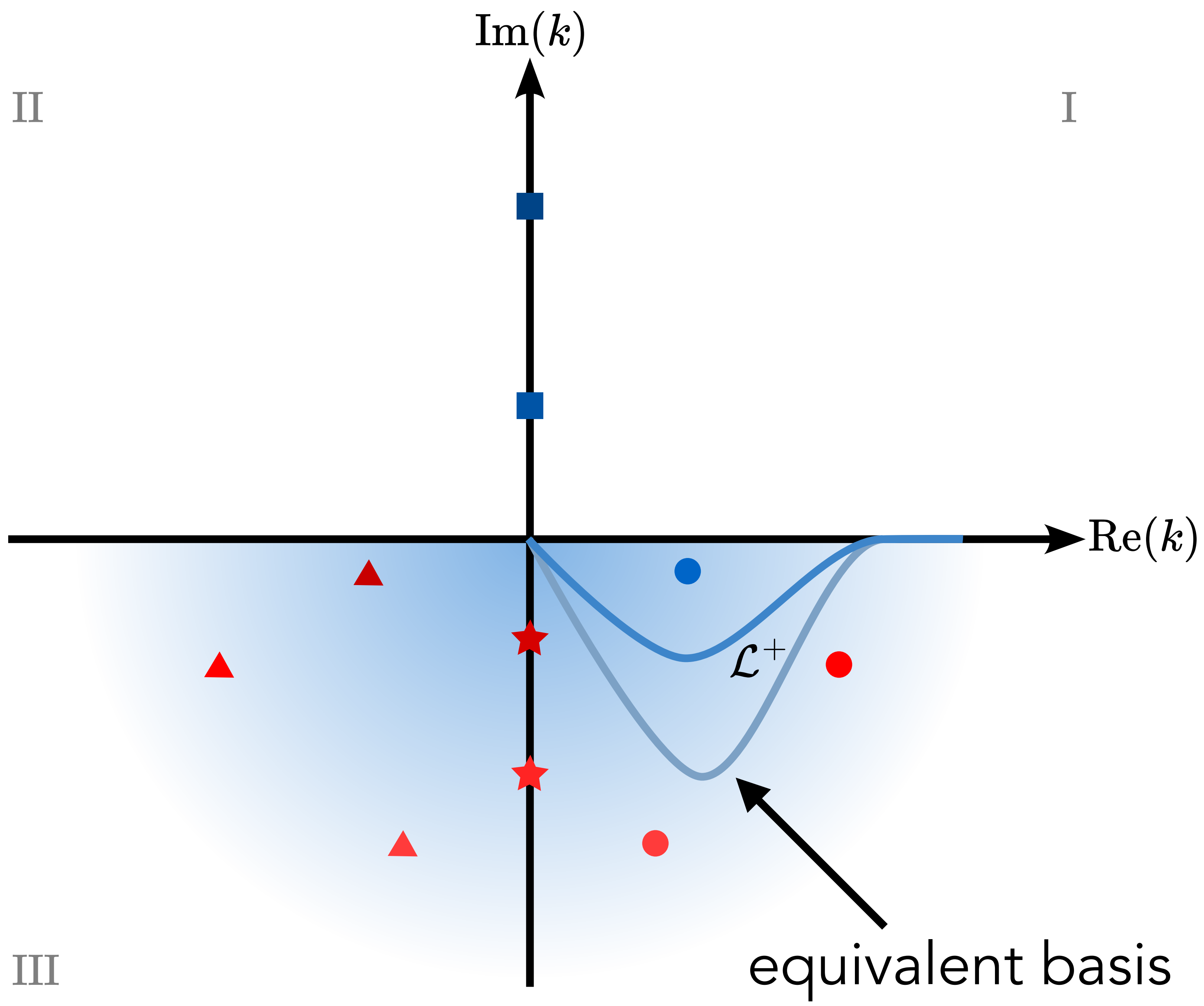
Berggren basis: Completeness relation over bound, resonant (Gamow), and scattering states.

T. Berggren, Nucl. Phys. A **109** 265 (1968)

$$\sum_{i=(b,r)} |k_i\rangle\langle\tilde{k}_i| + \int_{L^+} dk\, |k\rangle\langle\tilde{k}| = \hat{1}$$

Cauchy's integral theorem:





Gamow states treated on same footing as bound and scattering states.

Flexible basis that can be optimized to capture relevant physics.

Theoretical approaches for nuclear OQSs

Gamow shell model (GSM): complex-energy configuration-interaction.

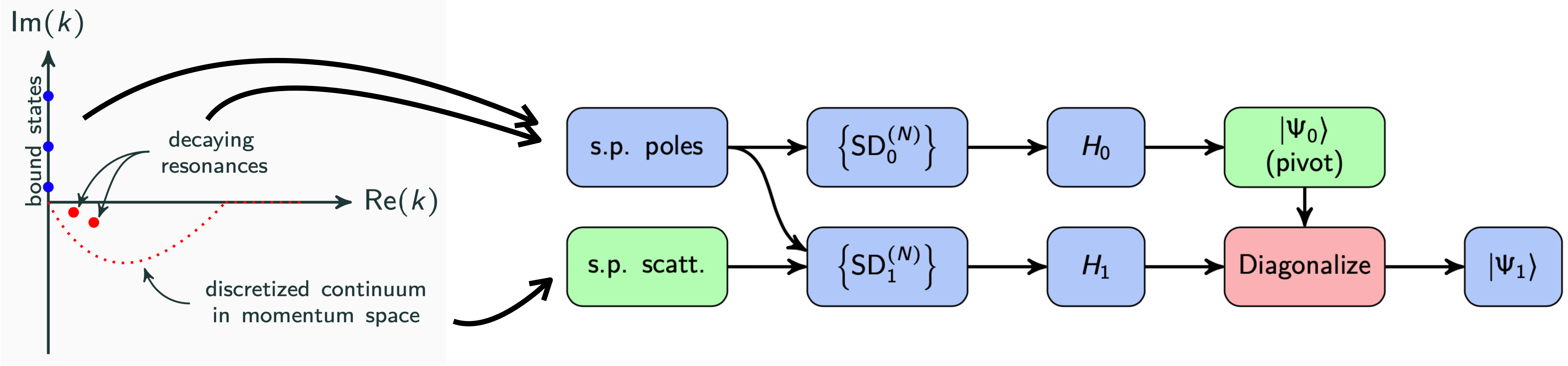
N. Michel *et al.*, *Gamow Shell Model* (2021)

Discretize the continuum in k-space for each partial-wave (l, j) considered:

$$\int_{L^+} dk f(k) \approx \sum_i w_i f(k_i)$$

Build Slater determinant (SD) basis, complex-symmetric H matrix, diagonalize:

$$\hat{H}|\Psi\rangle = \tilde{E}|\Psi\rangle \qquad |\Psi\rangle = \sum_i c_i |\mathrm{SD}_i\rangle \qquad \tilde{E} = E - i\frac{\Gamma}{2}$$

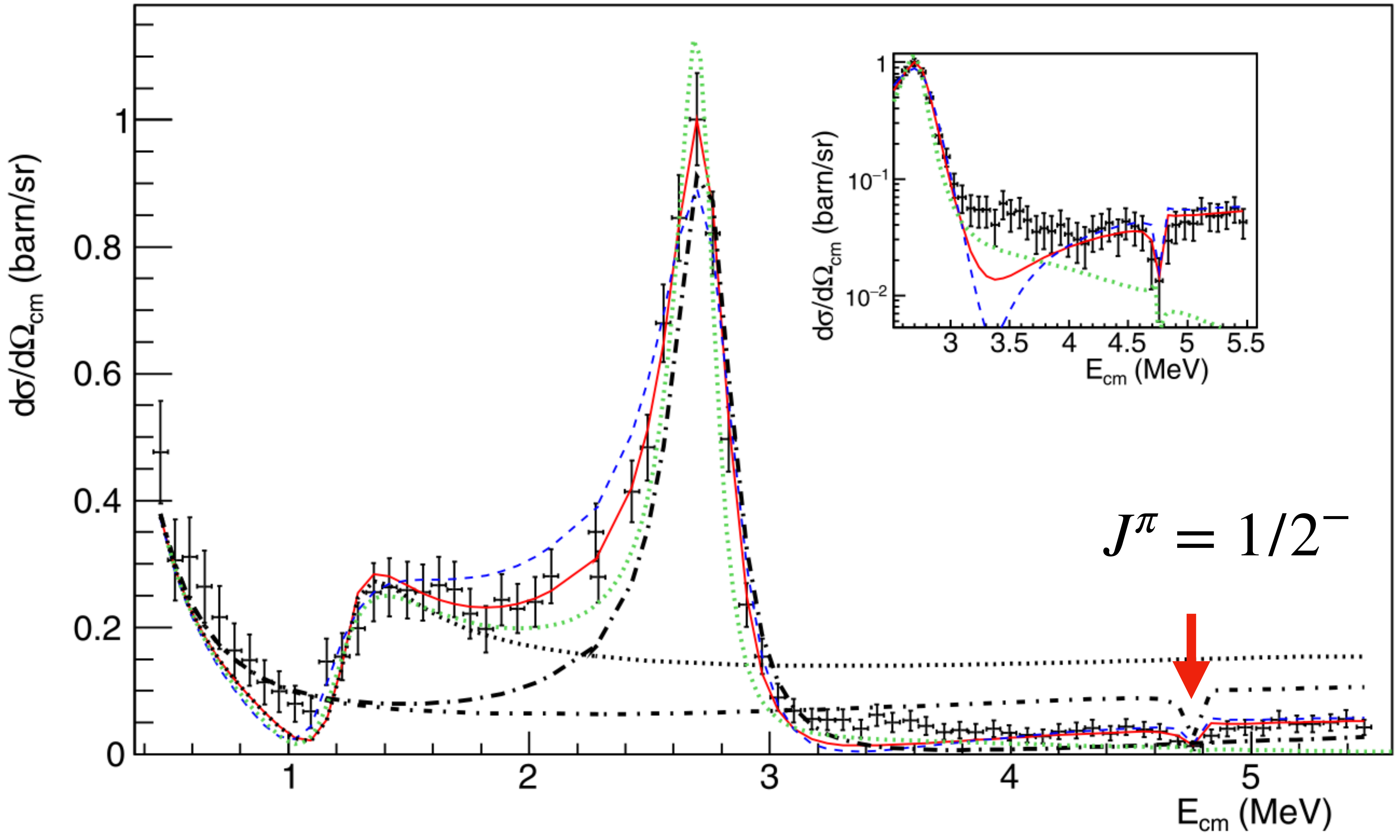


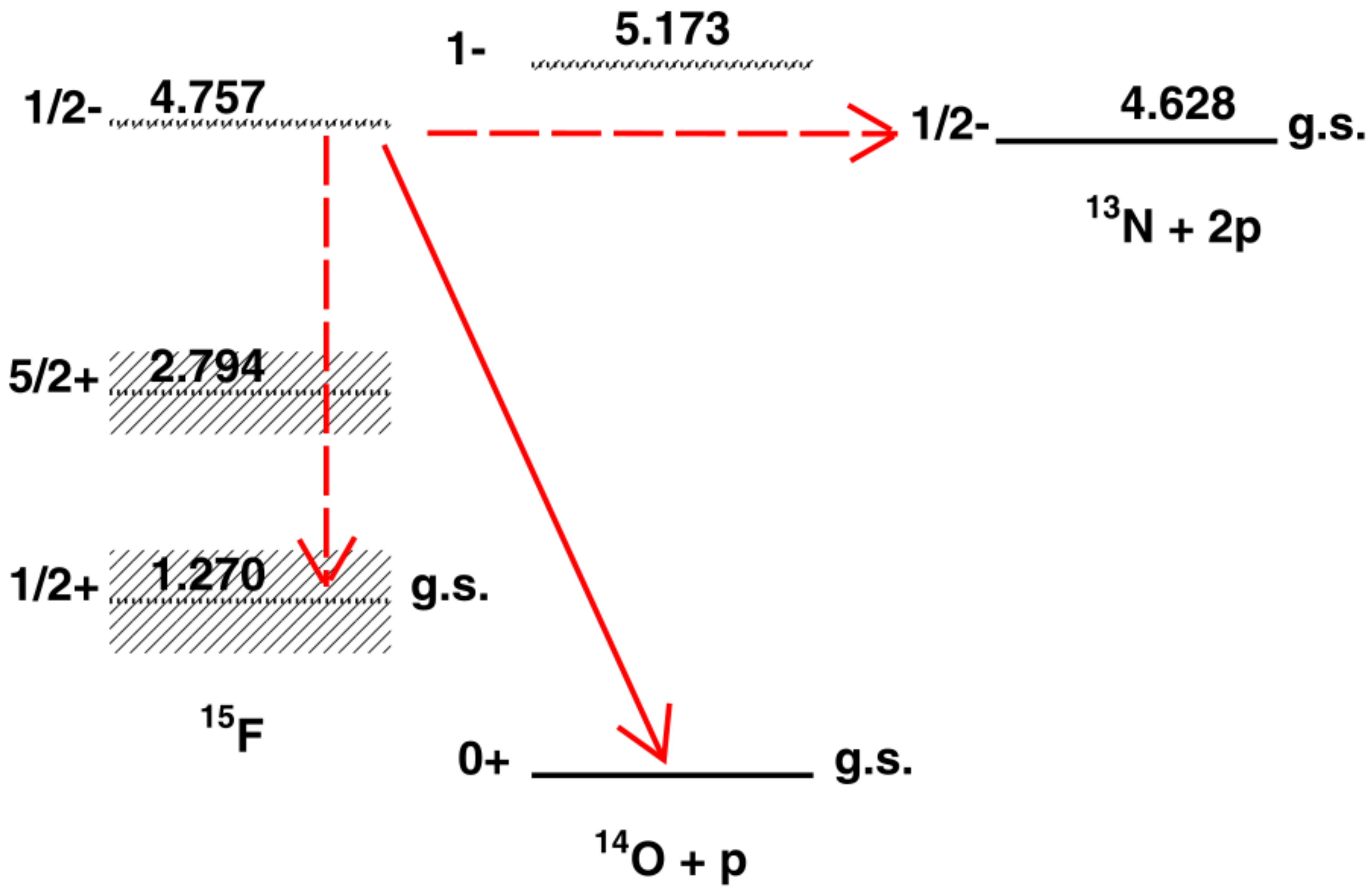
Only one diagonalization needed, but high computational cost due to discretization.

Trapped resonances

The case of a trapped resonance: Narrow proton resonance in 15F well above the Coulomb barrier.

F. de Grancey *et al.*, Phys. Lett. B **758**, 26 (2016).

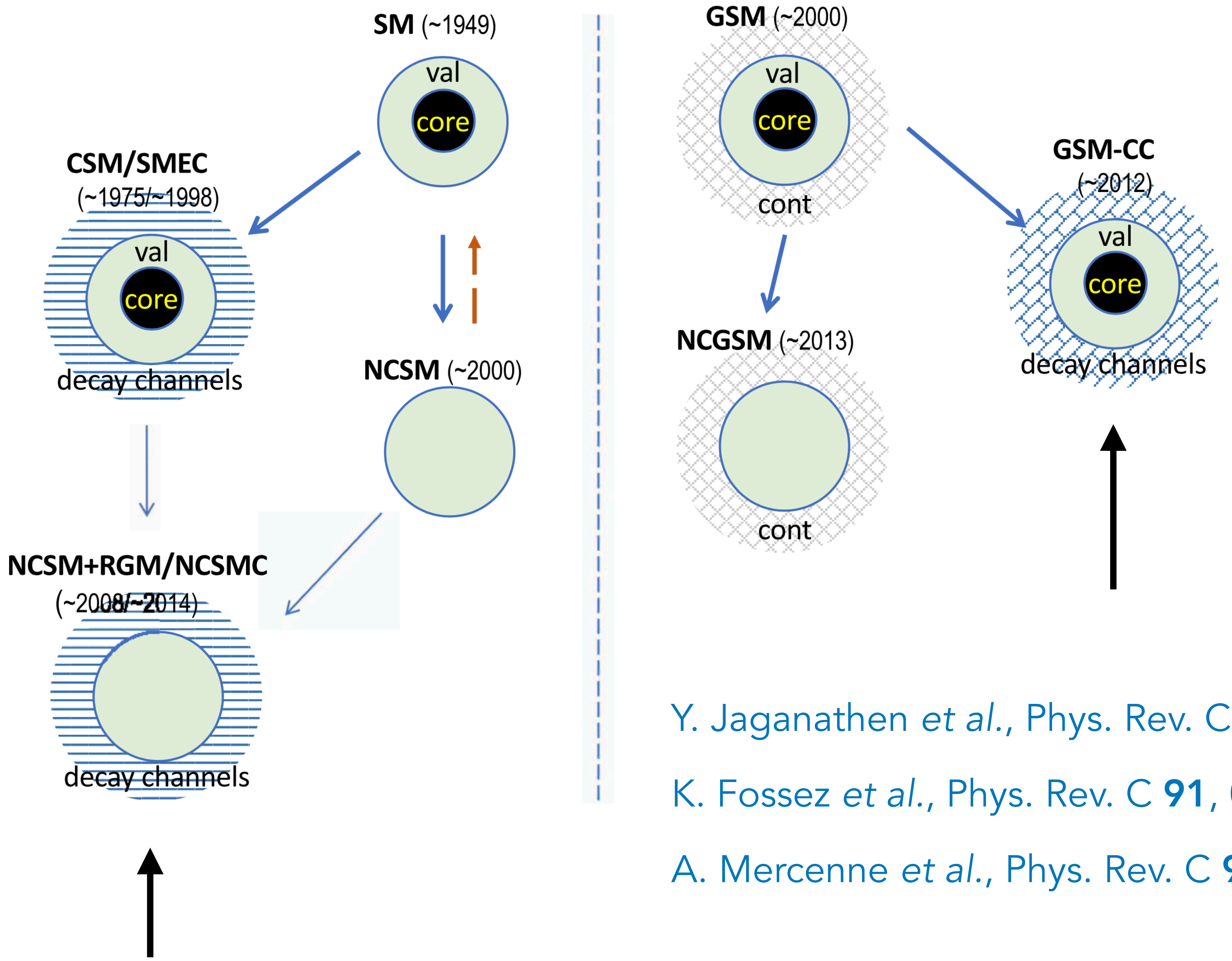




The $1/2^-$ wave function aligns with the 13N+2p threshold, reducing dramatically γ and $1p$ decays.

Theoretical approaches for nuclear OQSs

Resonating group method. J. A. Wheeler, Phys. Rev. **52**, 1107 (1937)



S. Baroni *et al.*, Phys. Rev. Lett. **110**, 022505 (2013)

P. Navràtil *et al*, Phys. Scr. **91**, 053002 (2016)

Y. Jaganathen *et al.*, Phys. Rev. C **89**, 034624 (2014)

K. Fossez *et al.*, Phys. Rev. C **91**, 034609 (2015)

A. Mercenne *et al.*, Phys. Rev. C **99**, 044606 (2019)

Microscopic reaction theory:

1. Many-body target and projectile wave functions.
2. For each reaction channel considered, exact continuum (relative motion in r-space).

Precise, but all reaction/decay channels must be included explicitly with their asymptotic.

Figure from C. W. Johnson *et al.*, J. Phys. G **47**, 123001 (2020)

Density matrix renormalization group (DMRG)

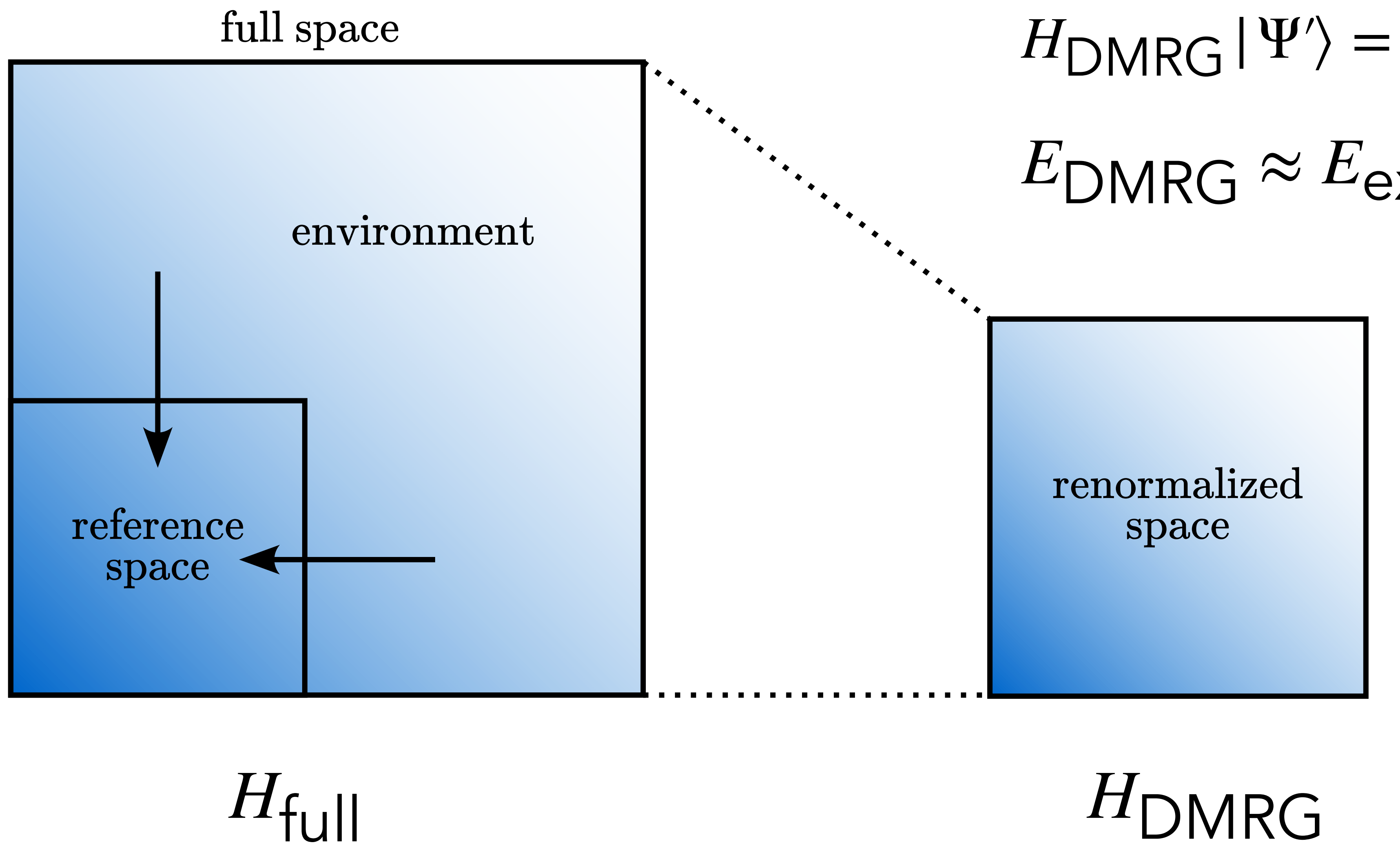
The DMRG method was introduced in condensed matter to approximate the ground state of infinite 1D lattices.

Exploits low entanglement between system and environment.

S. R. White, Phys. Rev. Lett. **69**, 2863 (1992)

$$\mathcal{H} = \mathcal{H}_{\text{system}} \otimes \mathcal{H}_{\text{evironment}}$$

In its original formulation, DMRG finds a compact representation of the Hamiltonian that approximates the ground state (Wilsonian renormalization).



$$H_{\text{DMRG}}\,|\Psi'\rangle = E_{\text{DMRG}}\,|\Psi'\rangle$$

$$E_{\text{DMRG}} \approx E_{\text{exact}}$$

In its (equivalent) modern formulation, the ansatz wave function is a matrix product state (MPS) optimized to minimize the energy.

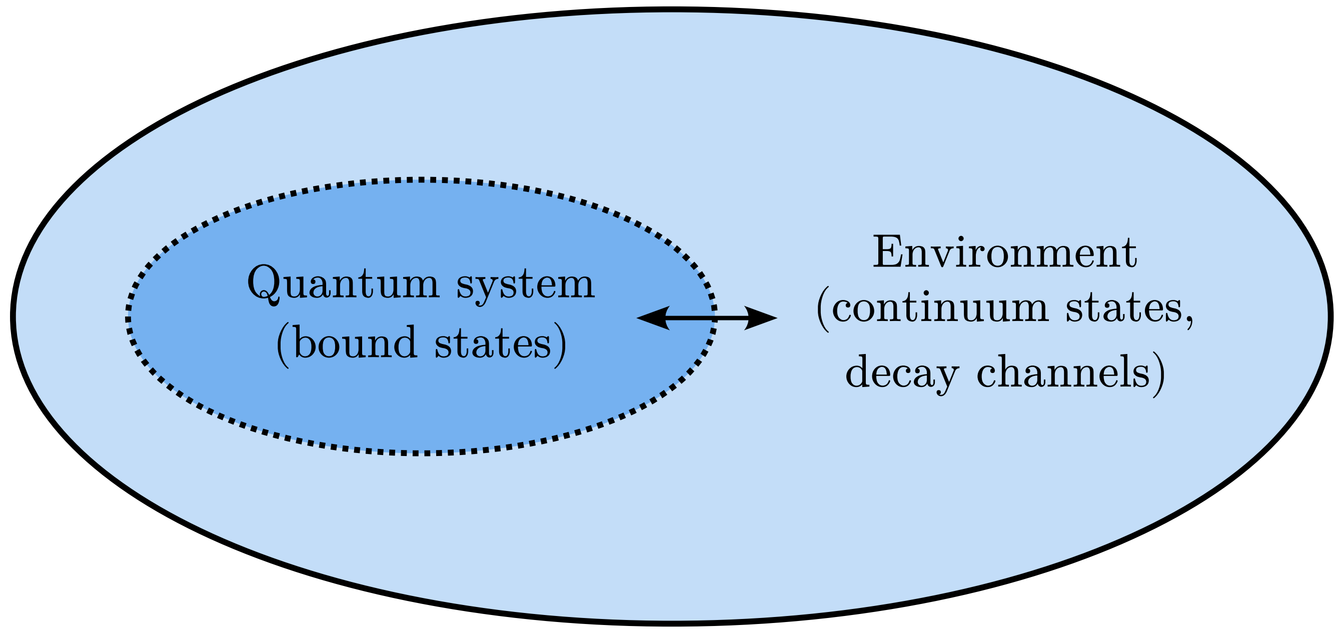
$$|\Psi\rangle = \sum_{\sigma_1,\sigma_2,\ldots,\sigma_N} A^{(1)}_{\sigma_1} A^{(2)}_{\sigma_2} \ldots A^{(N)}_{\sigma_N} \,|\sigma_1, \sigma_2, \ldots, \sigma_N\rangle$$

with $\sigma_i = 0{,}1$ and N is the number of orbitals.

Theoretical approaches for nuclear OQSs

Gamow density matrix renormalization group: complex-energy DMRG.

J. Rotureau *et al.*, Phys. Rev. Lett. **97**, 110603 (2006)



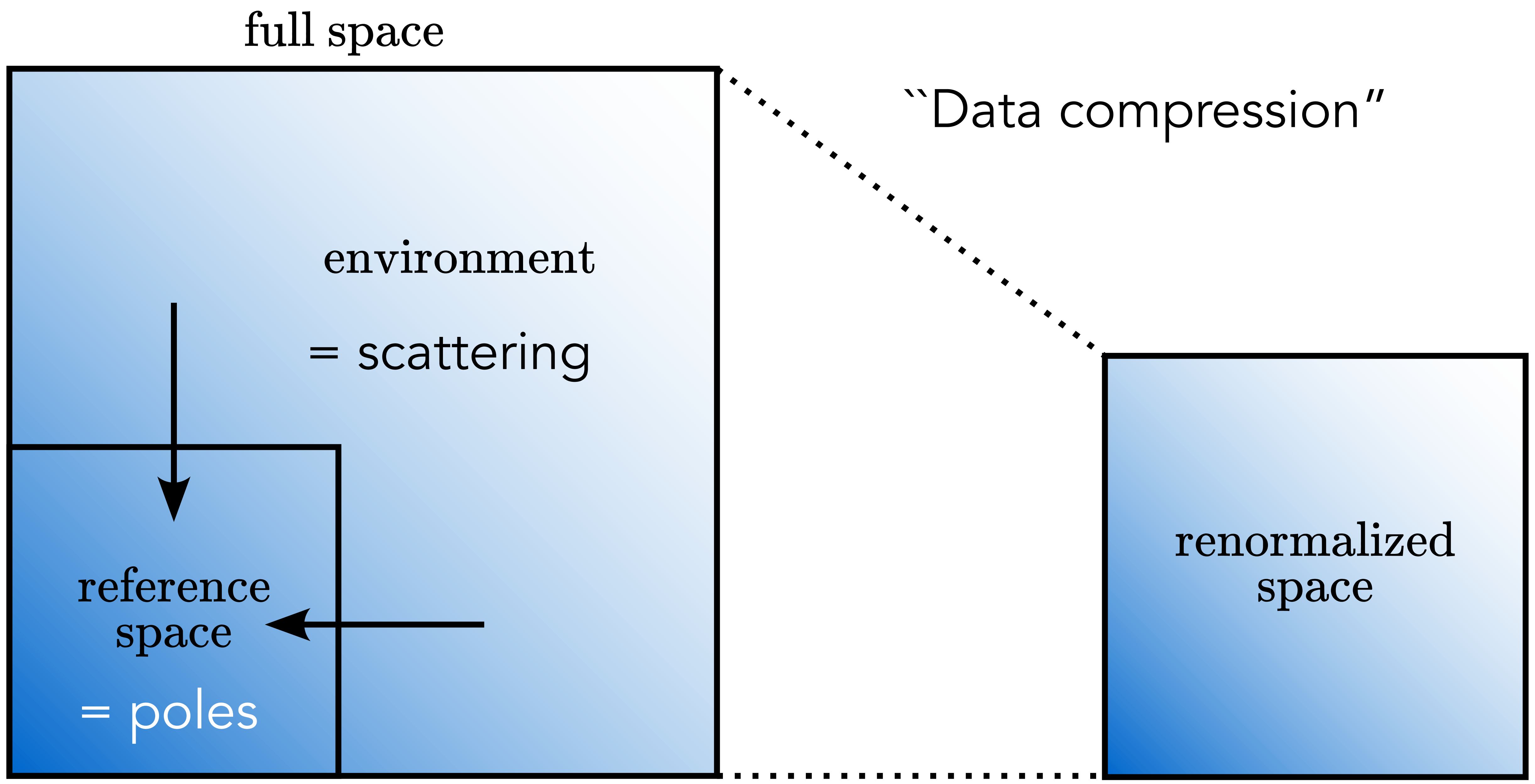
$$\mathcal{H} = \mathcal{H}_{\text{system}} \otimes \mathcal{H}_{\text{evironment}}$$

$$\downarrow$$

$$\mathcal{H} = \mathcal{H}_{\text{discrete}} \otimes \mathcal{H}_{\text{scatt}}$$

$$|\Psi^{A,J^\pi}\rangle_1 = \sum_{a,b} C^a_{b,i=1} \{ |\mathrm{SD}_a^{f_\mathscr{A}}\rangle_0^{\mathscr{A}} \otimes |\mathrm{SD}_b^{f_\mathscr{B}}\rangle_1^{\mathscr{B}} \}^{A,J^\pi}$$

reference space   medium



Gamow-DMRG

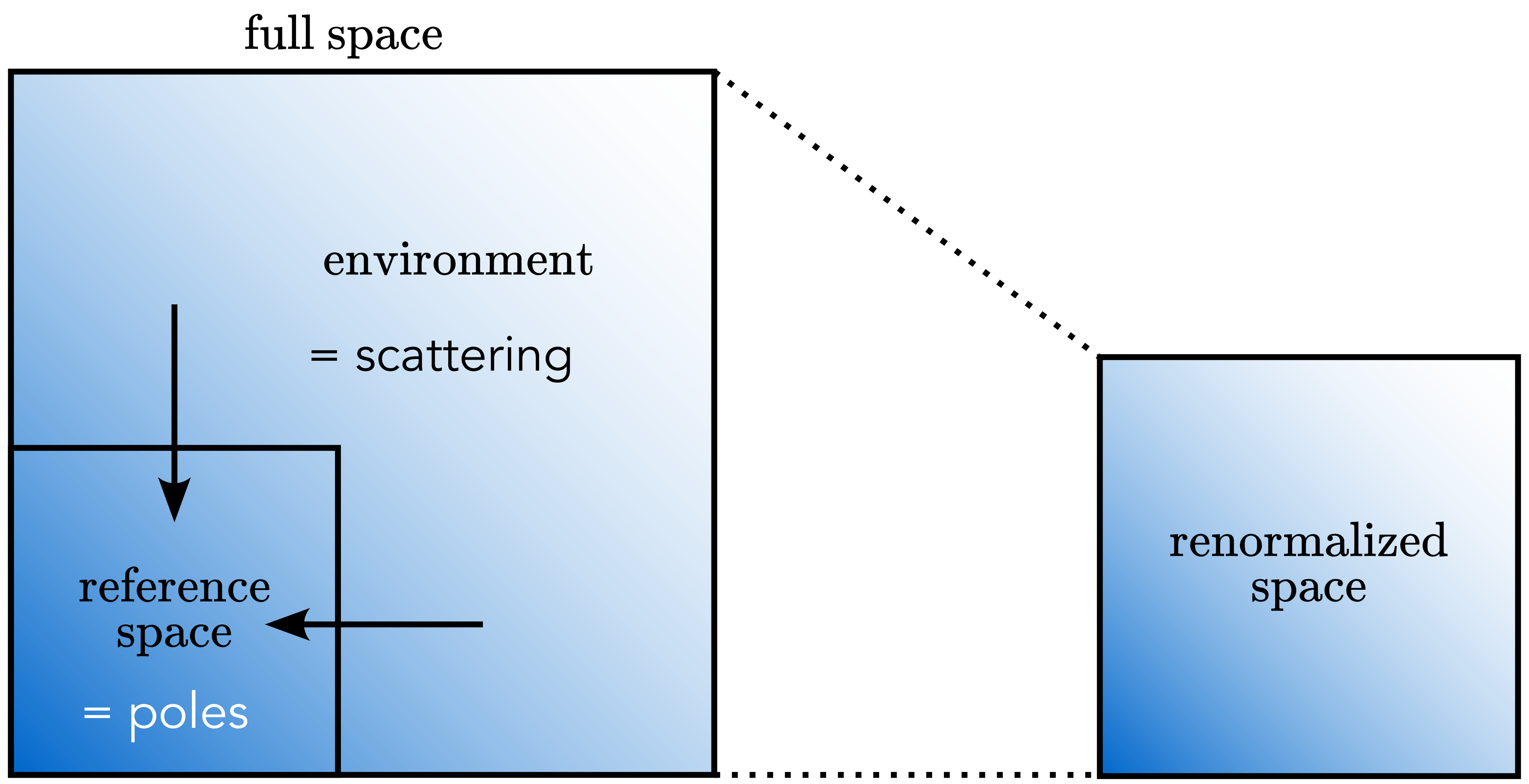
The most important steps:

Build the density matrix reduced in the medium:

$$\rho^{\mathscr{B}}_{b,b',i}(j_B^{\pi_B}) = \sum_a C^i_{a(j_A^{\pi_A}),b(j_B^{\pi_B})} C^i_{a(j_A^{\pi_A}),b'(j_B^{\pi_B})}$$

Diagonalize it to obtain occupations in the medium:

$$\hat{\rho}^{\mathscr{B}}_i |\phi_\alpha\rangle_i = \omega_{\alpha,i} |\phi_\alpha\rangle_i$$



Select the most important configurations:

$$\left| 1 - \mathrm{Re}\left(\sum_{\alpha=1}^{N} \omega_{\alpha,i=1} \right) \right| < \epsilon$$

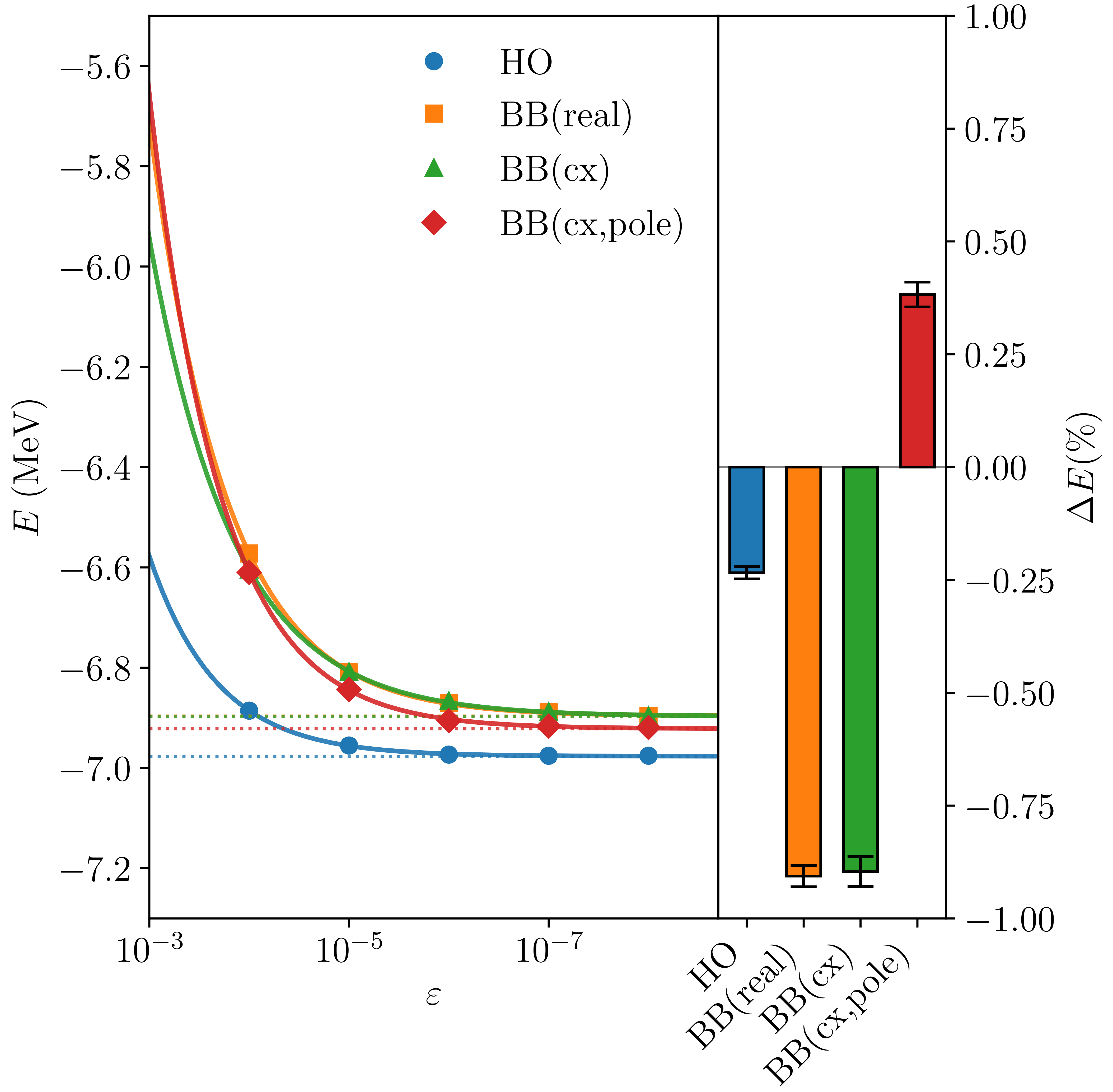
The truncation ϵ controls the error.
Exact result if $\epsilon \to 0$.

Gamow-DMRG

Example of convergence with DMRG truncation ε in harmonic oscillator (HO) and different Berggren bases (BB).

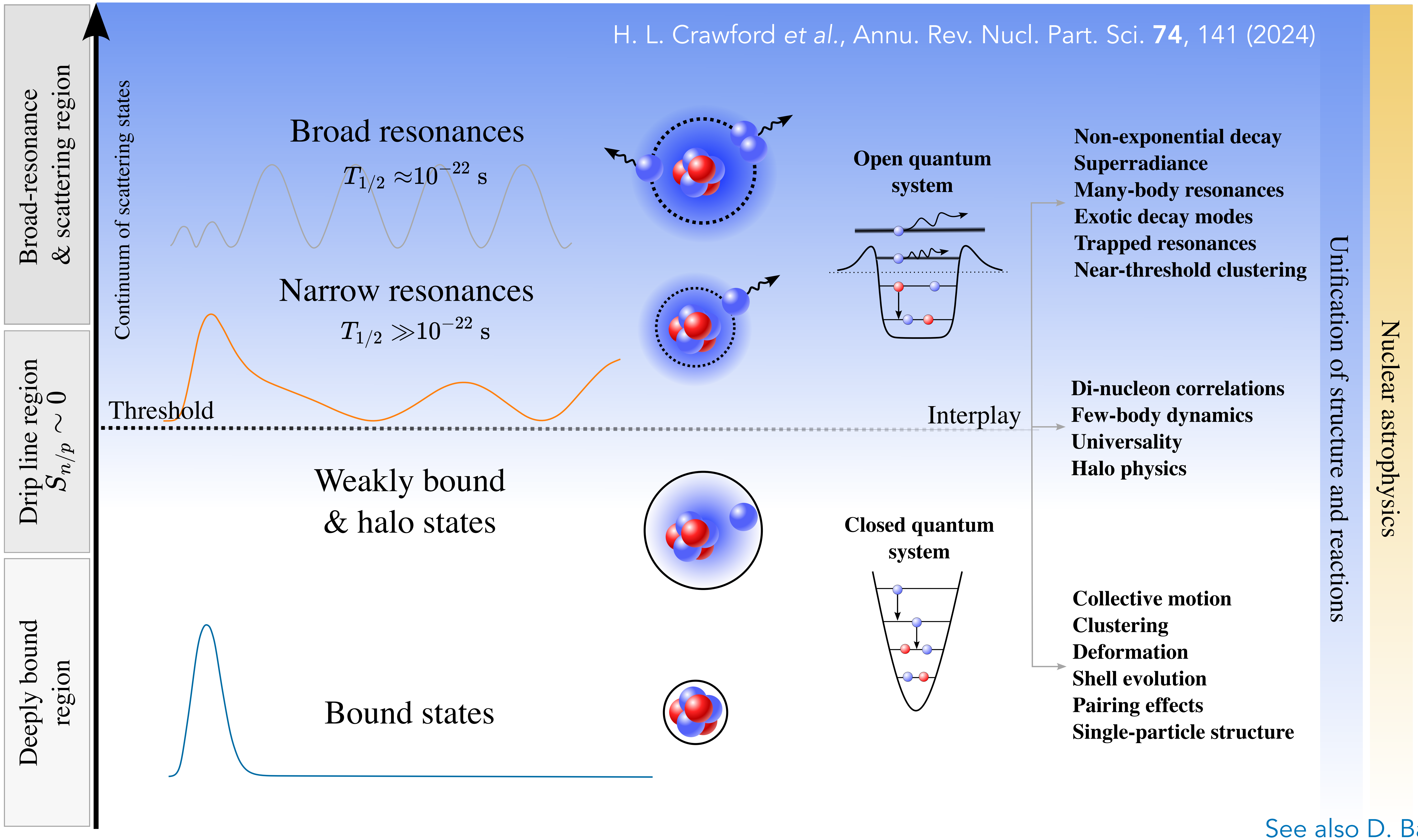
Bound $J^\pi = 1/2^+$ ground state of ^{3}He.

Within 1% of FCI (no-core GSM).



FLORIDA STATE UNIVERSITY

Physics of exotic nuclei: Challenges



Broad, many-body resonances.

Interplay between collective phenomena and continuum couplings.

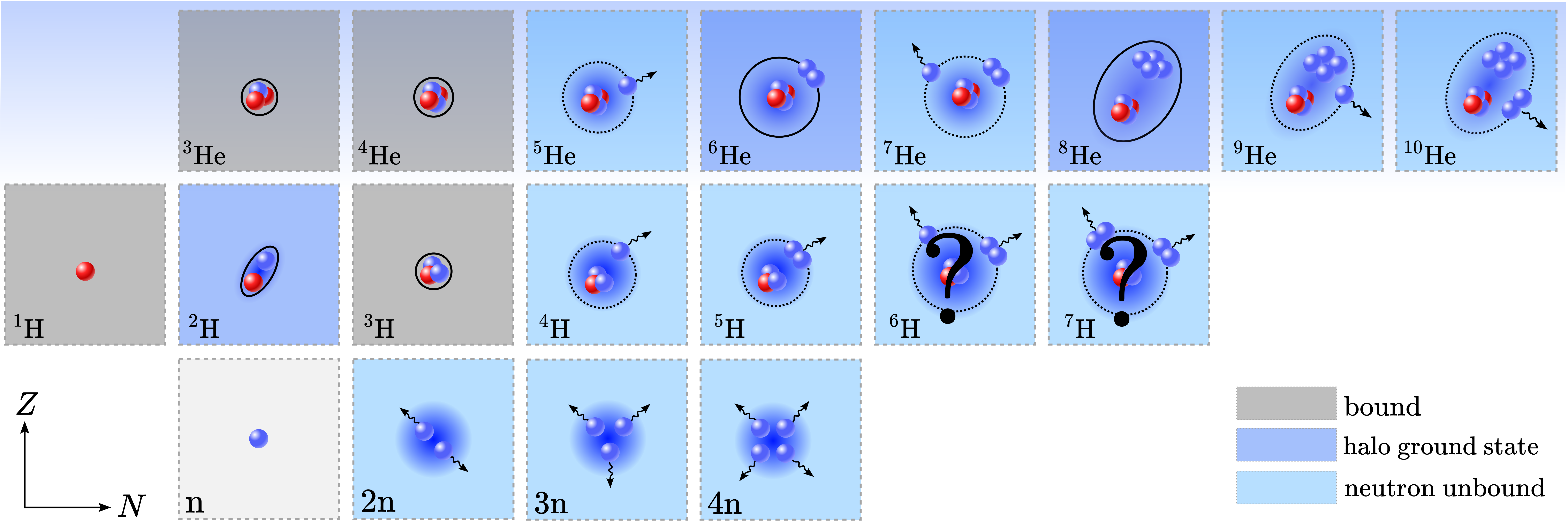
See also D. Bazin et al., Few-Body Syst. **64**, 25 (2023)

C. W. Johnson et al., J. Phys. G **47**, 123001 (2020)

Ab initio description of $^{4-7}$H (work in progress)

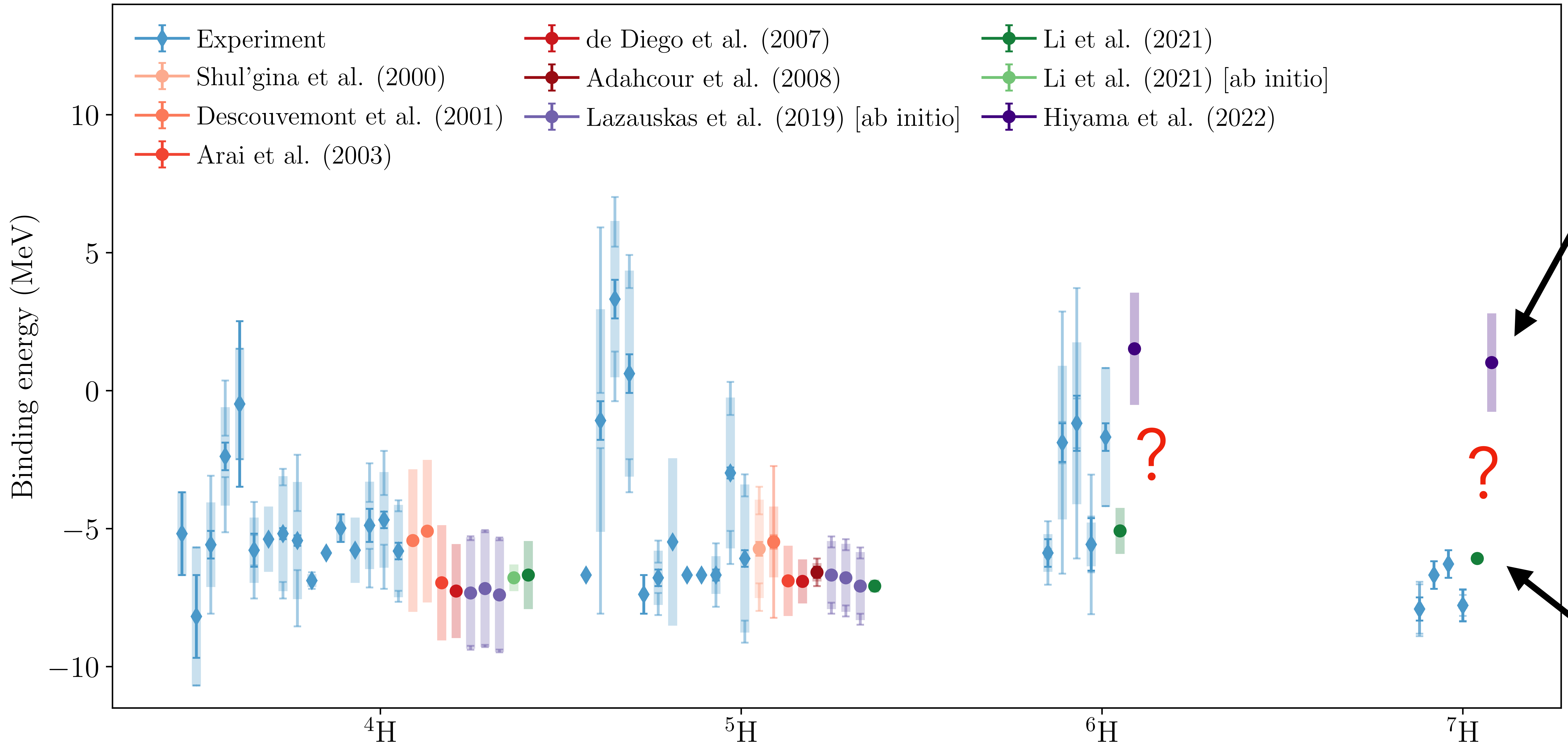
Work lead by
A. Sehovic (FSU)

Long-term goal: Testing nuclear forces in extreme N/Z conditions where quasi-exact calculations are feasible.



Challenge: Obtain the first *ab initio* description of the H chain and determine the nature of ^{7}H g.s. ($4n$ decay).

Discrepancies in $^{6,7}H$



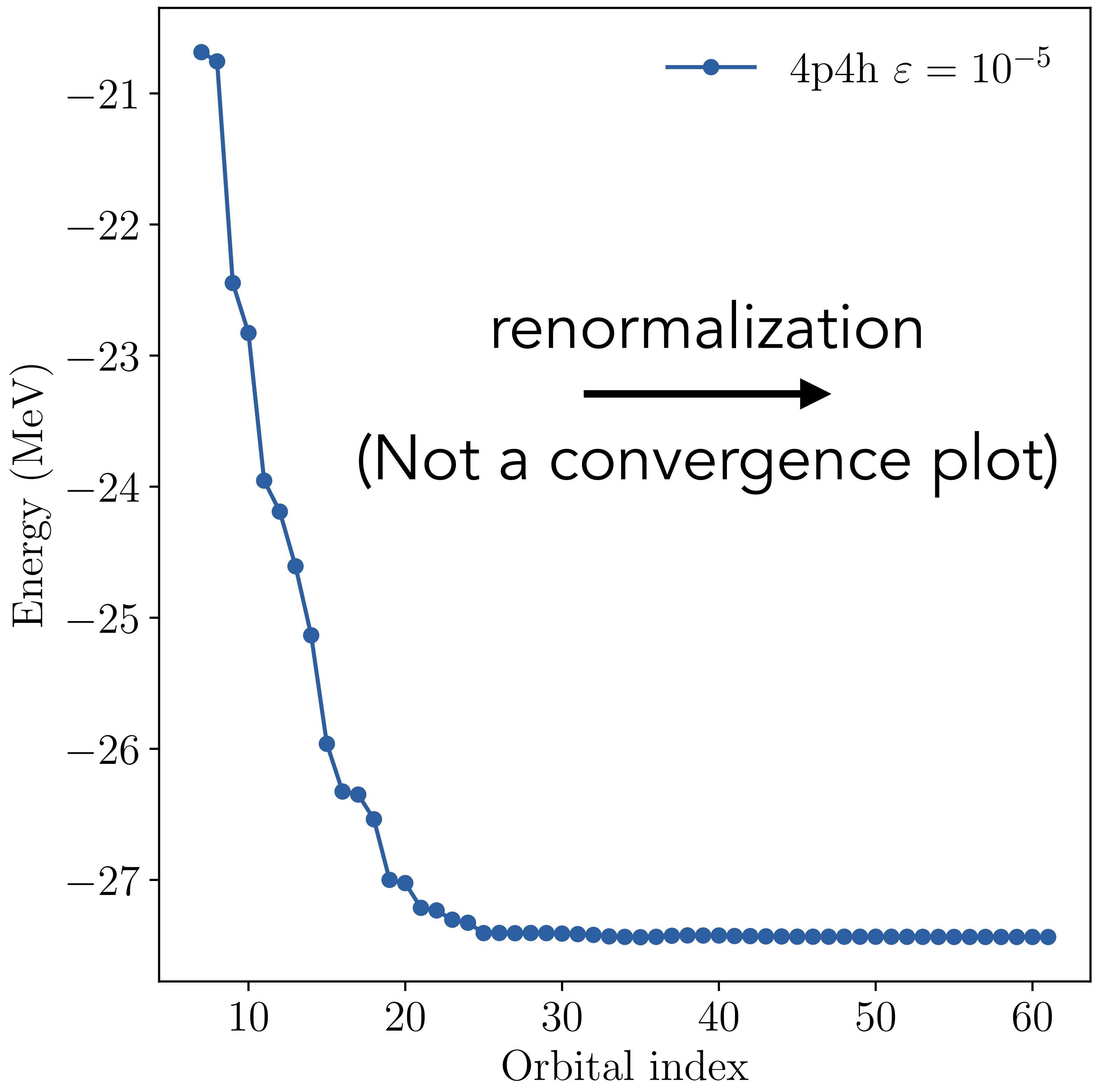
Faddeev-Yakubowski + complex-scaling, ^{3}H-*n* potential adjusted on phase shifts and *n*-*n* interaction adjusted on ^{5}H *ab initio* results.

Gamow shell model with model adjusted on He chain predicts a narrow ^{7}H g.s.

Ideal case: $J^\pi = 0^+$ ^{4}He g.s.

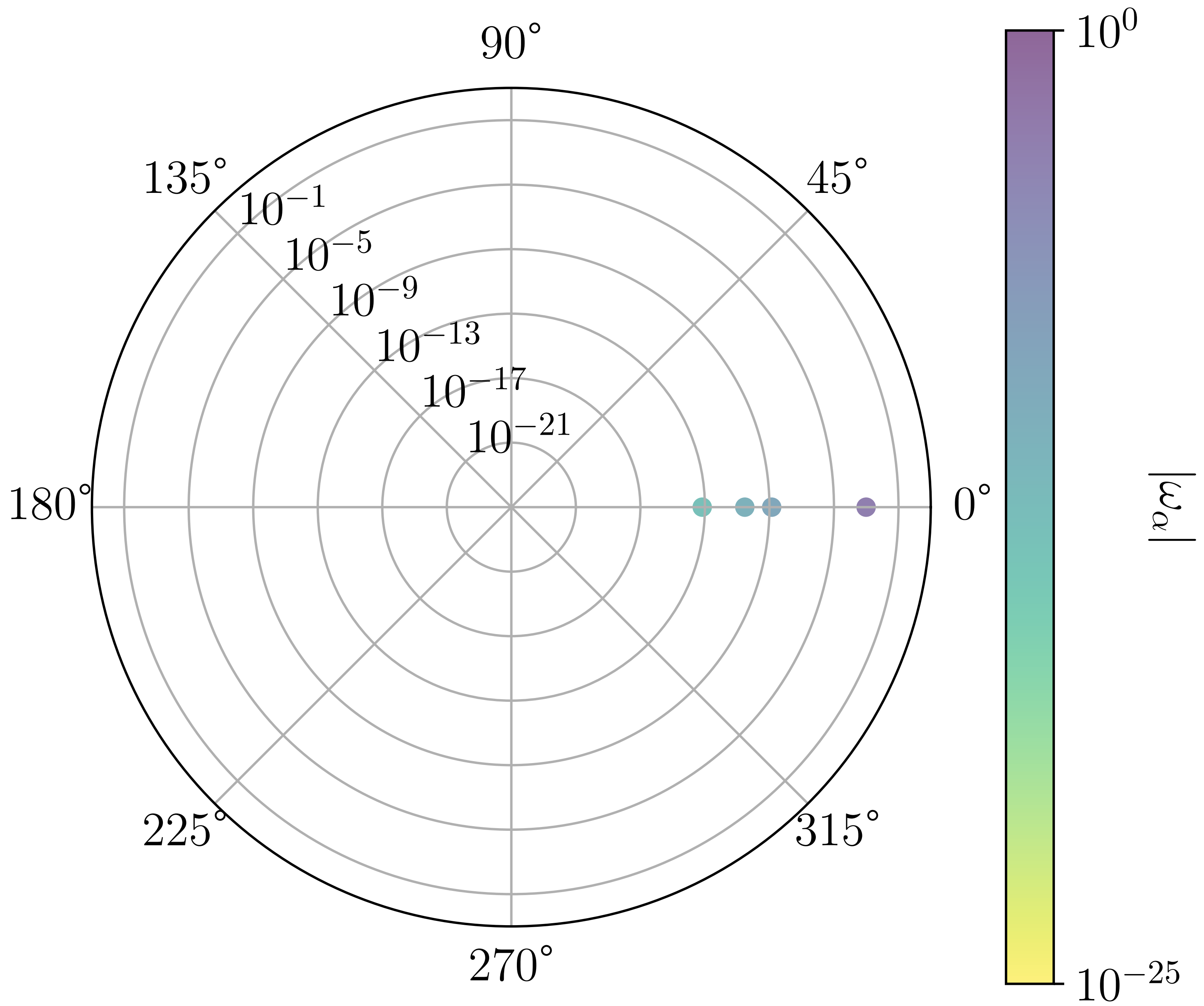
Well-bound state ($E = -28.30$ MeV), harmonic oscillator basis, variational principle.

Smooth, near-exponential convergence of the energy with the number of shells included:



Eigenvalues ω_α of the reduced density matrix (occupations) show excellent factorization:

$$|\Psi^{A,J^\pi}\rangle \approx C^a_{0,i}\{|\mathrm{SD}^{f_\mathscr{A}}_a\rangle^\mathscr{A}_0 \otimes |\mathrm{SD}^{f_\mathscr{B}}_0\rangle^\mathscr{B}_1\}^{A,J^\pi}$$

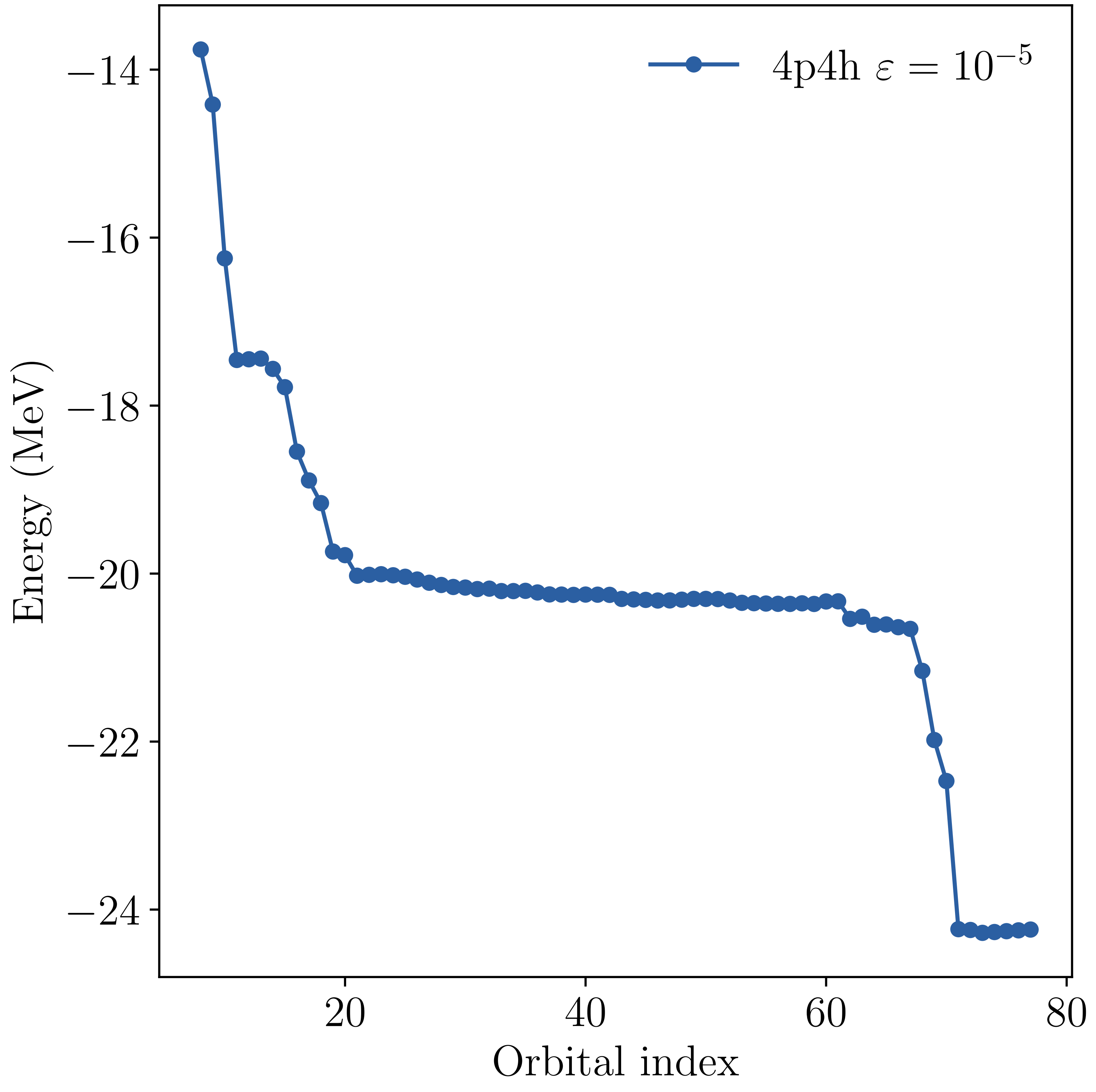


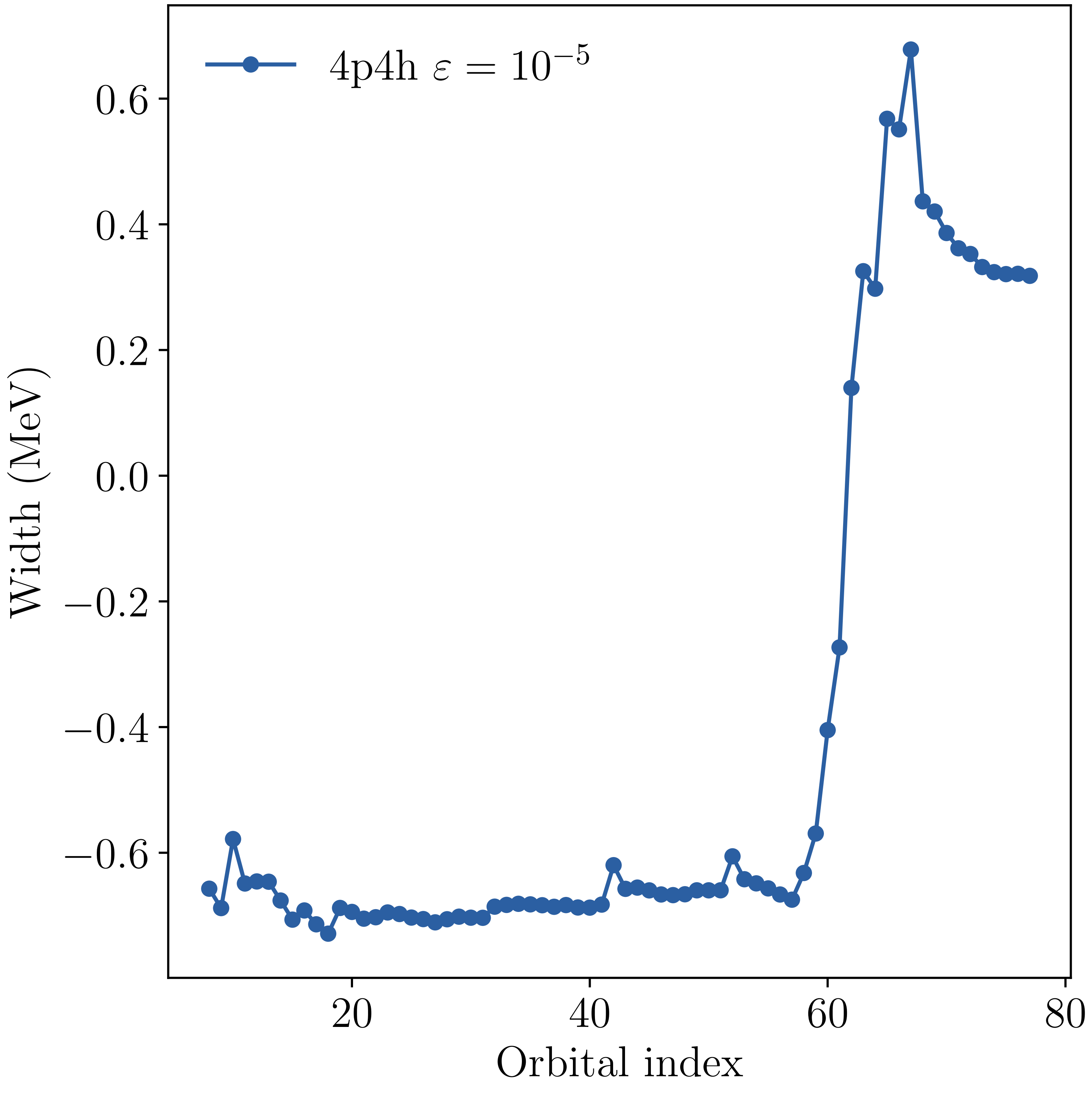
$$\omega_\alpha = |\omega_\alpha| e^{i\theta}$$

$J^\pi = 3/2^-$ g.s. resonance in ^{5}He

Single-particle resonance, neither narrow nor broad ($S_n = -0.735$ MeV, $\Gamma = 0.648$ MeV). Berggren basis.

Similar to ^{4}He at first, but then drop in energy when the width increases.





The wave function reorganizes due to continuum couplings!

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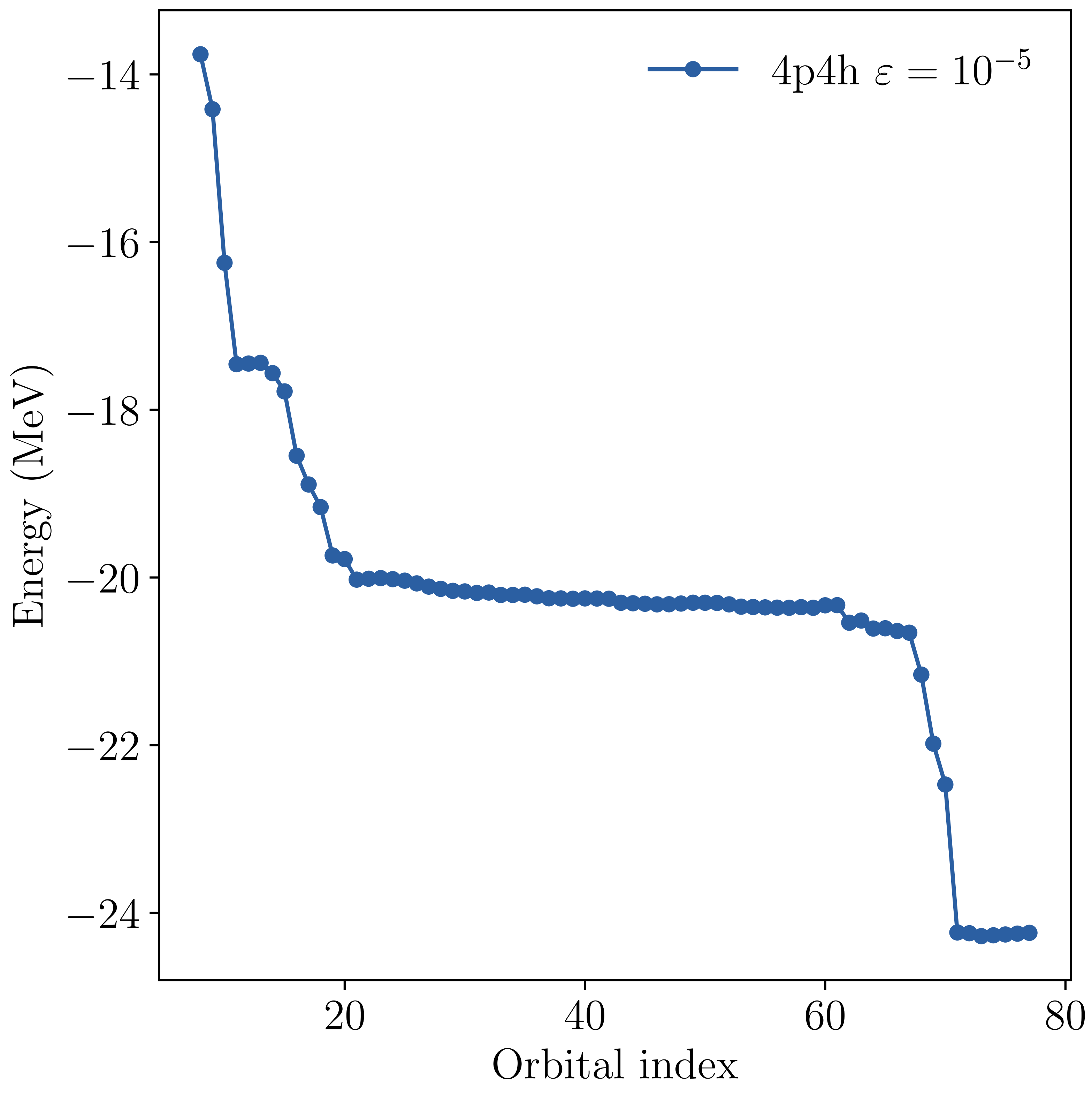
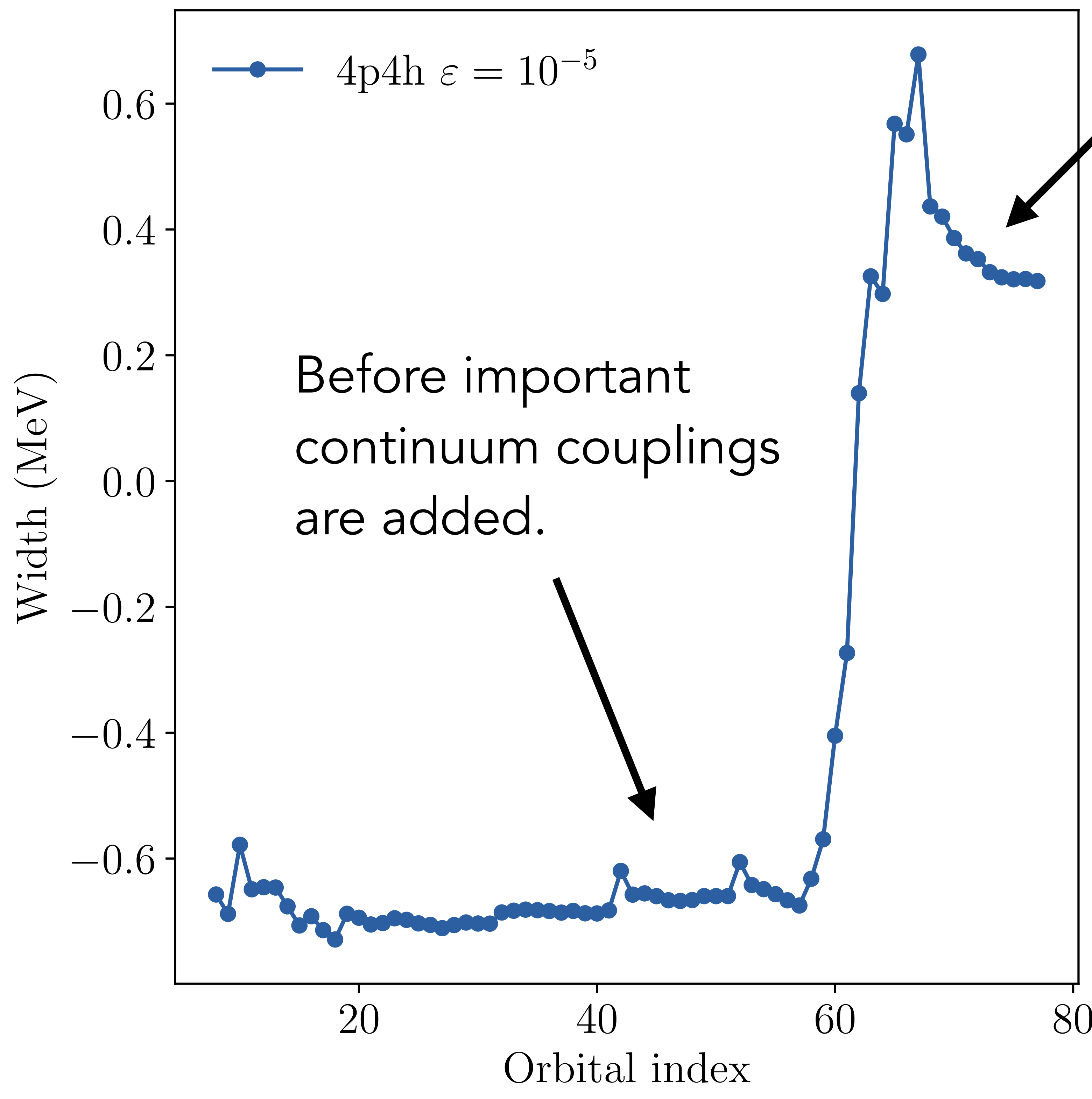


After.

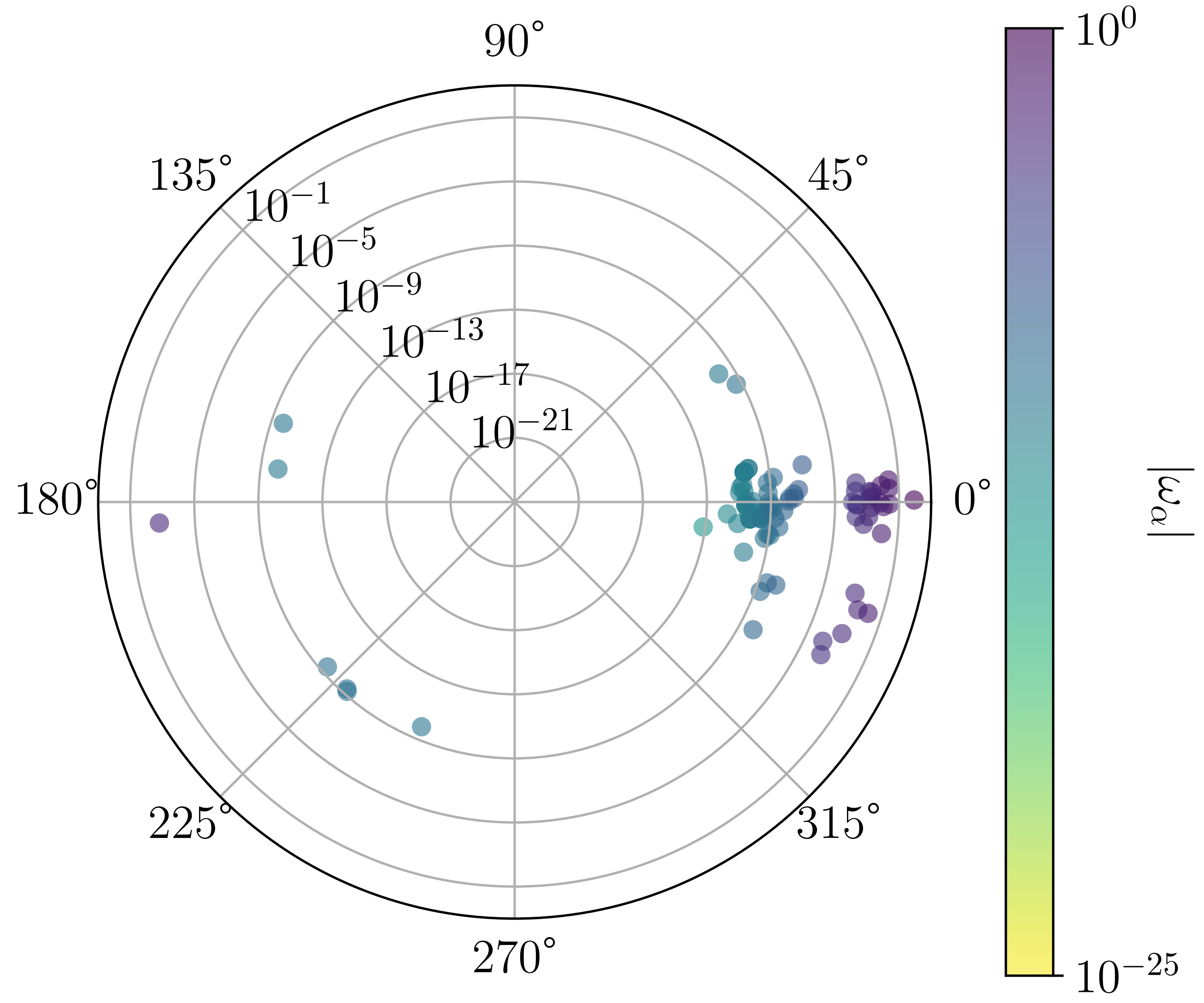


The wave function reorganizes due to continuum couplings!

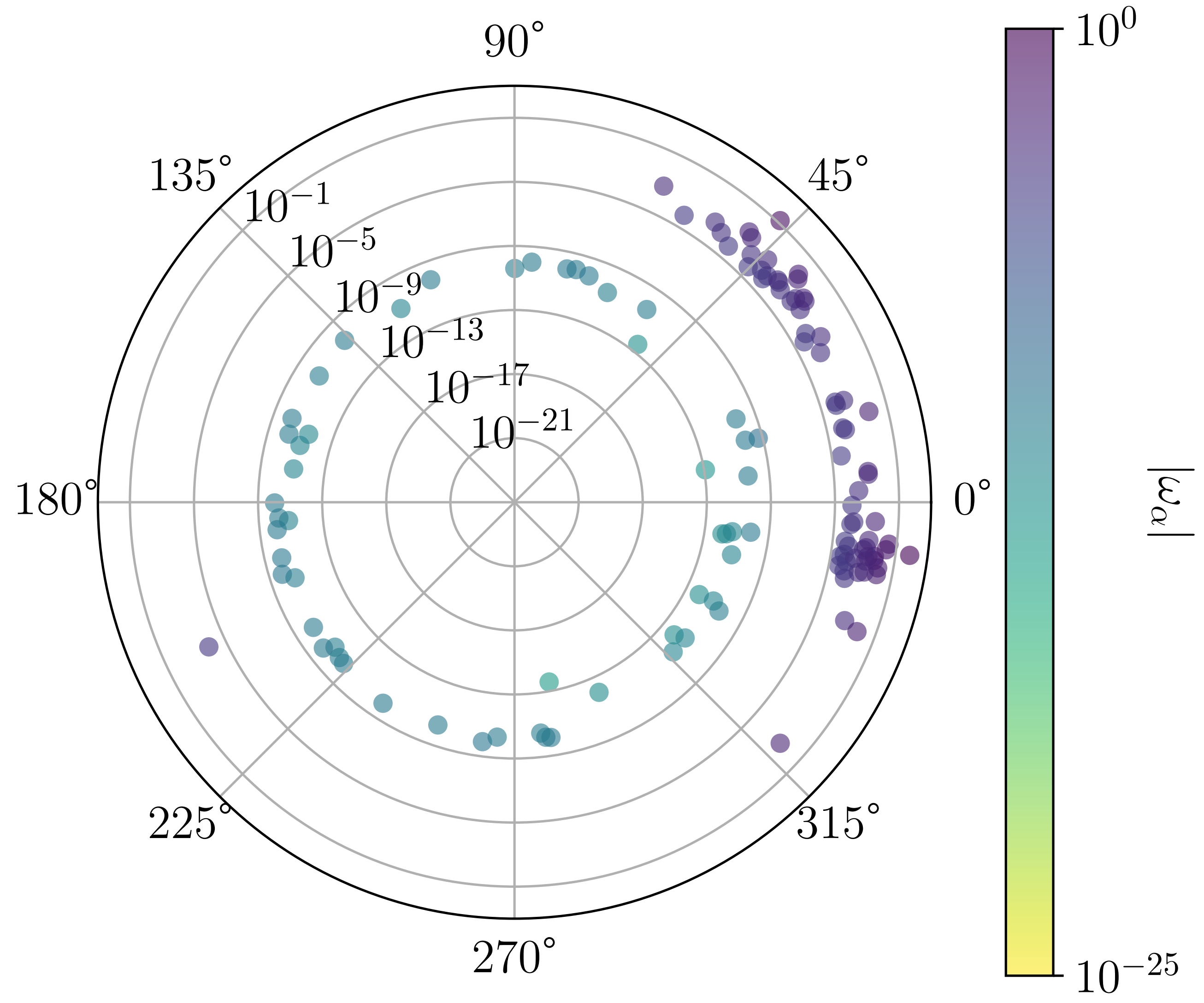
$J^\pi = 3/2^-$ g.s. resonance in ^{5}He

The reduced density matrix becomes complex-symmetric, but $\mathrm{Im}(\mathrm{Tr}[\rho]) = 0.$

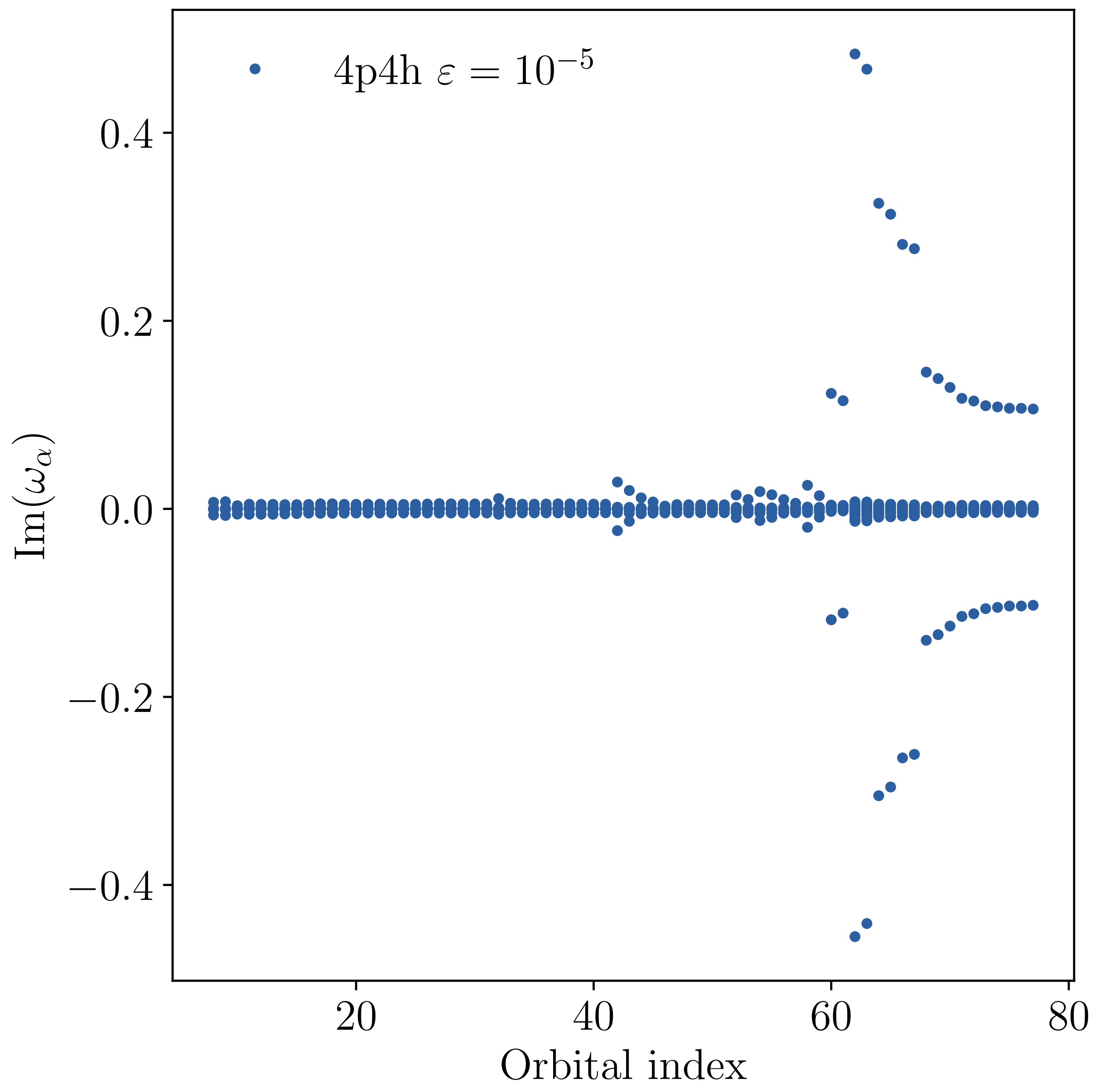
Before



After



$\mathrm{Tr}(\rho) = 1$



The absolute value of the imaginary part of the eigenvalues of the reduced density matrix represent uncertainties on the occupations due to continuum couplings.

We still have a good factorization, but the wave function becomes fragmented.

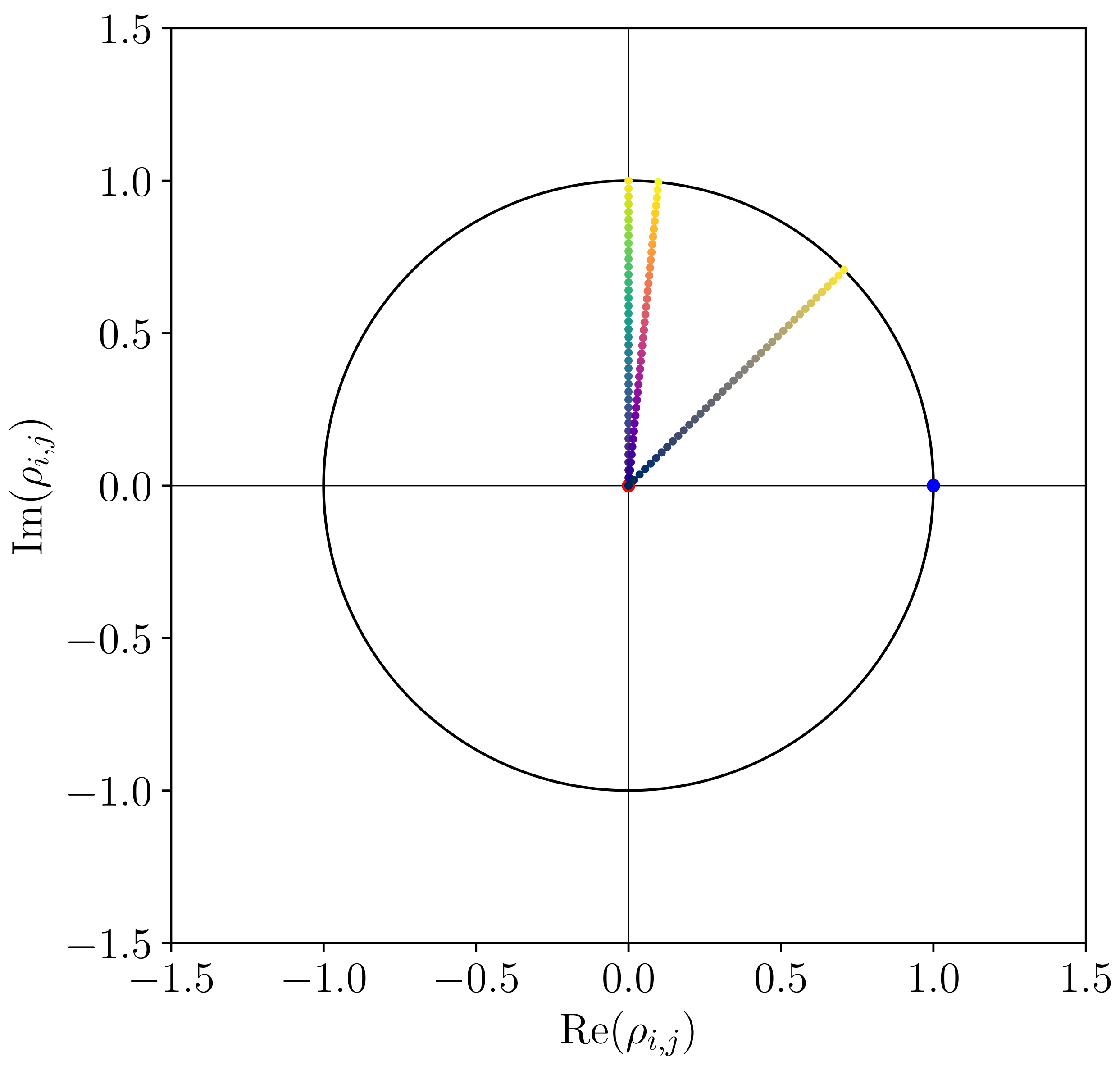
Continuum couplings and entanglement

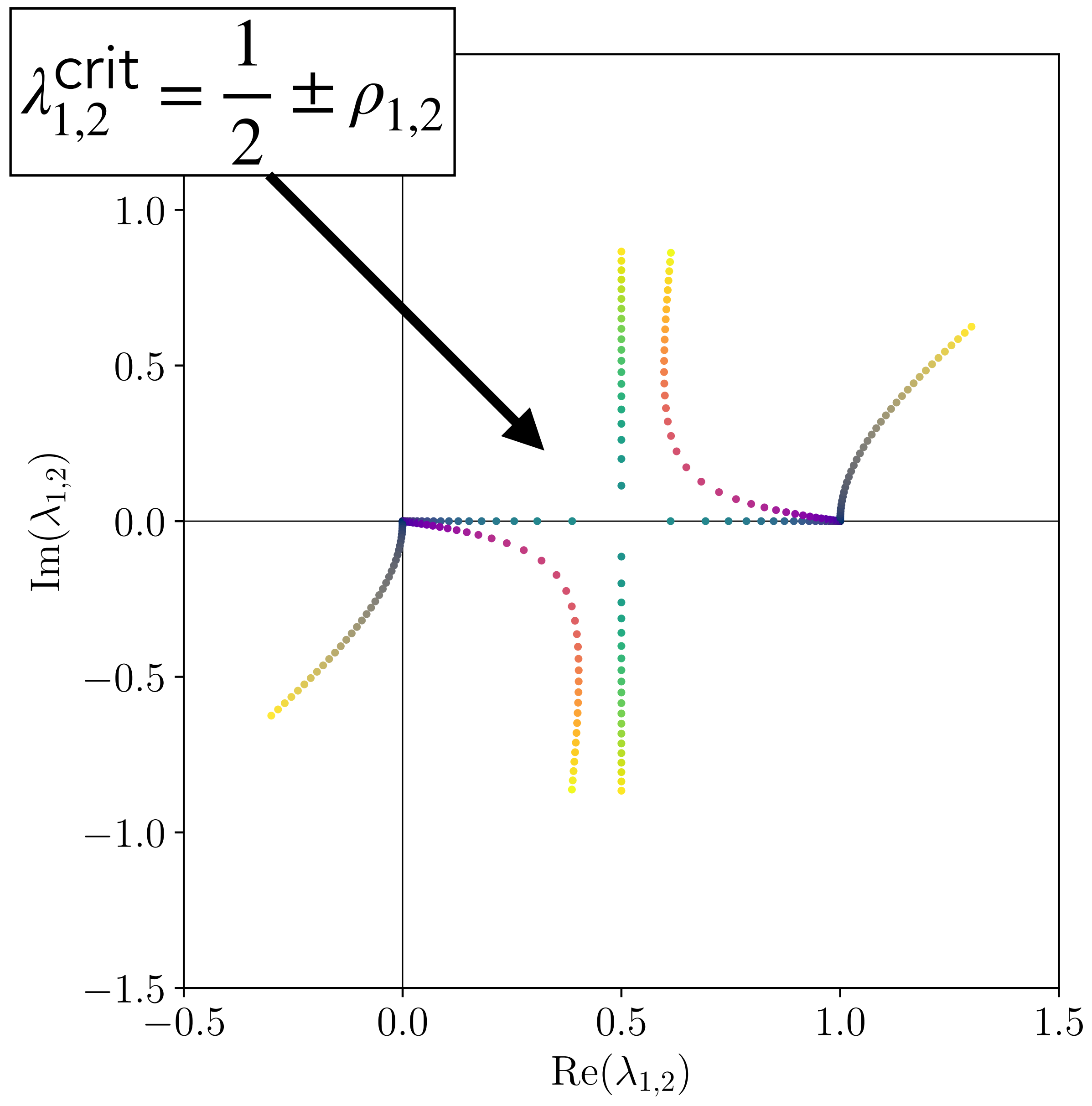
Continuum couplings increase entanglement.

$$\rho = \begin{pmatrix} \rho_{1,1} & \rho_{1,2} \\ \rho_{1,2} & 1-\rho_{1,1} \end{pmatrix} \qquad \mathrm{Tr}(\rho) = 1 \qquad \lambda_{1,2} = \frac{1}{2} \pm \frac{1}{2}\sqrt{(2\rho_{1,1}-1)^2 + 4\rho_{1,2}^2}$$

Making $\rho_{1,2}$ imaginary is akin to increasing continuum couplings.

Fix $\rho_{1,1} = 1$, vary $\rho_{1,2} = |\rho_{1,2}|e^{i\theta}$.



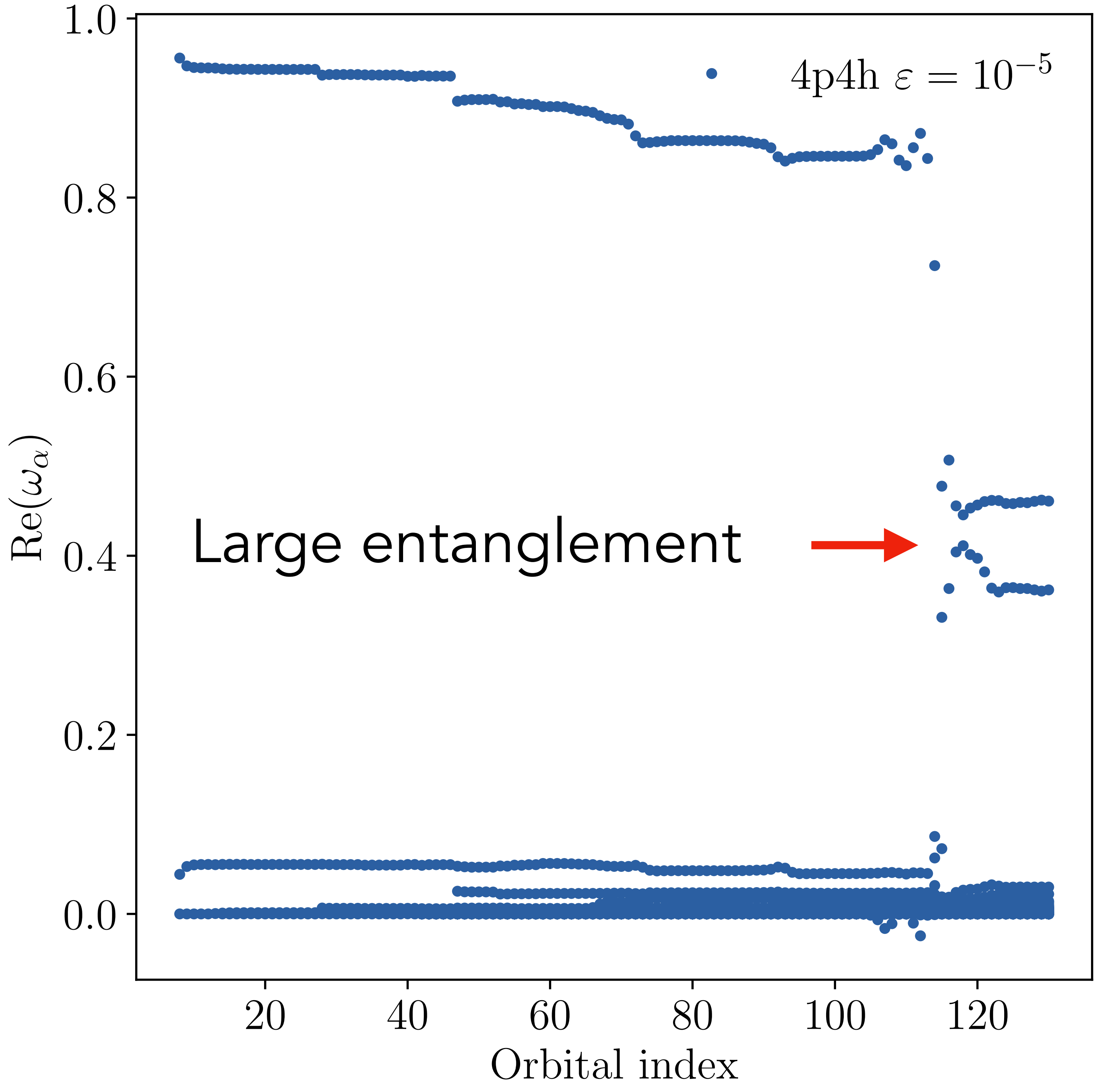


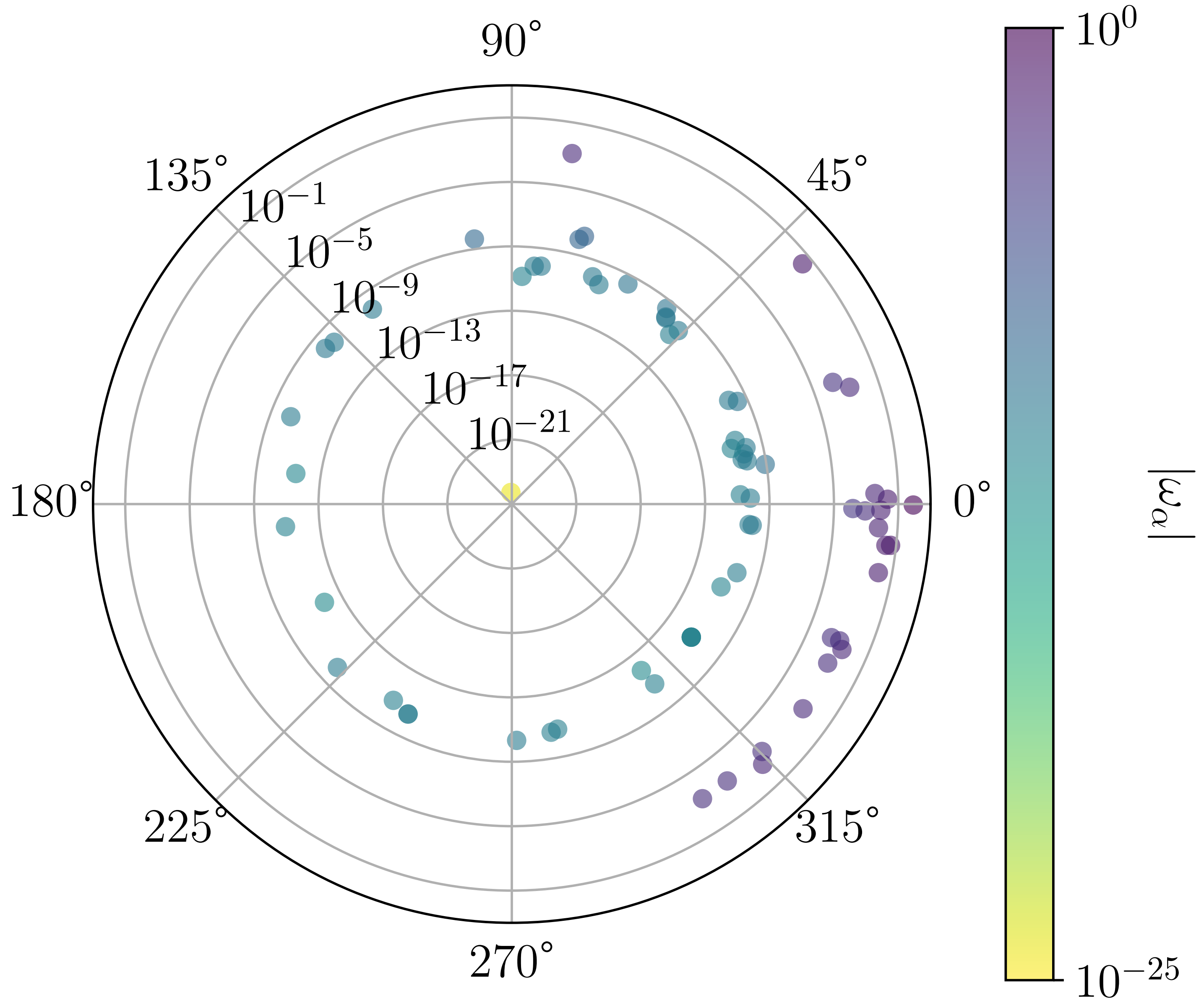
Entanglement saturates at the critical point ($\lambda_{1,2} = 0.5$), then occupations acquire an imaginary part, *i.e.* an uncertainty due to the time-dependent nature of the state.

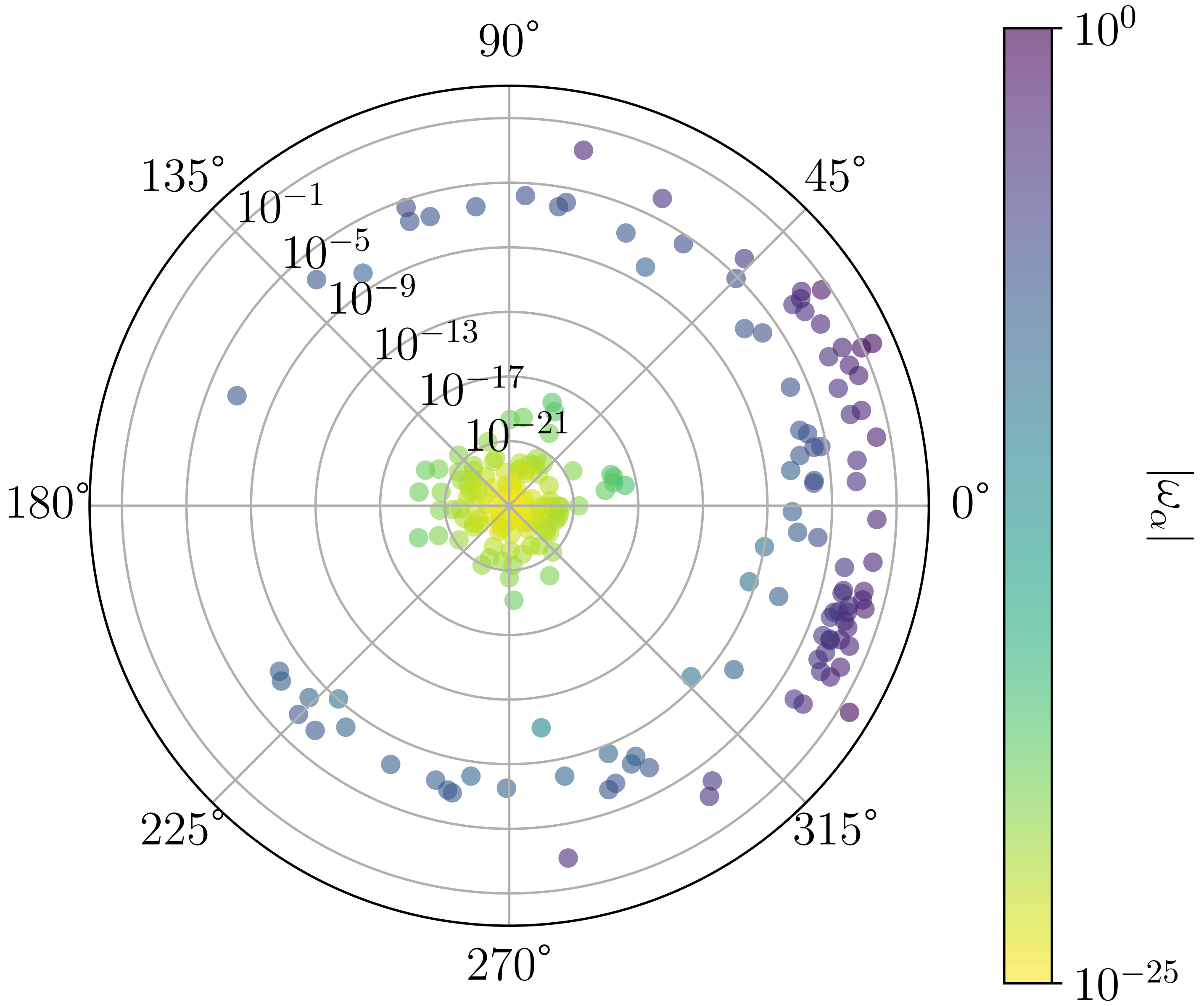
$J^{\pi} = 2^{-}$ neutron resonance in ^{4}H

Broad single-particle resonance. Berggren basis with contour **descending rapidly into 4th quadrant (to illustrate).**

Continuum couplings increase too rapidly. The renormalization fails to optimize the representation.

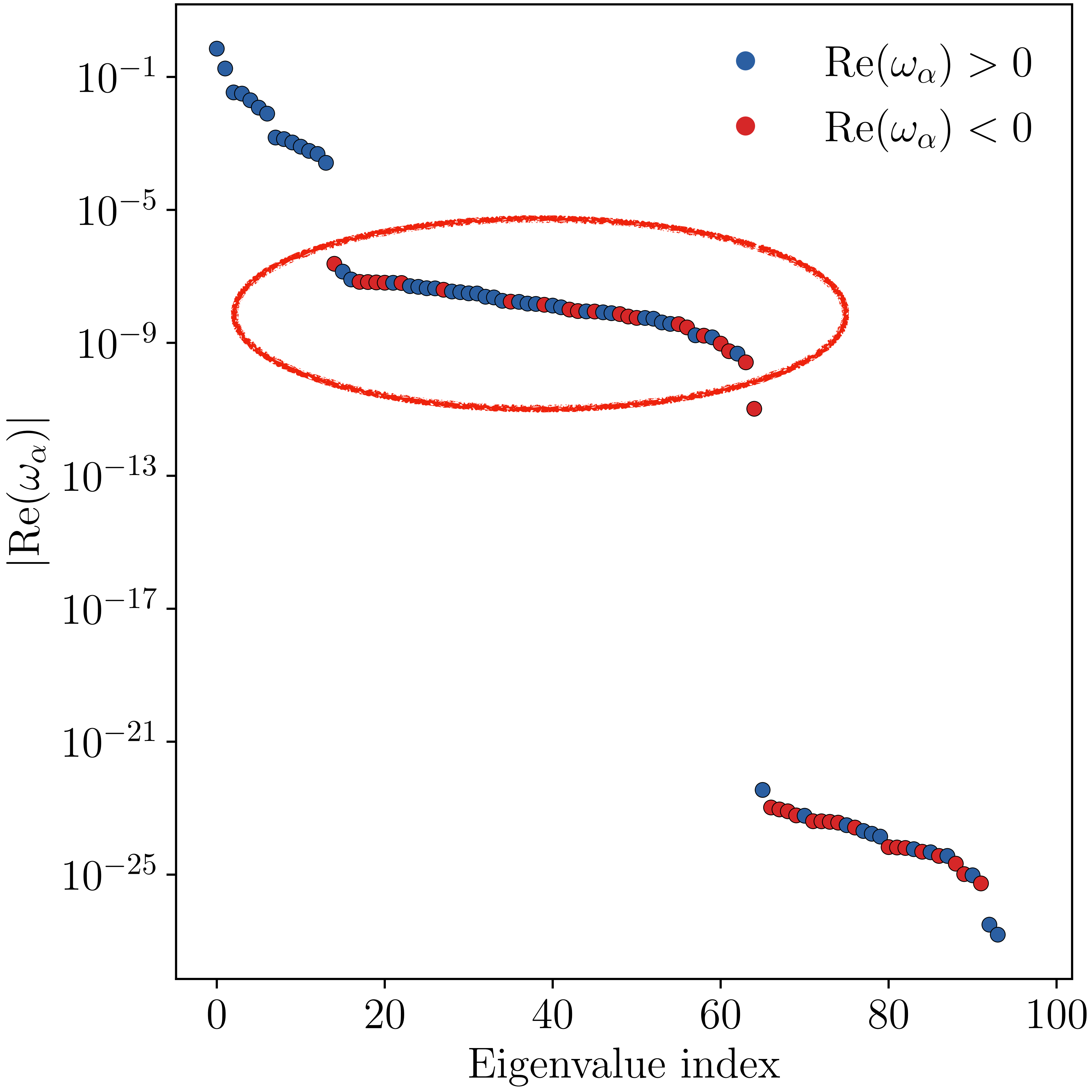






Two equiprobable states translates into nearly degenerate Hamiltonian eigenstates. $|\psi\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm |-\rangle)$

Continuum couplings and entanglement



The magnitude of occupations reveals three groups:

1. Large $|\omega_\alpha|$, near-exponential decrease, configurations dominated by discrete orbitals.

2. Small $|\omega_\alpha|$, plateau, configurations dominated by scattering orbitals.

3. Below numerical accuracy.

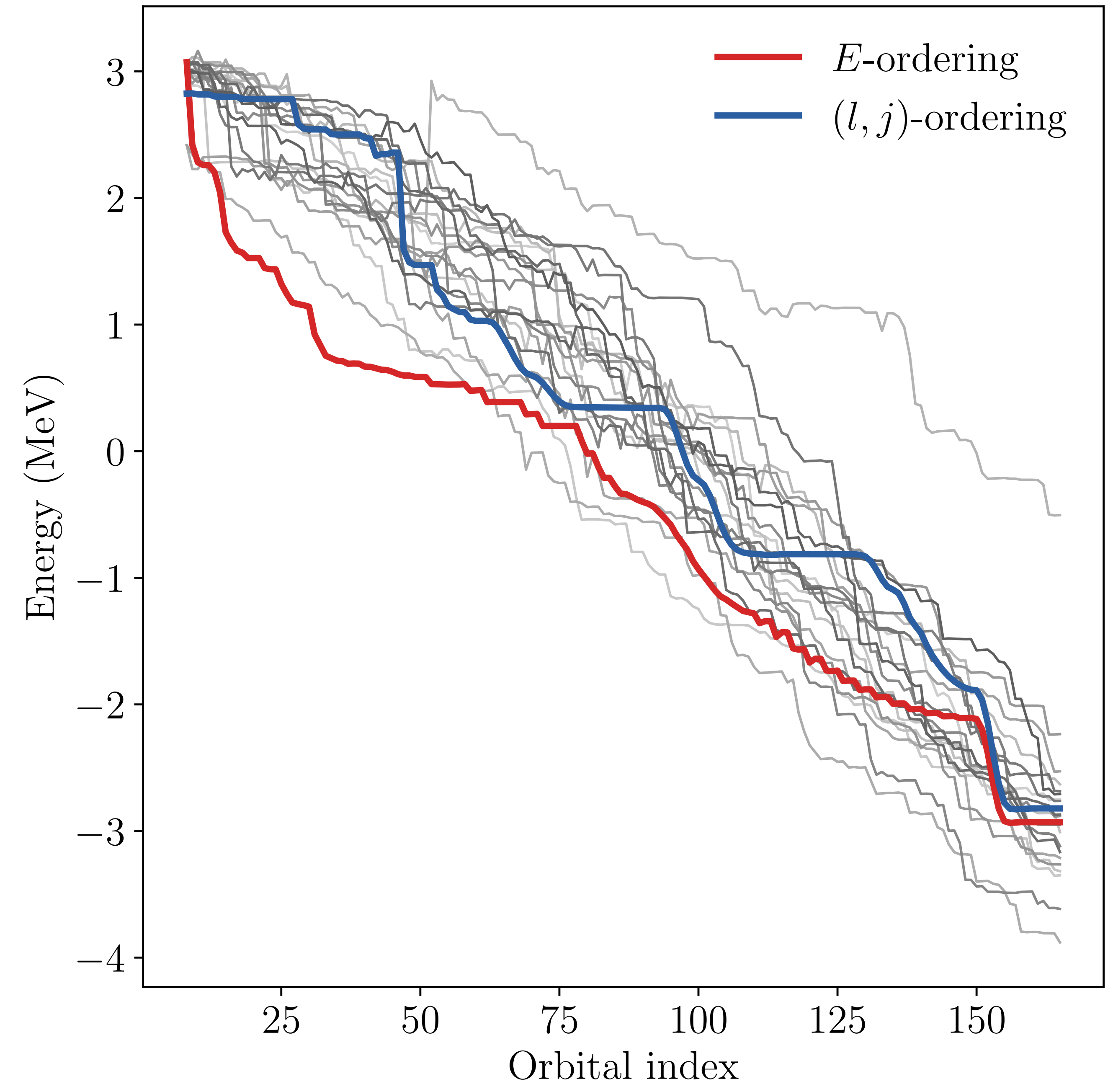
Removing all eigenvalues $|\omega_\alpha| < \kappa$, with $\kappa_{\text{max}} = \varepsilon/10$, stabilizes calculations.

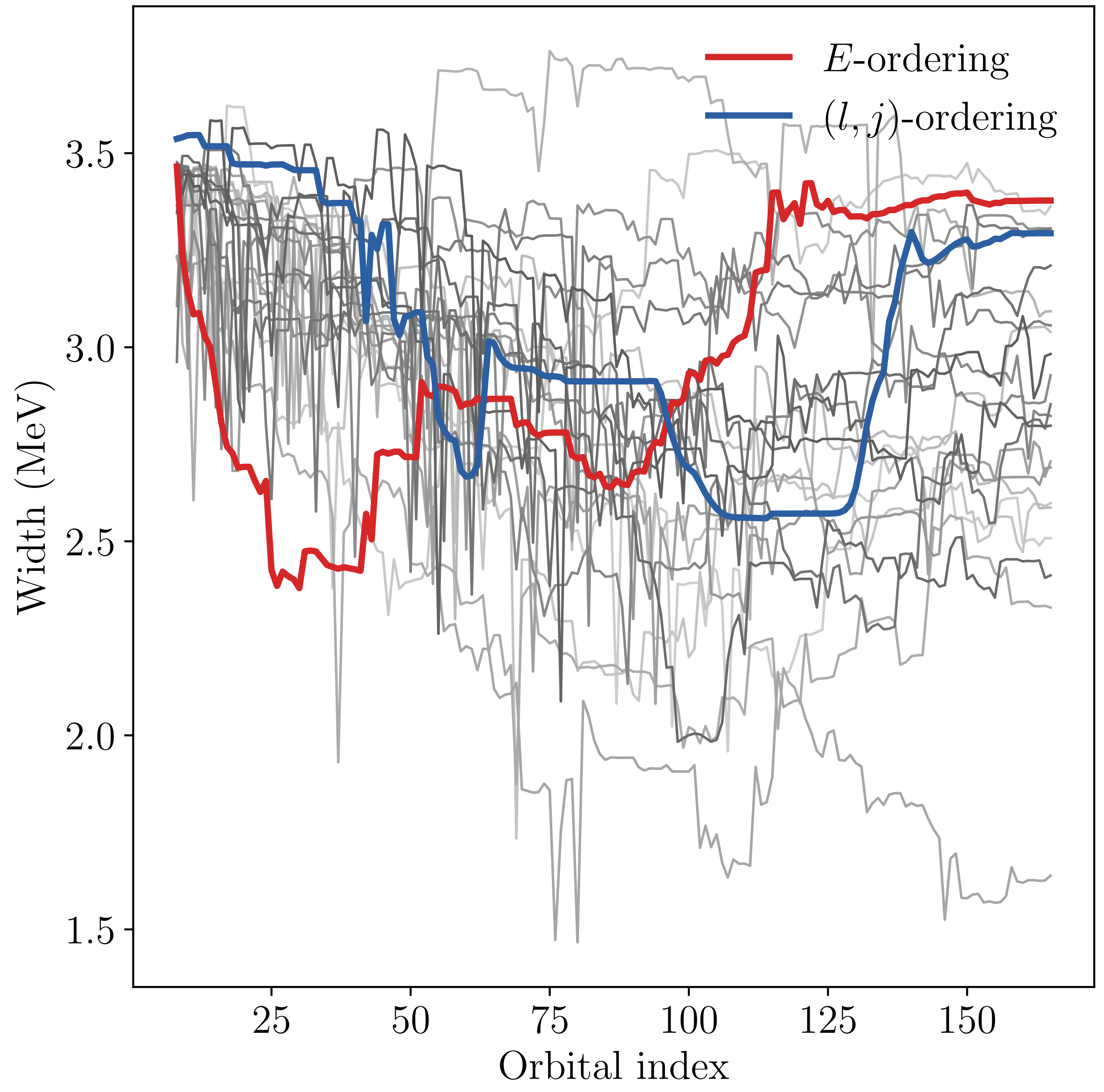
Reductionof entanglement between the system and the environment of scattering states.

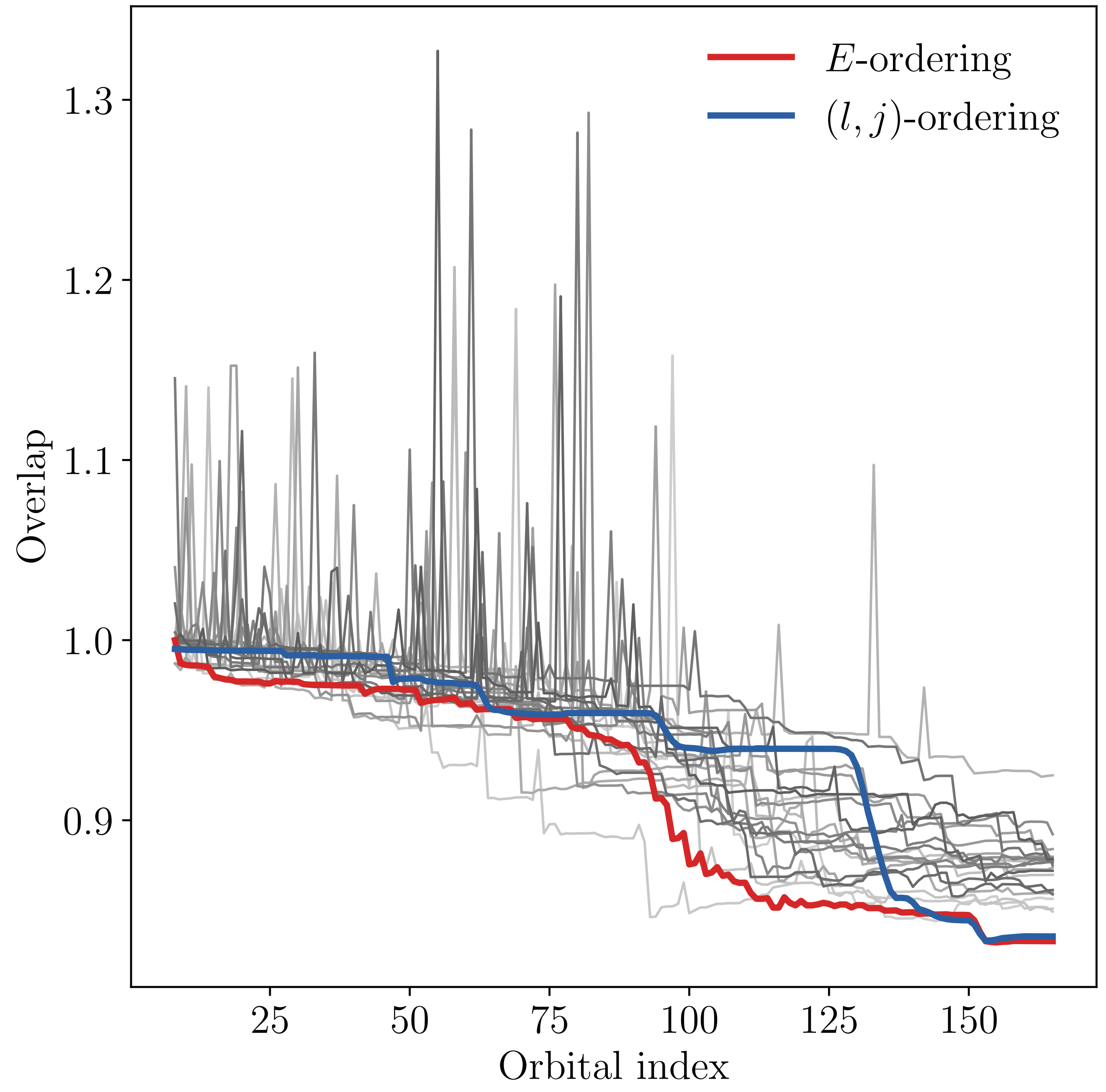
Effect of orbital ordering

The stability of calculations is also affected by how entanglement is constructed.

E-ordering vs. (l, j)-ordering (according to partial waves, separating p/n orbitals).







We found that (l, j)-ordering is more forgiving and stable (builds shell model shells), but E-ordering gives better results and natural orbitals once the basis has been optimized.

Natural orbitals (NAT)

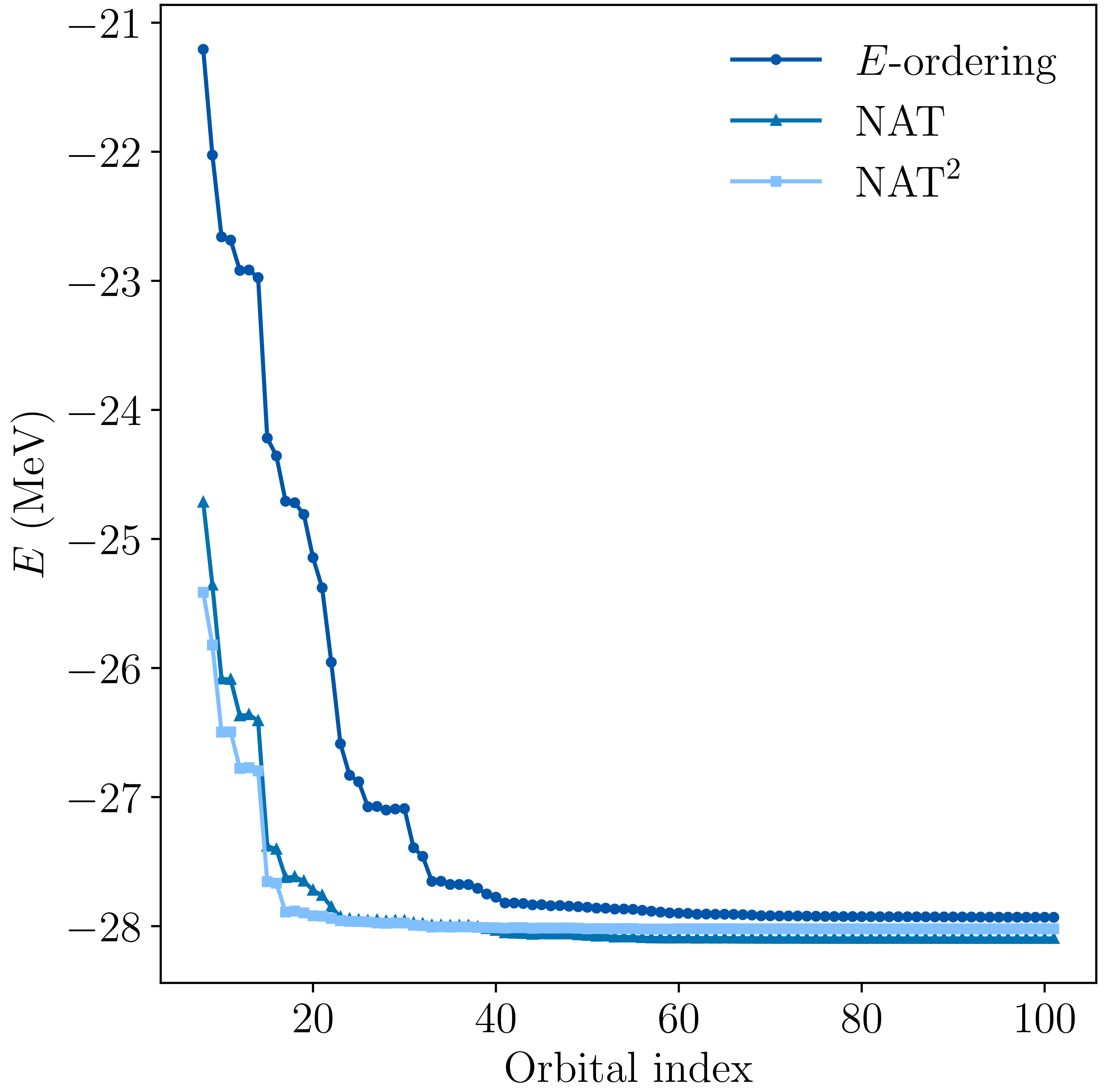
Once a regular calculation in the Berggren basis has been obtained, it is possible to build the natural orbital basis, defined here as the eigenstates of the 1-body density matrix.

$$\hat{\rho}^{(1)} = \sum_{\alpha,\beta} |\alpha\rangle\langle\psi| a_\alpha a^\dagger_\beta |\psi\rangle\langle\beta|$$

At the orbital level, the NAT basis provides a near-optimal representation for the state of interest. However, the NAT basis mostly help converge the inner part of the wave function (energy).

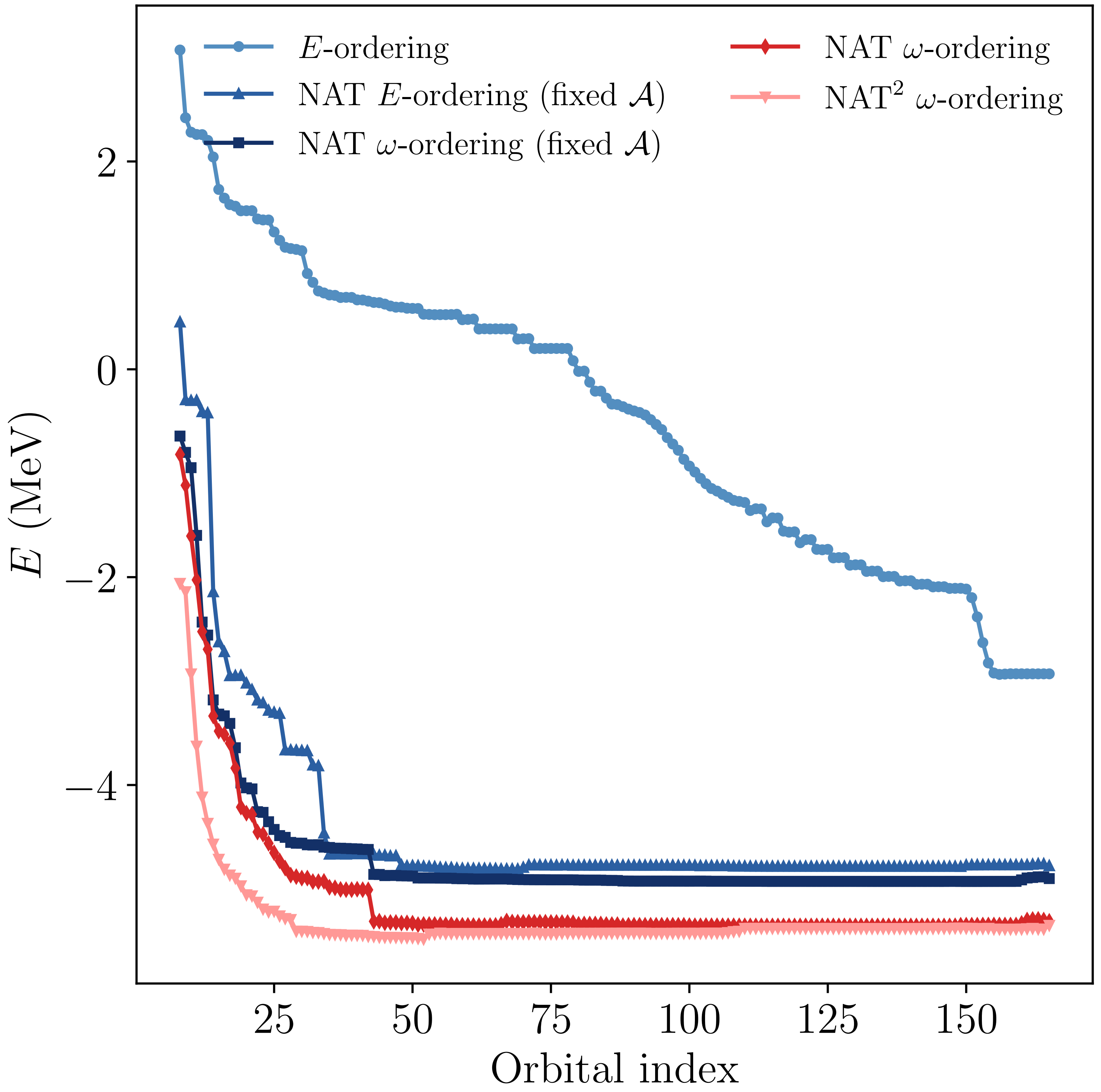
For the g.s. of ^{4}He in the HO basis, the NAT representation provides almost no benefit.

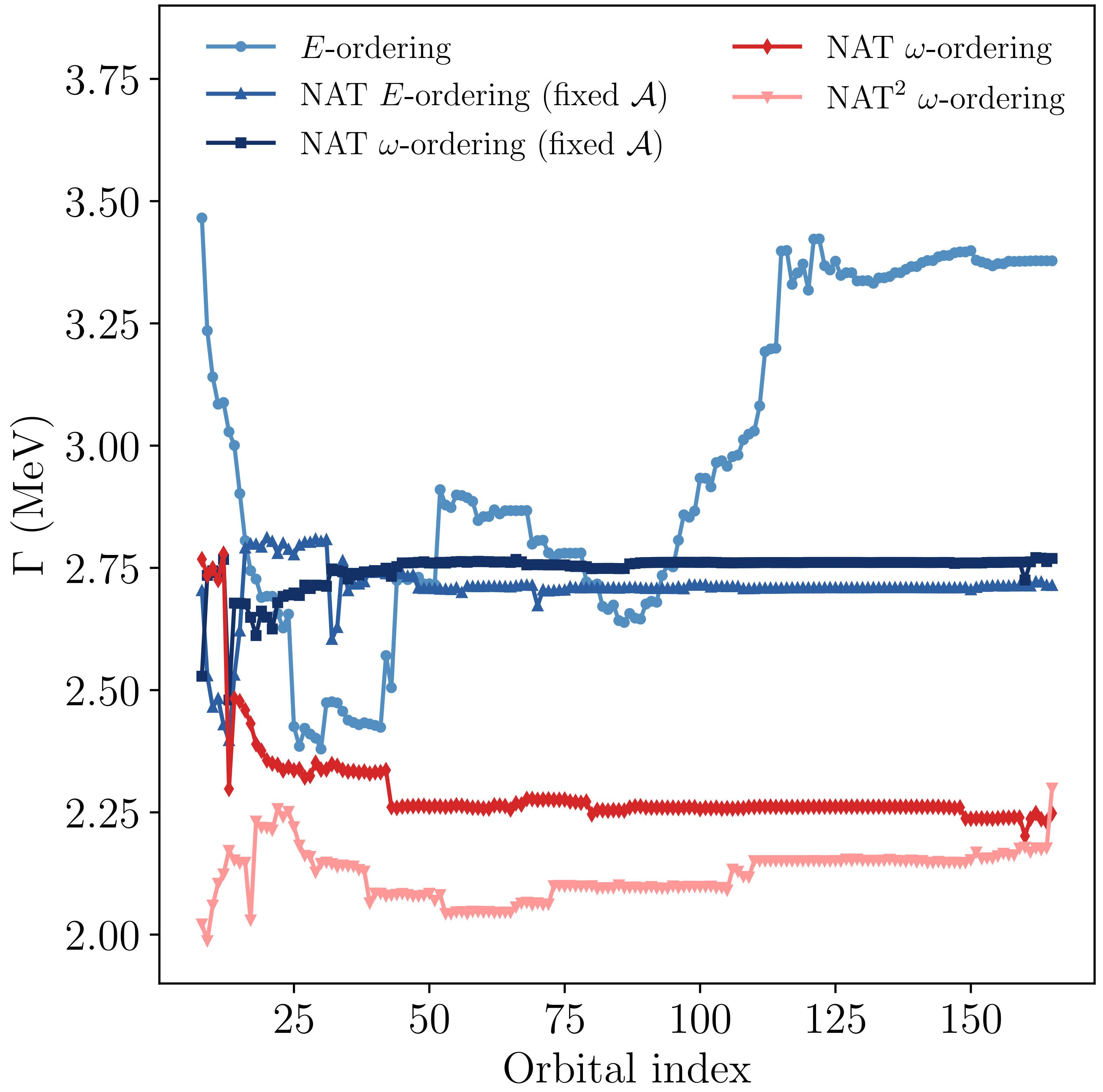
Generating new NAT (NAT^2) from a calculation in the NAT basis has again no effect.



Natural orbitals (NAT) — broad resonance

Generating NAT for the $J^\pi = 2^-$ state of ^{4}H greatly improves convergence, but requires full occupation-ordering (ω-ordering) for optimal result.

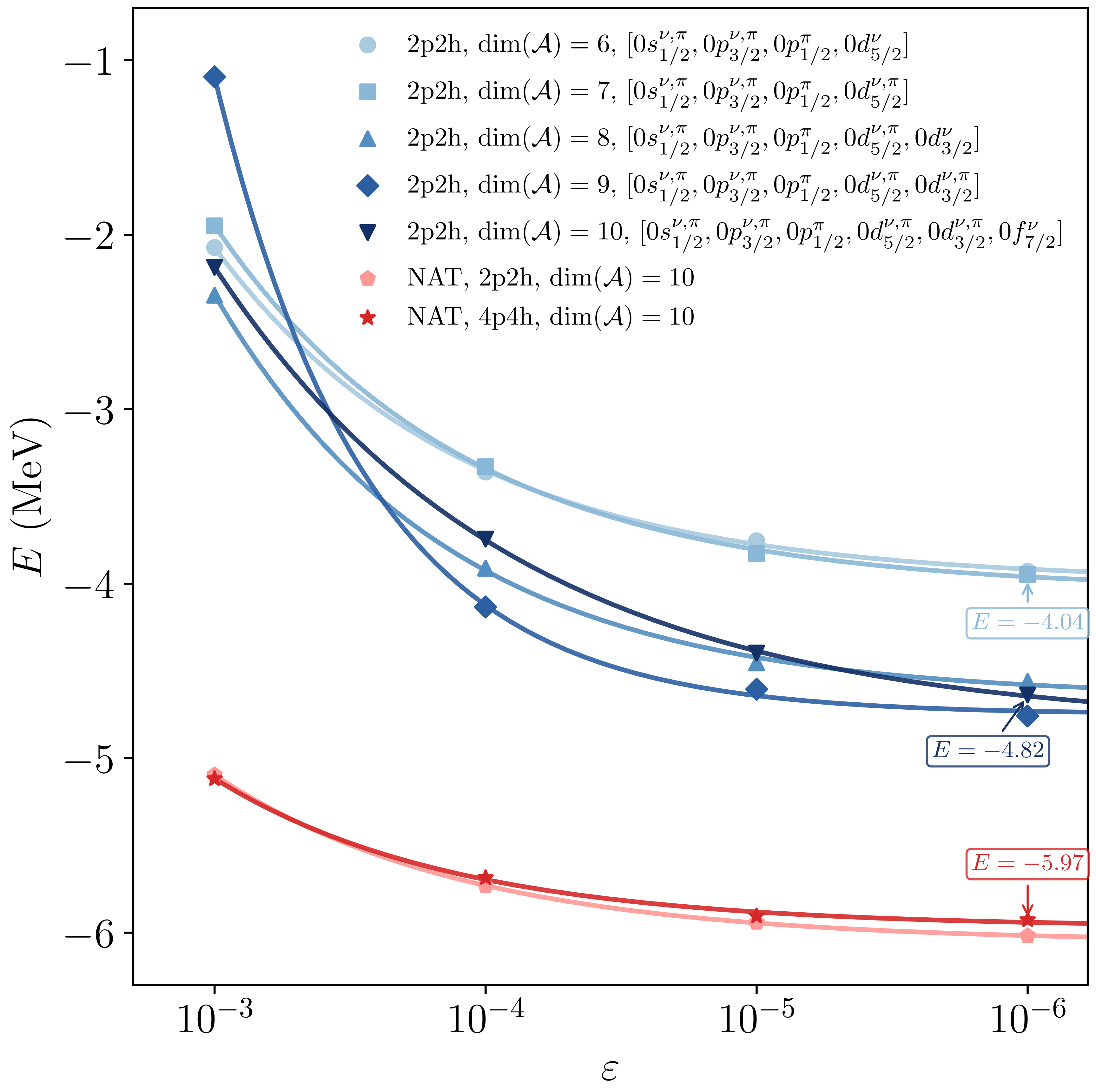


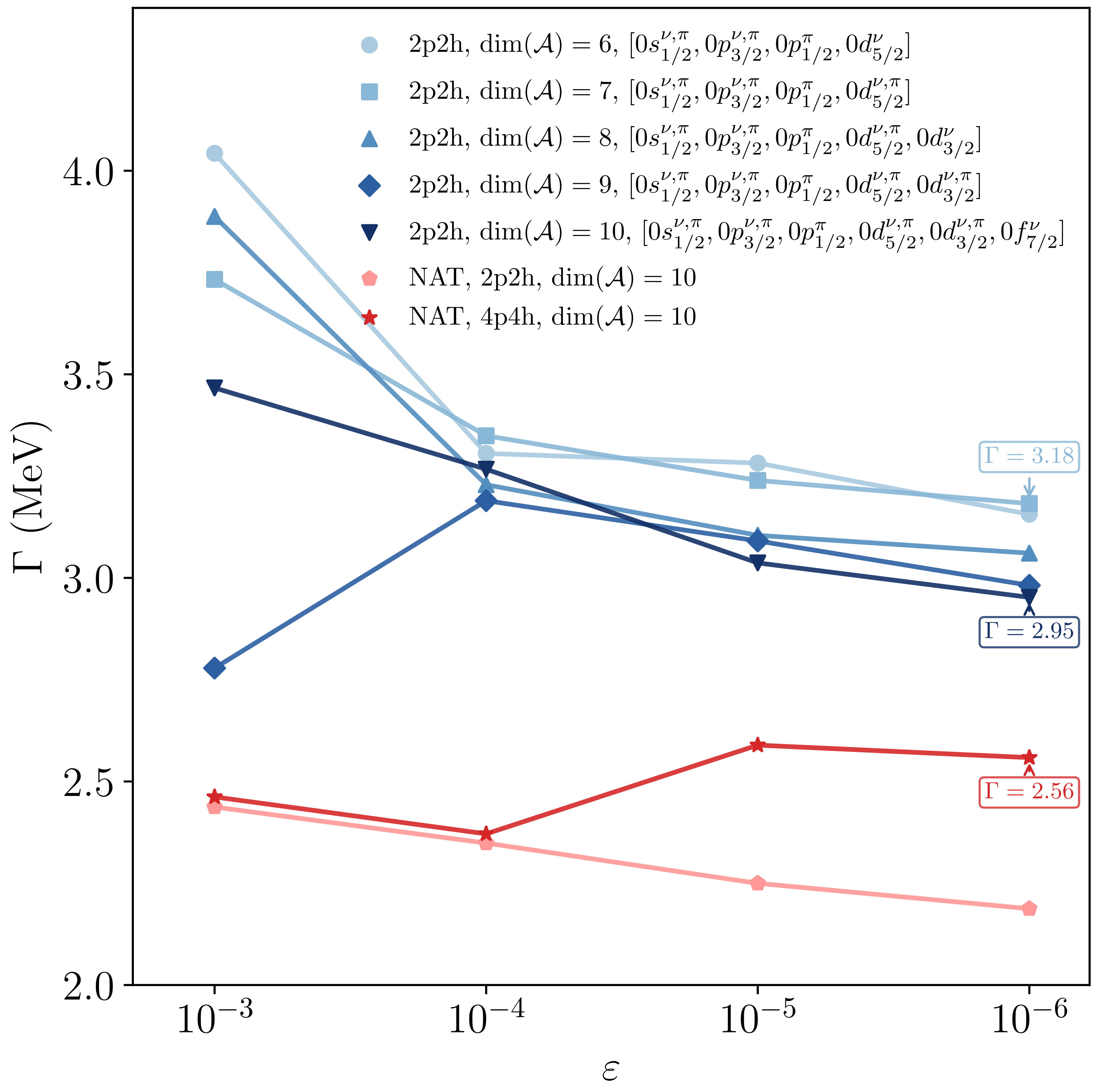


Preliminary results: $J^\pi = 2^-$ state in ^{4}H

Renormalized N2LO$_{\text{opt}}$, $l_{\text{max}} = 5$ with s, p waves in Berggren basis and $N_{\text{max}} = 12$ otherwise.

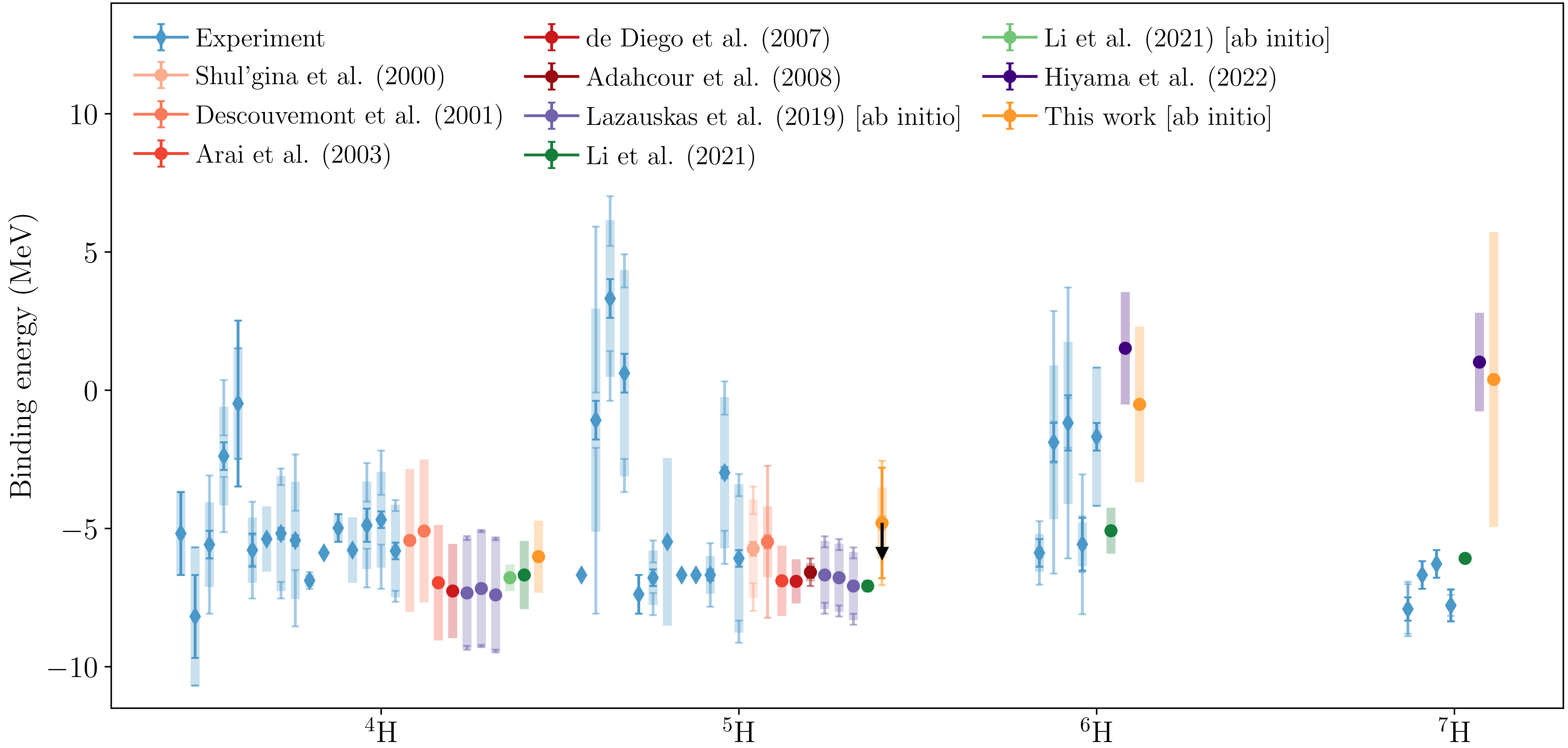
Calculations on only ~130 cores...





Summary (preliminary)

More work is needed to improve convergence but, using *ab initio* theory, we can already **rule out narrow ^{6,7}H g.s.**



We hypothesize that all ^{7}H experiments, based on ^{8}He proton knockout, saw four correlated neutrons.

Thank you for your attention!