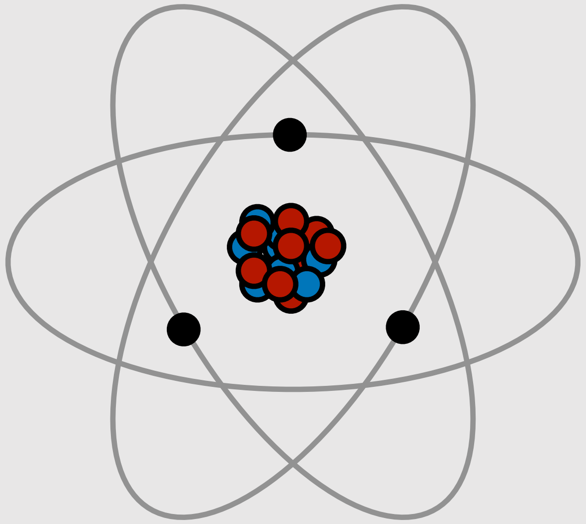
Symmetry reduction of tensor networks in nuclear many-body theory

ESNT workshop

'Automated tools for many-body theory'

June 6th, 2023



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Overview

Part I

Ab initio nuclear structure

State-of-the-art, complexity, role of symmetries, …

Part II

Symmetry reduction

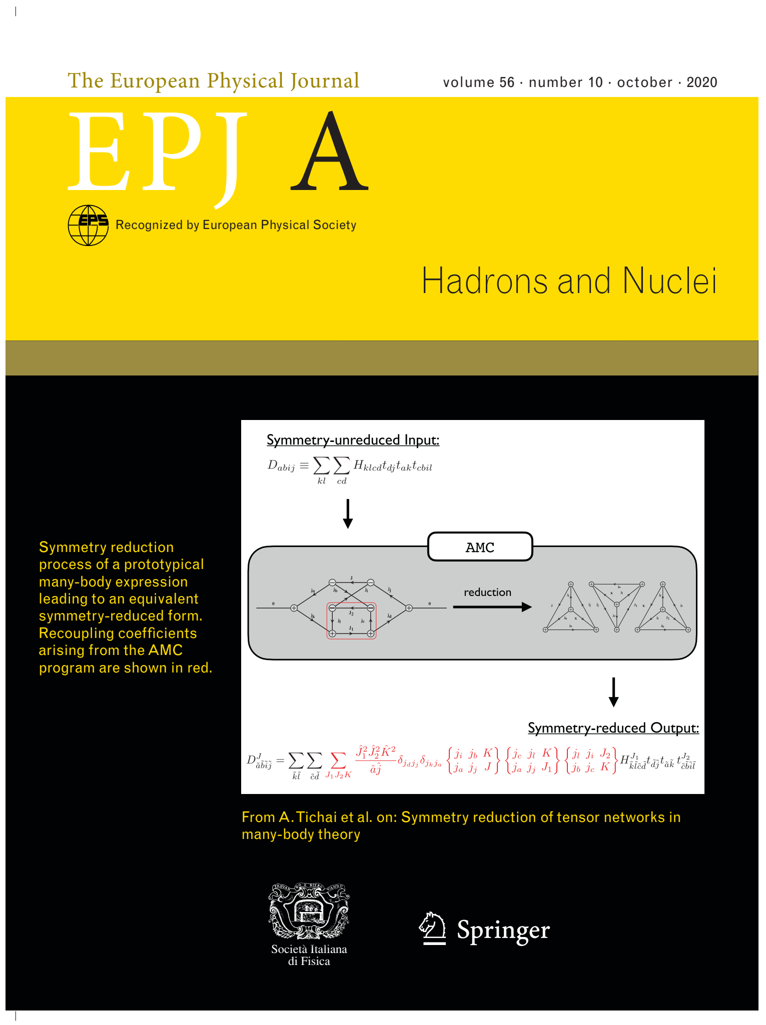
Angular-momentum coupling, Yutsis graphs, …

Part III

The AMC program

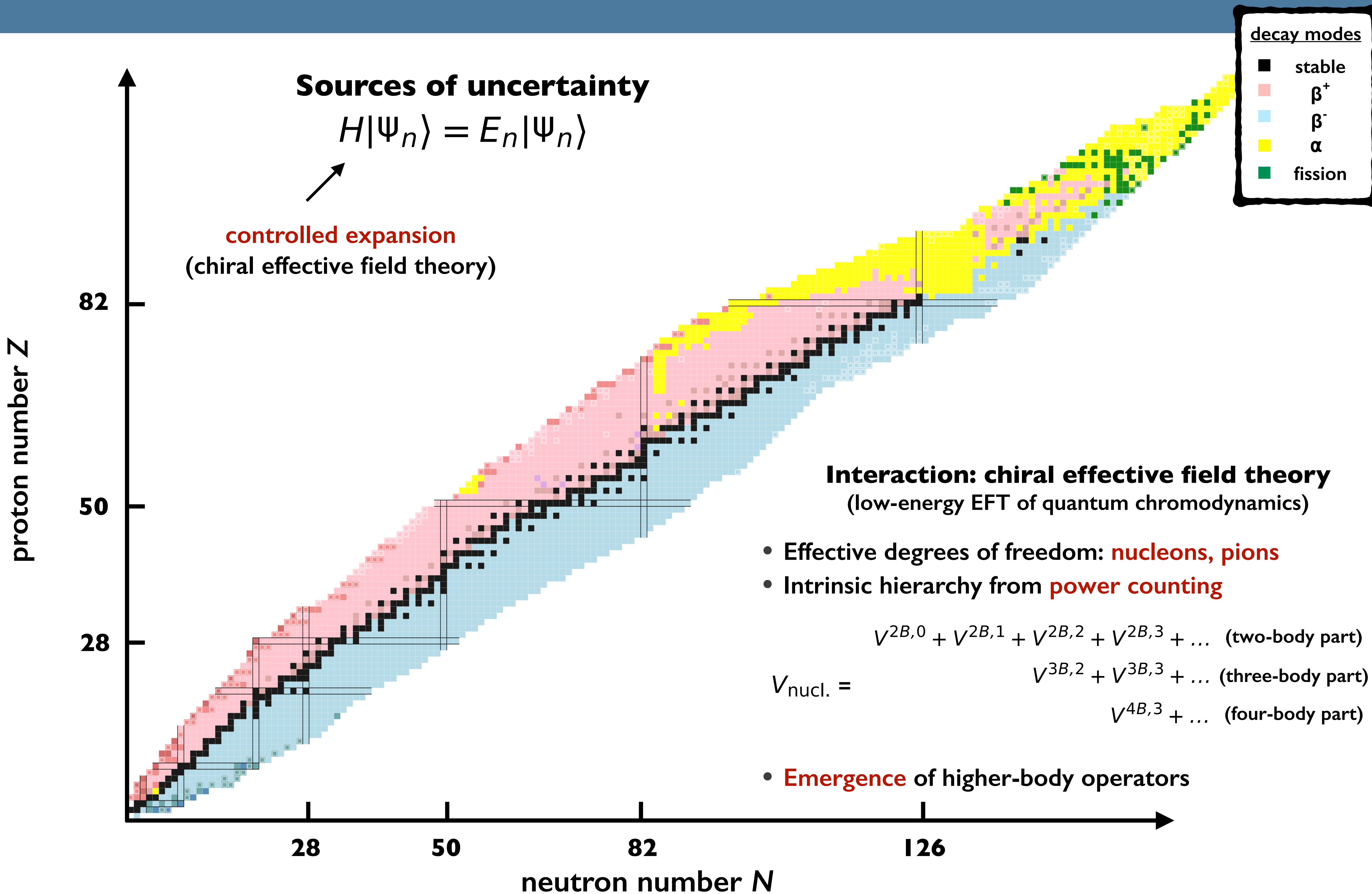
Structure of the program, Usage, Examples, …

Conclusion and outlook



Tichai, Wirth, Ripoche, Duguet
EPJA (2020)

What is ‘*ab initio*’ nuclear structure?



Sources of uncertainty

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

controlled expansion
(chiral effective field theory)

Interaction: chiral effective field theory
(low-energy EFT of quantum chromodynamics)

- Effective degrees of freedom: nucleons, pions
- Intrinsic hierarchy from power counting

$$V_{\text{nucl.}} = \begin{cases} V^{2B,0} + V^{2B,1} + V^{2B,2} + V^{2B,3} + \dots & \text{(two-body part)} \\ V^{3B,2} + V^{3B,3} + \dots & \text{(three-body part)} \\ V^{4B,3} + \dots & \text{(four-body part)} \end{cases}$$

- Emergence of higher-body operators

What is ‘*ab initio*’ nuclear structure?

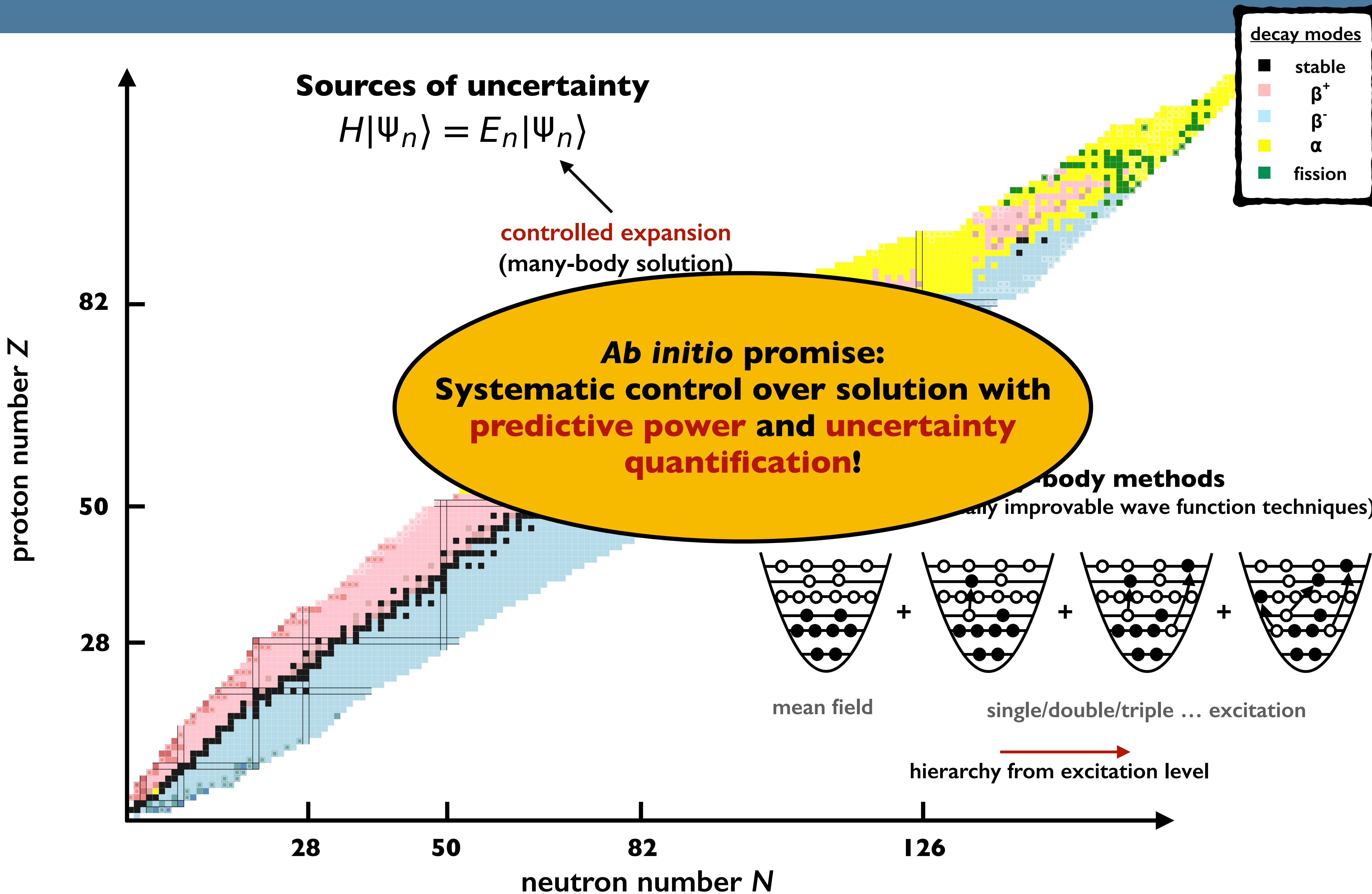
Sources of uncertainty

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

controlled expansion
(many-body solution)

***Ab initio* promise:**
Systematic control over solution with predictive power and uncertainty quantification!

-body methods
ally improvable wave function techniques)

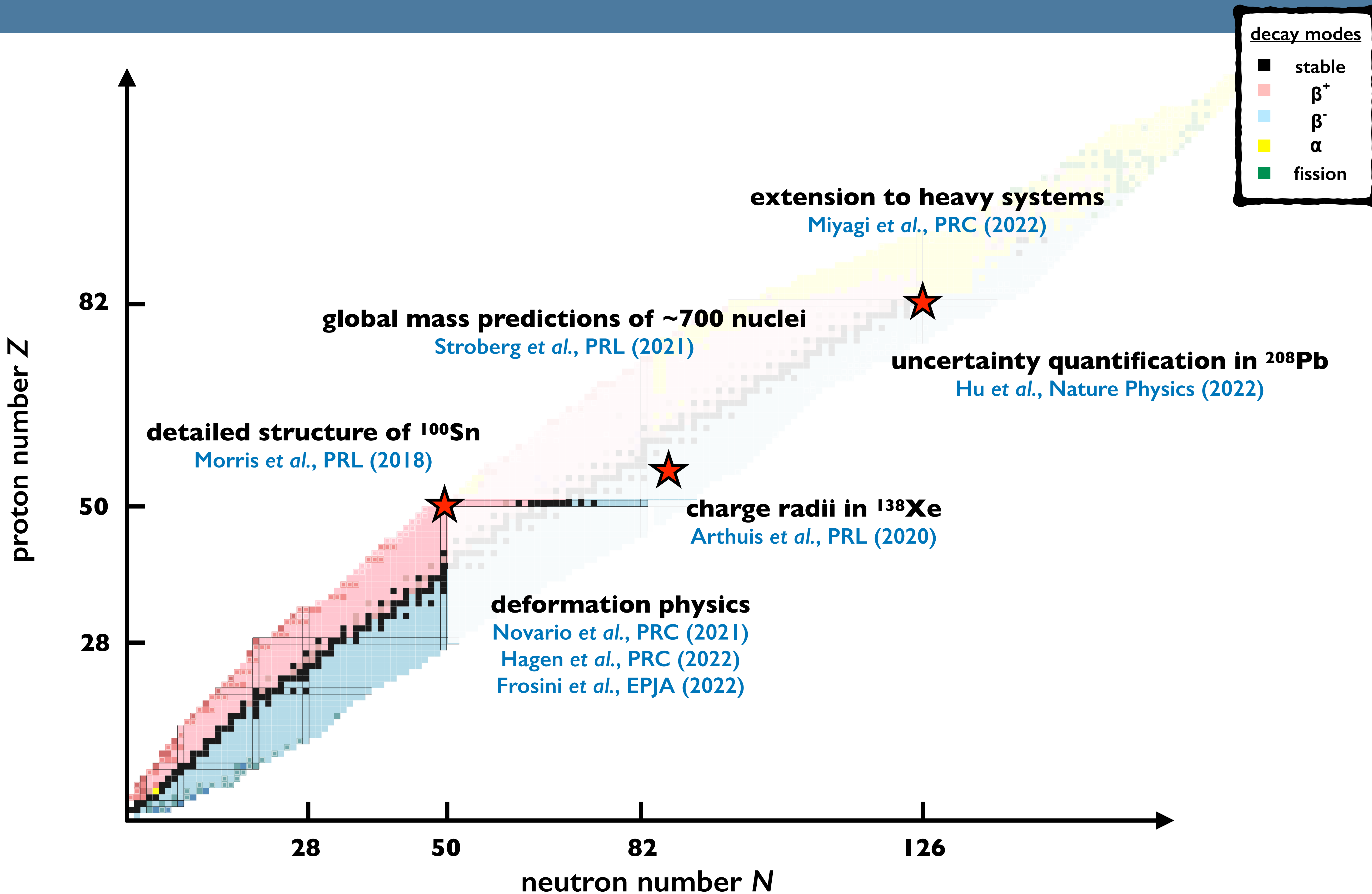


mean field

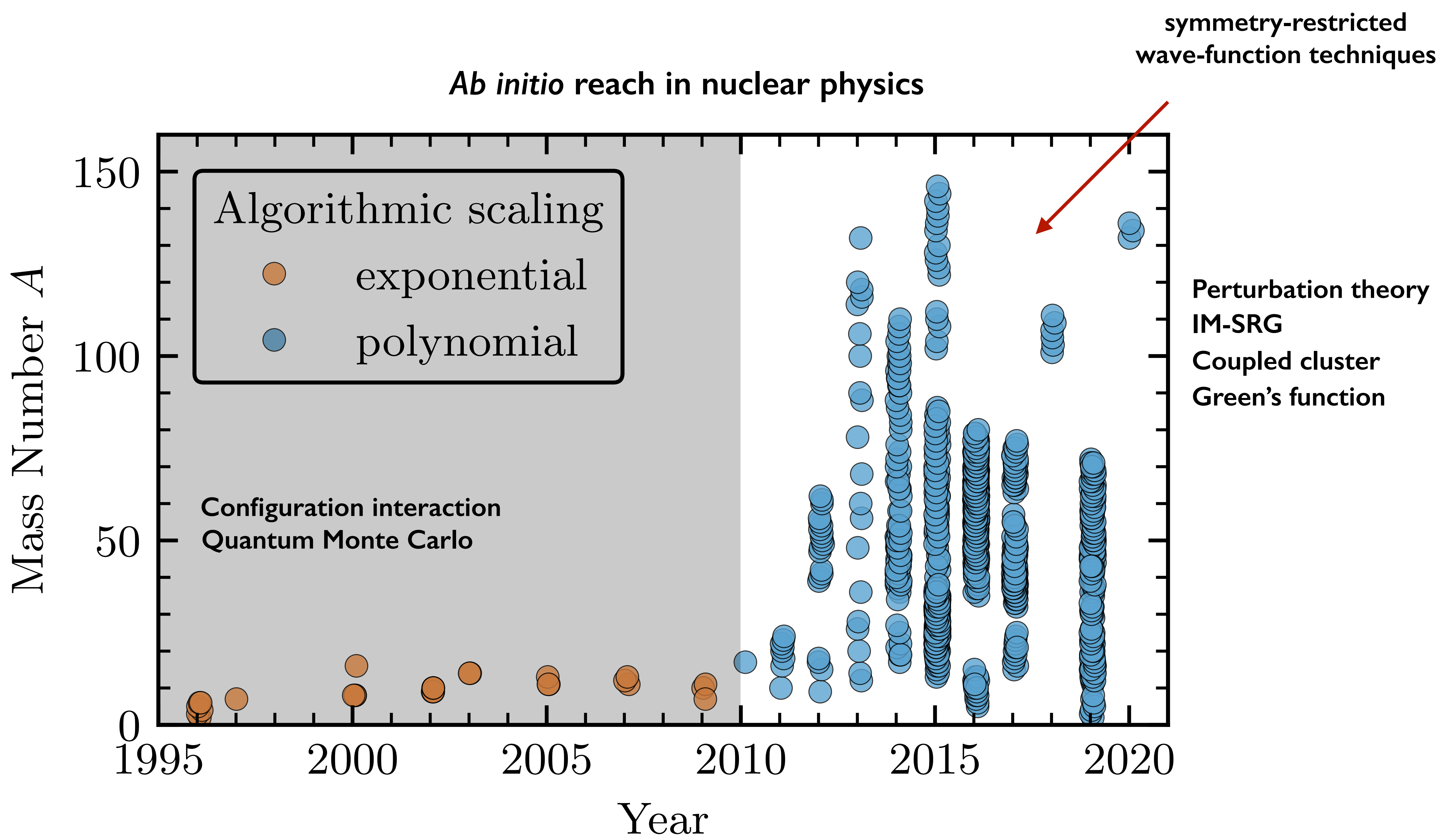
single/double/triple … excitation

hierarchy from excitation level

Ab initio today!

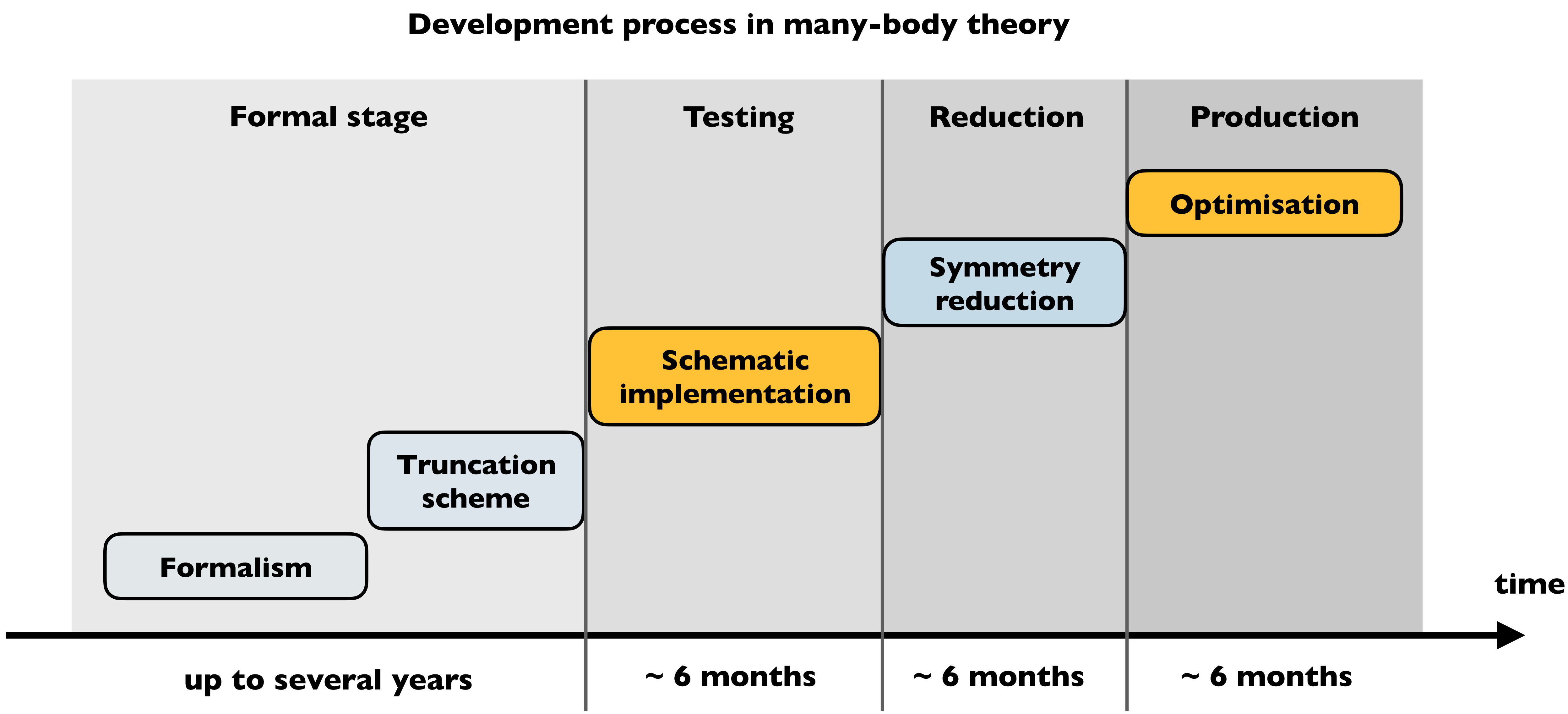


Scaling, Complexity and Symmetries



Drischler, Bogner, Few-Body Systems (2021)

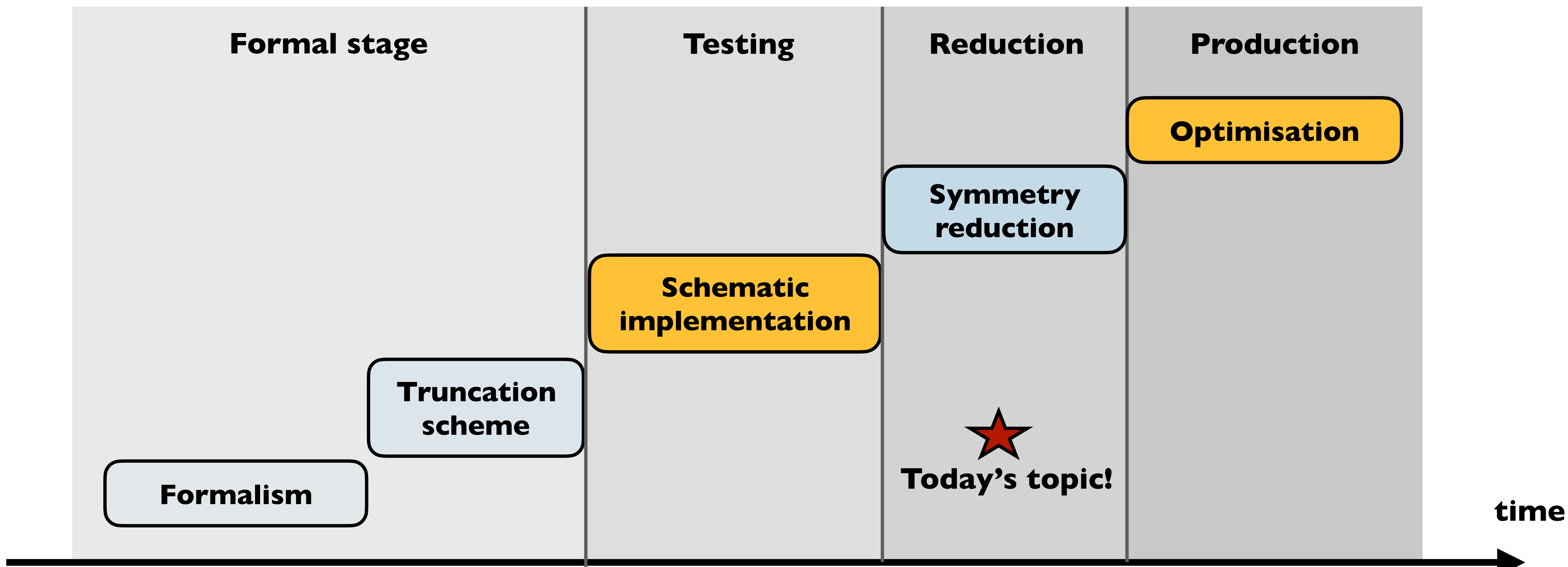
How to get a production code



Testing of (potentially great) ideas can easily take 2 years of work!

How to get a production code

Development process in many-body theory



ADG
'Automatic Diagram Generator'

Arthuis *et al.*, CPC (2019/2020)
Tichai *et al.*, EPJA (2022)

AMC
'Angular-Momentum Coupling'

Tichai et al., EPJA (2020)

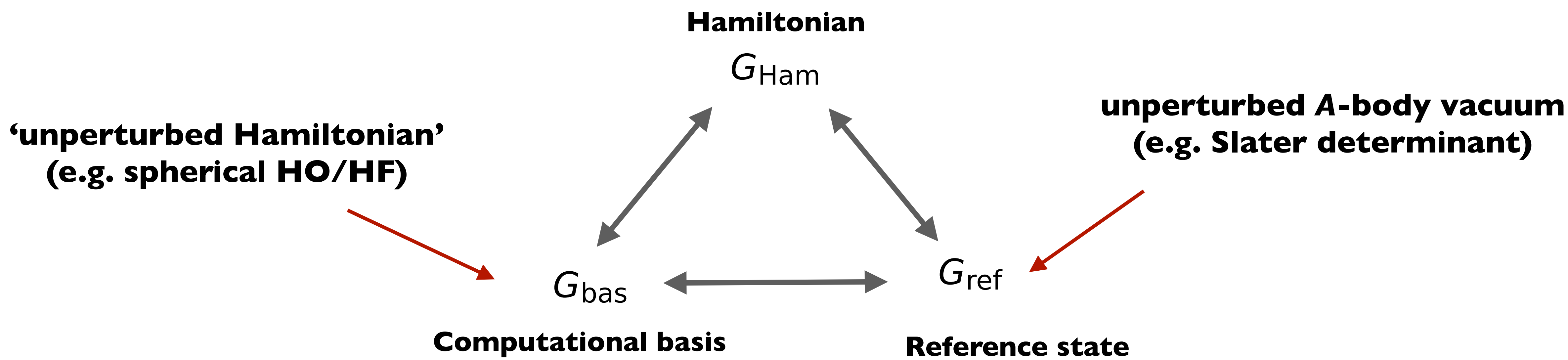
⟶ **see talk by P. Arthuis!**

Interplay of symmetries

- Symmetries encode fundamental invariances of a (quantum) system
- Encoded via linear representations of symmetry groups (*SU(2), U(1), Z₂*, …)

$$[H, U(g)] = 0 \quad (\forall g \in G)$$

- Symmetry groups affect many-body treatment at various stages of the formalism



- Simplifications can be done in the case where a common symmetry group exists

$$G_{\text{sym}} = G_{\text{Ham}} = G_{\text{bas}} = G_{\text{ref}}$$

What is a symmetry reduction?

- Starting point: formulation using symmetry-unrestricted tensor network (SU-TN)

symmetry-unrestricted tensors (SU-T's)

$$R_{abij} = \ldots + \sum_{kl}\sum_{cd} H_{klcd} t_{dj} t_{ak} t_{cbil} + \ldots$$

(CCSD residual)

external indices

internal summations (contractions)

holes: *i,j,k,l,…*
particles: *a,b,c,d,…*

- Reduction mediated by transformation generating symmetry-restricted tensors (SR-T)

$$T_{k_1\ldots k_n} \xrightarrow{f_{G_\text{sym}}} \tilde{T}^{\lambda}_{\tilde{k}_1\ldots\tilde{k}_n} \qquad \sum_{k} A_{\ldots k\ldots} B_{\ldots k\ldots} C_{\ldots k\ldots} \xrightarrow{f_{G_\text{sym}}} \sum_{\lambda\tilde{k}} \tilde{A}^{\lambda}_{\ldots\tilde{k}\ldots} \tilde{B}^{\lambda}_{\ldots\tilde{k}\ldots} \tilde{C}^{\lambda}_{\ldots\tilde{k}\ldots}$$

- Computational requirements are reduced by (up to) several orders of magnitudes

- Many-body objects are manifestly invariant with respect to symmetry properties

Symmetries numerically enforced!

Symmetries of nuclear matrix elements

- Treatment/processing of symmetries of matrix elements crucial

$$\frac{1}{4}\sum_{pqrs} v_{pqrs} c^\dagger_p c^\dagger_q c_s c_r$$

- Parity conservation linked to discrete group Z_2

$$[H, \Pi] = 0 \qquad \ldots \text{mod}2 = l_r + l_s \ \text{mod}2$$

- Isospin conservatio… strong interaction!)

$$[H, T_z] \ldots = m_{t_r} + m_{t_s}$$

Size of symmetry group dictates possible computational gains!

- Angular-momentum projection conservation linked to abelian U(1)

$$[H, J_z] = 0 \qquad m_{j_p} + m_{j_q} = m_{j_r} + m_{j_s}$$

- Rotational invariance linked to non-abelian SU(2) symmetry

$$[H, J^2] = 0$$

Angular-momentum coupling

- *SU(2)* symmetry encodes rotational invariance of quantum objects

$$|k\rangle = |n_k l_k j_k t_k m_k\rangle = |\tilde{k} m_k\rangle$$

- Definition of angular-momentum-coupled states from symmetry transformation

$$|k_1\rangle \otimes |k_2\rangle \xrightarrow{f_{SU(2)}} |\tilde{k}_1 \tilde{k}_2 (J)\rangle \equiv \sum_{m_{k_1} m_{k_2}} \left(\begin{matrix} j_{k_1} & j_{k_2} \\ m_{k_1} & m_{k_2} \end{matrix} \middle| \begin{matrix} J \\ M \end{matrix} \right) |k_1 k_2\rangle$$

Clebsch-Gordan coeff. (CGC)

- Symmetry-restricted tensors: angular-momentum-coupled matrix elements

$$\tilde{O}^J_{\tilde{k}_1 \tilde{k}_2 \tilde{k}_3 \tilde{k}_4} = \sum_{m_{k_1} \dots m_{k_4}} \bar{o}_{k_1 k_2 k_3 k_4} \left(\begin{matrix} j_{k_1} & j_{k_2} \\ m_{k_1} & m_{k_2} \end{matrix} \middle| \begin{matrix} J \\ M \end{matrix} \right) \left(\begin{matrix} j_{k_3} & j_{k_4} \\ m_{k_3} & m_{k_4} \end{matrix} \middle| \begin{matrix} J \\ M \end{matrix} \right)$$

- *SU(2)*-irreducible tensor operators can be processed via Wigner-Eckart theorem

$$\langle \xi_1 j_1 m_1 | T^J_M | \xi_2 j_2 m_2 \rangle = (-1)^{2J} \frac{1}{\hat{j}_1} \left(\begin{matrix} j_2 & J \\ m_2 & M \end{matrix} \middle| \begin{matrix} j_1 \\ m_1 \end{matrix} \right) (\xi_1 j_1 | \mathbf{T}^J | \xi_2 j_2)$$

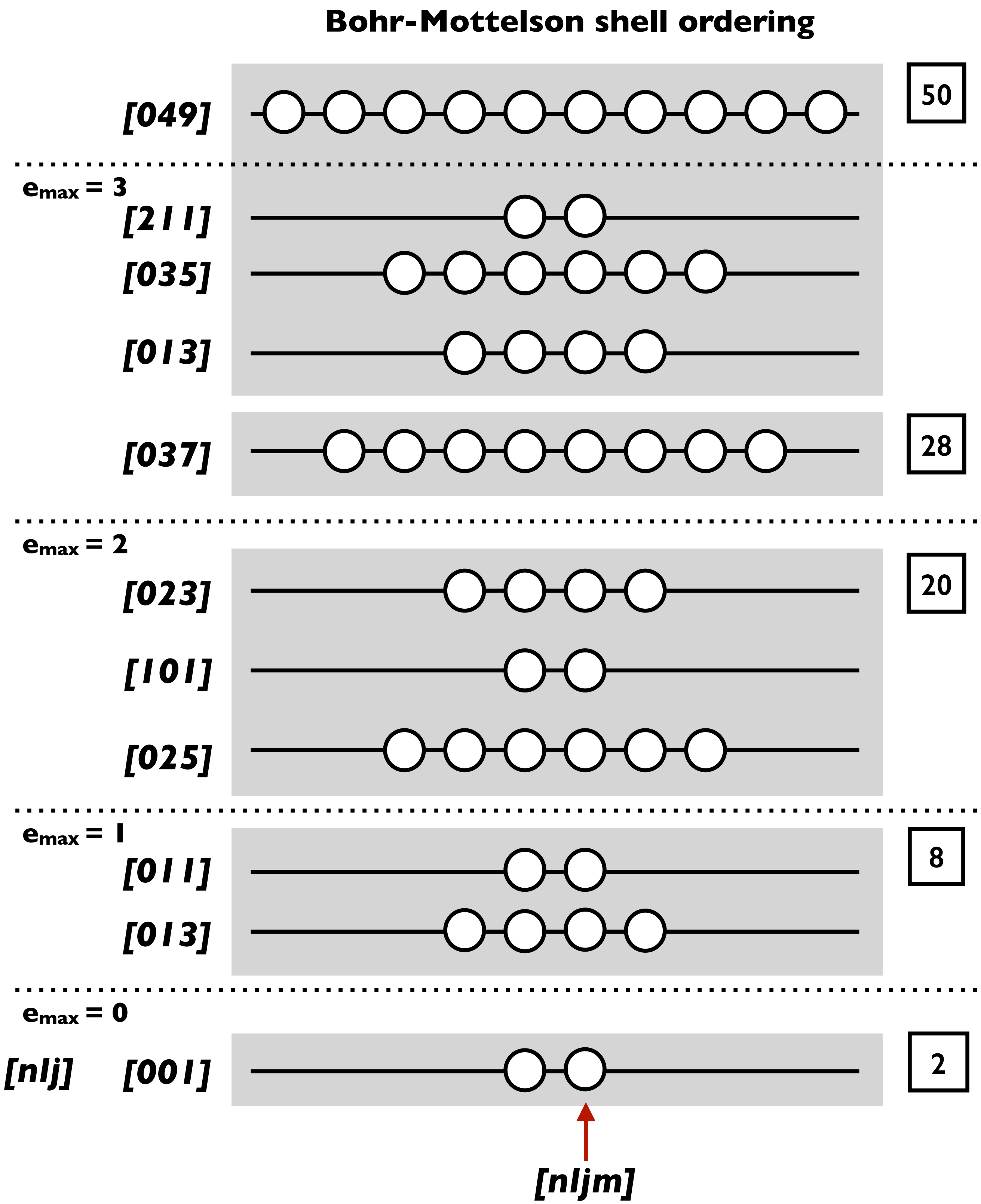
'geometry' *'physics'*

Why is it such a big deal?

- Symmetry: degenerate s.p. energies
- Substates *[nljm]* correspond to the same physics but different geometry
- Goal: sum over orbits *[nlj]* instead of individual substates *[nljm]*

e_{max}	#[nlj]	#[nljm]	ratio	$(ratio)^{-6}$
2	40	12	0.3	~1300
4	140	30	0.214	~10400
6	336	56	0.166	~48000
8	660	90	0.136	$1.6 \cdot 10^5$
10	1140	132	0.116	$4.1 \cdot 10^5$
12	1820	182	0.1	10^6
14	2740	240	0.088	$2.1 \cdot 10^6$

$$e = 2n + l \leq e_{max}$$



A peek behind the curtain

- Angular-momentum coupling leverages use of non-perturbative frameworks
  (Green's functions, coupled cluster, IMSRG, …)

- Formal expression for coupled-cluster amplitude equations look like this …

$$R_{abij} = \ldots + \sum_{kl} \sum_{cd} H_{klcd} t_{dj} t_{ak} t_{cbil} + \ldots$$

- … but what is contained in large-scale codes looks like this!

multiplicity labels

$$R^{J}_{\tilde{a}\tilde{b}\tilde{i}\tilde{j}} = \ldots + \sum_{J_1 J_2 K} \frac{\hat{J}_1^2 \hat{J}_2^2 \hat{K}^2}{\hat{j}_a \hat{j}_j} \sum_{\tilde{k}\tilde{l}\tilde{c}\tilde{d}} \delta_{j_d j_j} \delta_{j_k j_a} H^{J_1}_{\tilde{k}\tilde{l}\tilde{c}\tilde{d}} (\tilde{d}|\mathbf{T_1}|\tilde{j})(\tilde{a}|\mathbf{T_1}|\tilde{k})\, t^{J_2}_{\tilde{c}\tilde{b}\tilde{i}\tilde{l}} \begin{Bmatrix} j_i & j_b & K \\ j_a & j_j & J \end{Bmatrix} \begin{Bmatrix} j_c & j_l & K \\ j_a & j_j & J_1 \end{Bmatrix} \begin{Bmatrix} j_l & j_i & J_2 \\ j_b & j_c & K \end{Bmatrix} + \ldots$$

reduced matrix elements
(Wigner-Eckart theorem)

Wigner 6j-symbols

- Nuclear applications involve time-consuming symmetry adaption of equations

Example - IMSRG(2)

- **Symmetry-unrestricted contribution to IMSRG commutator (see talk by M. Heinz!)**

$$C_{pqrs} = \frac{1}{2}\sum_{tu} \bar{n}_t \bar{n}_u S_{pqtu} T_{turs}$$

- **Plugging in all Clebsch-Gordan coefficients in the case of non-scalar operators yields**

$$(\tilde{p}\tilde{q}J_1|\mathbf{C}^{\lambda}|\tilde{r}\tilde{s}J_2) = \frac{1}{2}\sum_{\mu_1\mu_2\mu}\sum_{\{m_i\}}\sum_{\substack{J_1,\dots,J_6\\M_1,\dots,M_6}} \frac{1}{\hat{J}_1\hat{J}_3\hat{J}_5}\left(\begin{matrix}\lambda_1 & \lambda_2\\ \mu_1 & \mu_2\end{matrix}\middle|\begin{matrix}\lambda\\ \mu\end{matrix}\right)$$
$$\times \left(\begin{matrix}j_p & j_q\\ m_p & m_q\end{matrix}\middle|\begin{matrix}J_1\\ M_1\end{matrix}\right)\left(\begin{matrix}j_r & j_s\\ m_r & m_s\end{matrix}\middle|\begin{matrix}J_2\\ M_2\end{matrix}\right)\left(\begin{matrix}J_2 & \lambda\\ M_2 & \mu\end{matrix}\middle|\begin{matrix}J_1\\ M_1\end{matrix}\right)$$
$$\times \left(\begin{matrix}j_p & j_q\\ m_p & m_q\end{matrix}\middle|\begin{matrix}J_3\\ M_3\end{matrix}\right)\left(\begin{matrix}j_t & j_u\\ m_t & m_u\end{matrix}\middle|\begin{matrix}J_4\\ M_4\end{matrix}\right)\left(\begin{matrix}J_4 & \lambda_1\\ M_4 & \mu_1\end{matrix}\middle|\begin{matrix}J_3\\ M_3\end{matrix}\right)$$
$$\times \left(\begin{matrix}j_t & j_u\\ m_t & m_u\end{matrix}\middle|\begin{matrix}J_5\\ M_5\end{matrix}\right)\left(\begin{matrix}j_r & j_s\\ m_r & m_s\end{matrix}\middle|\begin{matrix}J_6\\ M_6\end{matrix}\right)\left(\begin{matrix}J_6 & \lambda_2\\ M_6 & \mu_2\end{matrix}\middle|\begin{matrix}J_5\\ M_5\end{matrix}\right)$$
$$\times\, \bar{n}_{\tilde{t}}\bar{n}_{\tilde{u}}(\tilde{p}\tilde{q}J_3|\mathbf{S}^{\lambda_1}|\tilde{t}\tilde{u}J_4)(\tilde{t}\tilde{u}J_5|\mathbf{T}^{\lambda_2}|\tilde{r}\tilde{s}J_6)$$

reduced matrix elements

from Wigner-Eckart theorem

- **IMSRG(3) involves ~100 additional terms with more couplings coefficients**

More systematic solution required !

How to do it manually

- **Identify substrings of CGCs and compare to documented identities**

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \sum_{m_1,\dots,m_6} (-1)^{\sum_{k=1}^{6}(j_k - m_k)} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_5 & j_6 \\ m_1 & -m_5 & m_6 \end{pmatrix} \begin{pmatrix} j_4 & j_2 & j_6 \\ m_4 & m_2 & -m_6 \end{pmatrix} \begin{pmatrix} j_4 & j_5 & j_3 \\ -m_4 & m_5 & m_3 \end{pmatrix}$$

- **Check position of minus signs and correct ordering of columns**

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

time reversal

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix}$$

odd permutation

- **Keeping track of phase factor is very tedious and error-prone**

- **Many more complicated angular-momentum identities arise in practice**

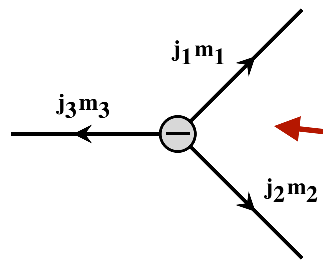
'Quantum Theory of Angular Momentum'
Khersonskii, Moskalev, Varshalovic

Diagrammatic notation

- Introduction of diagrammatic notion of angular-momentum-coupling objects

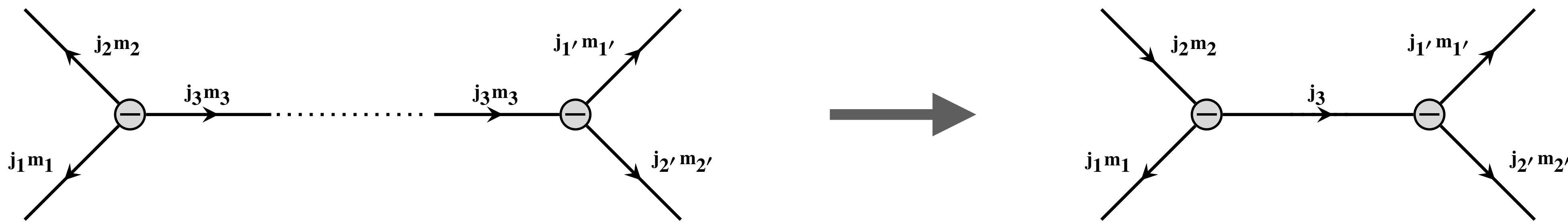
Wigner *3jm*-symbol

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} =$$



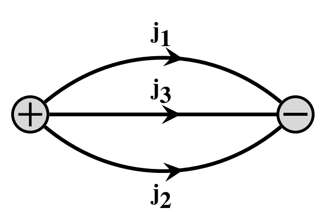
Vertex of degree three

- Contractions among vertices: summation over projection quantum numbers

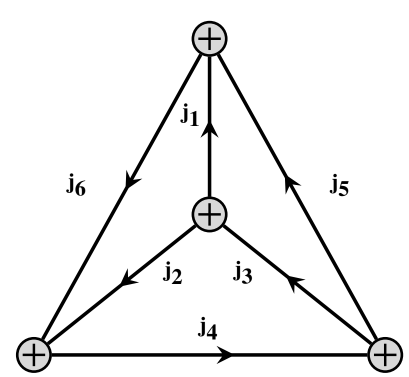


- Wigner *nj*-symbols yield irreducible topologies with *2,4,6,…* vertices

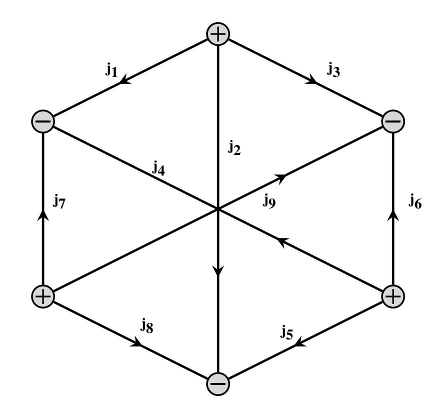
3*j*-symbol (triangular inequality)



6*j*-symbol



9*j*-symbol

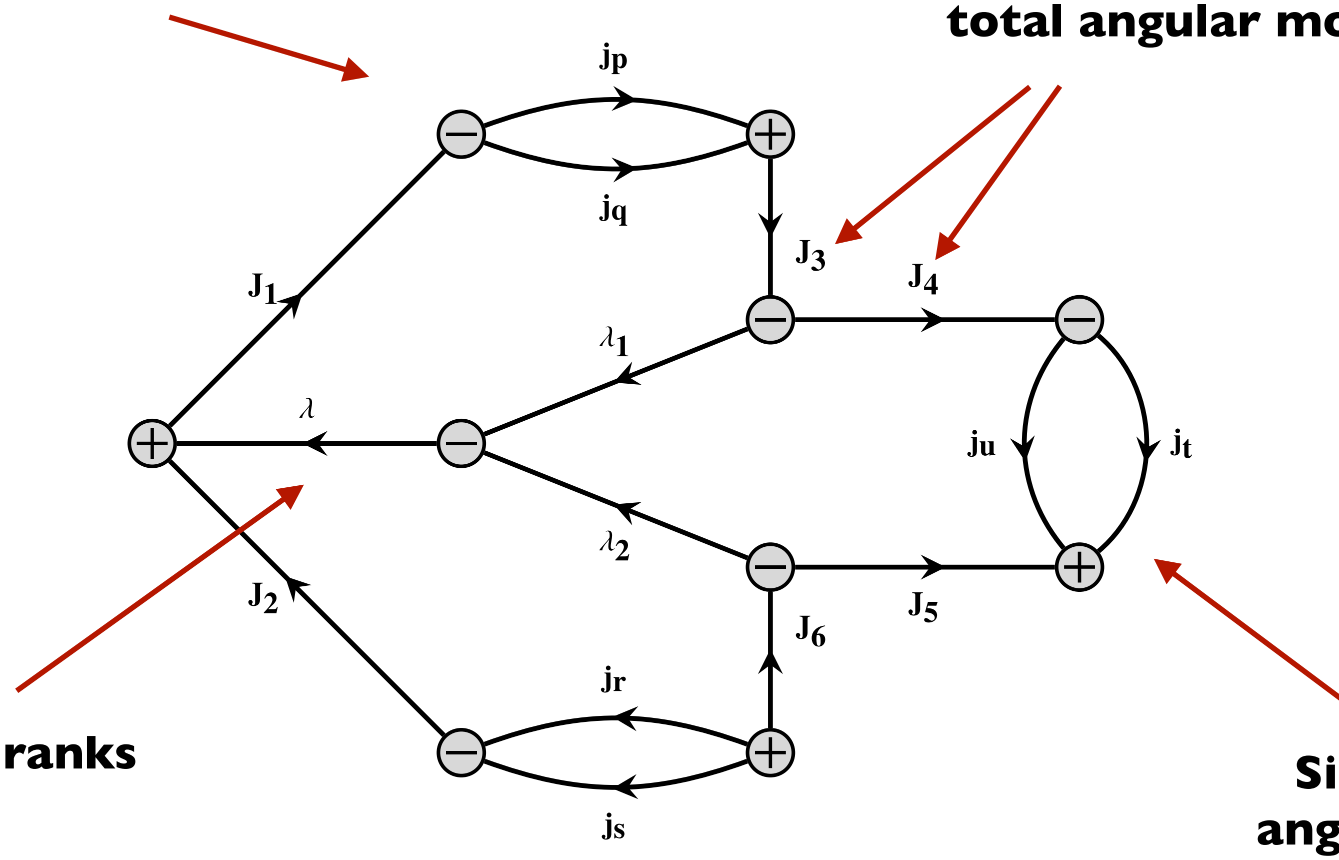


IMSRG(2) revisited

<u>**Angular-momentum network (Yutsis graph)**</u>

Subdiagram (apply 2-cycle rule)

Two-body total angular momenta

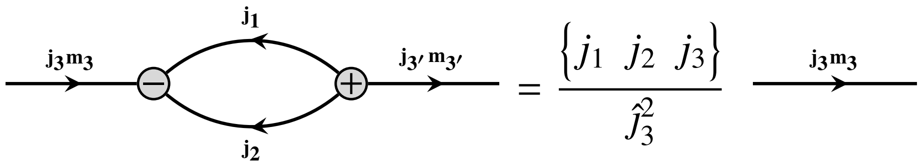


Spherical tensor ranks

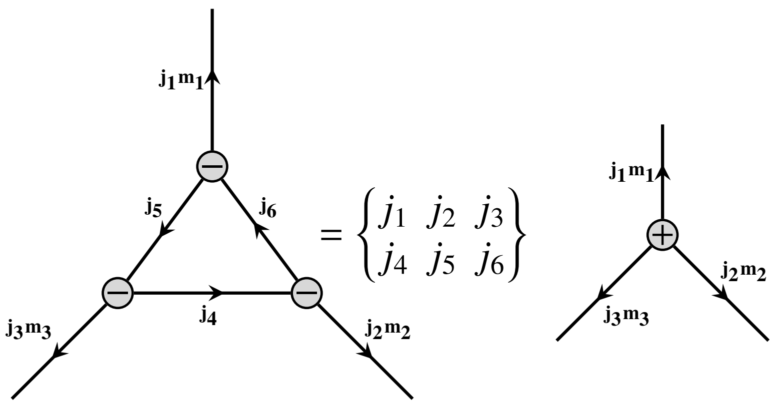
Single-particle angular momenta

Reduction rules

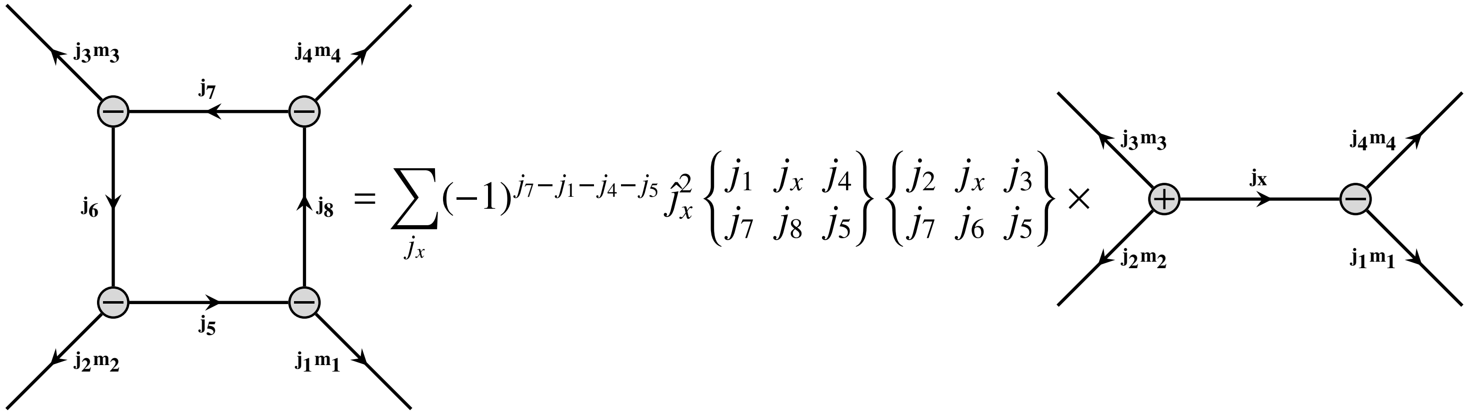
- Simplification of Yutsis graph while inducing irreducible 3*nj*-Wigner symbols
- 2-cycle rule: Simplest reduction corresponds to orthogonality relation



- 3-cycle rule: generation of 6j-symbol from removing three summations

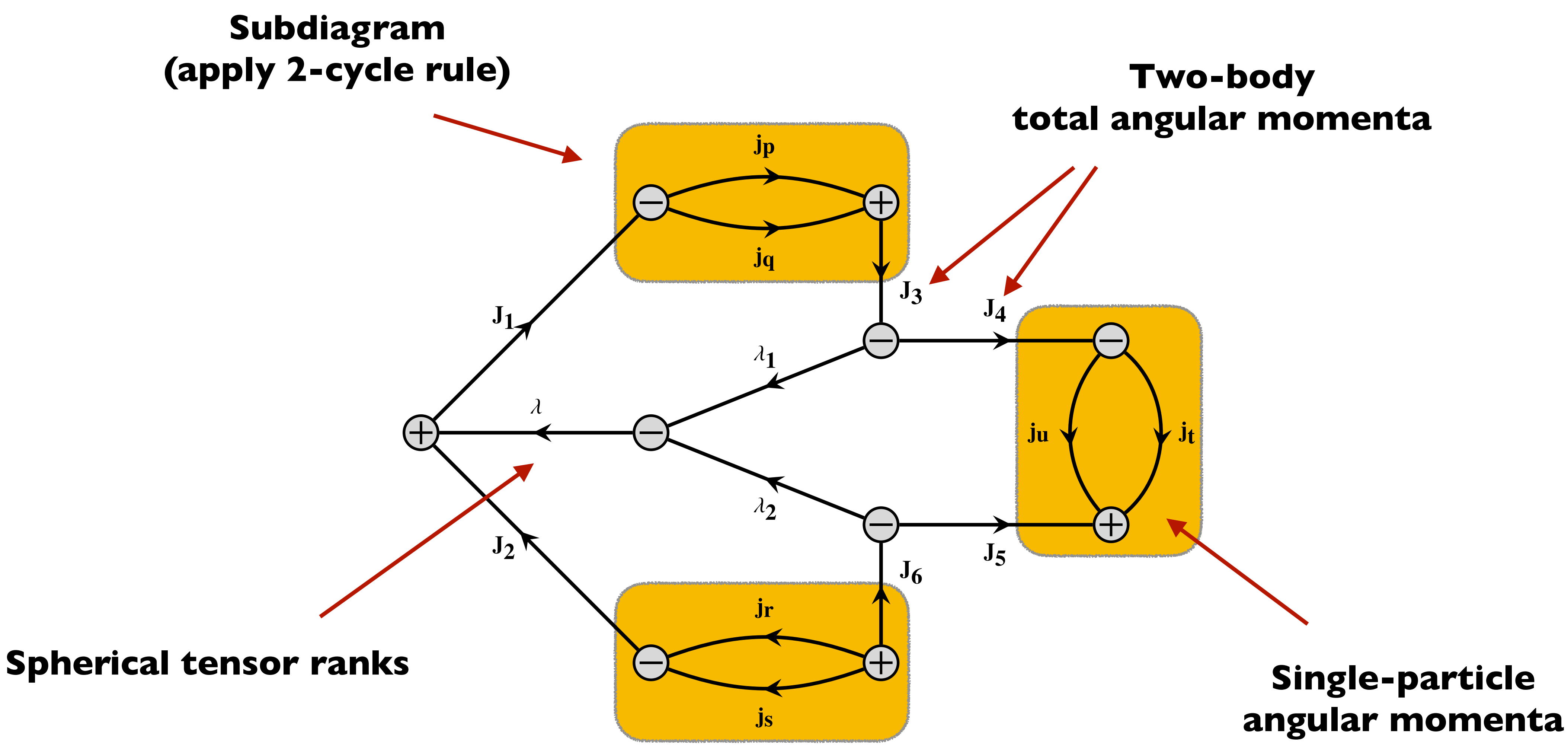


- 4-cycle: generation of two 6*j*-symbols and an additional dummy summation



IMSRG(2) revisited

Angular-momentum network (Yutsis graph)



Final result

$$(\tilde{p}\tilde{q}J_1|\mathbf{C}^{\lambda}|\tilde{r}\tilde{s}J_2) = \frac{1}{2}\hat{\lambda}(-1)^{J_1+J_2+\lambda}\sum_{J_3}\begin{Bmatrix}\lambda_1 & \lambda_2 & \lambda \\ J_2 & J_1 & J_3\end{Bmatrix}\sum_{\tilde{t}\tilde{u}}\bar{n}_{\tilde{t}}\bar{n}_{\tilde{u}}(\tilde{p}\tilde{q}J_1|\mathbf{S}^{\lambda_1}|\tilde{t}\tilde{u}J_3)(\tilde{t}\tilde{u}J_3|\mathbf{T}^{\lambda_2}|\tilde{r}\tilde{s}J_2)$$

Intrinsic workflow

- **Symmetry transformation**: replace *m*-scheme with *J*-scheme matrix elements
- **Canonicalization**: transform all CGCs to Wigner *3jm*-symbols

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \equiv \frac{1}{\hat{j}_1}(-1)^{j_2-j_3-m_1} \left(\begin{matrix} j_1 & j_2 \\ -m_1 & m_2 \end{matrix} \middle| \begin{matrix} j_3 \\ m_3 \end{matrix} \right)$$

- **Formation of Jutsis graph**: build contractions from internal summation

Output: cubic angular-momentum network

- **Symmetry reduction**: find closed subgraphs in the network

Application of 2-, 3- and 4-cycle rules

keep track of global prefactor → $\frac{1}{\hat{J}_{\text{global}}} \cdot \Phi_{\text{global}}$

- **Output**: generation of abstract expression of symmetry-reduced tensor network

Many-body framework written in terms of *SU(2)*-invariant objects

How to use AMC

- Text file: specify tensor mode, tensorial properties and LaTeX output

```
declare C { mode=(2,2), latex="C", scalar=False }
declare S { mode=(2,2), latex="S", scalar=False }
declare T { mode=(2,2), latex="T", scalar=False }
declare nbar { mode=2, diagonal=true, latex="\bar{n}" }
```

- Text file: symmetry-unrestricted working equations of many-body formalism

```
C_pqrs = 1/2 * sum_tu(nbar_t * nbar_u * S_pqtu * T_turs);
```

- Execution: call the AMC program to generate an output LaTeX file

```
amc imsrgtens.txt  imsrgtens.tex -option
```

- Possible options enable for fine-tuning of output for various end-users
  - Using *9j*-symbols instead of products of *6j*-symbols
  - Switches for using reduced/unreduced matrix elements
  - Various phase conventions for Wigner-Eckart theorem

Possible output: IMSRG(3)

2.9 Term 9

$$-\frac{1}{2}\,\delta_{j_1,j_0}\,\hat{J}_0 \sum_{abcJ_2J_3j_2j_3} (n_a\,n_b\,\bar{n}_c - \bar{n}_a\,\bar{n}_b\,n_c)\,\hat{J}_2\,\hat{j}_2^2\,\hat{j}_3^2 \times \begin{Bmatrix} j_r & j_q & J_2 \\ j_p & j_0 & J_0 \end{Bmatrix} \begin{Bmatrix} j_c & j_2 & J_2 \\ j_3 & J_3 & j_p \\ J_1 & j_u & j_0 \end{Bmatrix} A^{J_2j_2J_3j_20}_{rqcabu}\,B^{J_3j_3J_1j_30}_{abpstc}$$

2.10 Term 10

$$\frac{1}{2}\,\delta_{j_1,j_0}\,\hat{J}_0 \sum_{abcJ_2J_3j_2j_3} (n_a\,n_b\,\bar{n}_c - \bar{n}_a\,\bar{n}_b\,n_c)\,\hat{J}_2\,\hat{j}_2^2\,\hat{j}_3^2 \times \begin{Bmatrix} j_r & j_q & J_2 \\ j_p & j_0 & J_0 \end{Bmatrix} \begin{Bmatrix} j_c & j_2 & J_2 \\ j_3 & J_3 & j_p \\ J_1 & j_u & j_0 \end{Bmatrix} B^{J_2j_2J_3j_20}_{rqcabu}\,A^{J_3j_3J_1j_30}_{abpstc}$$

2.11 Term 11

$$\frac{1}{2}\,\delta_{j_1,j_0}\,(-1)^{J_1+j_t+j_u}\,\hat{J}_0\,\hat{J}_1 \sum_{abcJ_2J_3J_4j_2j_3} (n_a\,n_b\,\bar{n}_c - \bar{n}_a\,\bar{n}_b\,n_c)\,(-1)^{J_4}\,\hat{J}_2\,\hat{J}_4 \times \hat{j}_2^2\,\hat{j}_3^2 \begin{Bmatrix} j_r & j_q & J_2 \\ j_p & j_0 & J_0 \end{Bmatrix} \begin{Bmatrix} j_u & j_s & J_4 \\ j_t & j_0 & J_1 \end{Bmatrix} \begin{Bmatrix} j_c & j_2 & J_2 \\ j_3 & J_3 & j_p \\ J_4 & j_t & j_0 \end{Bmatrix} A^{J_2j_2J_3j_20}_{rqcabt}\,B^{J_3j_3J_4j_30}_{abpsuc}$$

plus 14 more pages ...
(derived in less than a second)

Bogoliubov coupled cluster

- Use of **Bogoliubov reference state**

$$|\Phi\rangle = \prod \beta_k |0\rangle$$

- **Quasi-particle extension** of CC theory

$$|\Psi\rangle = e^{\mathcal{T}} |$$

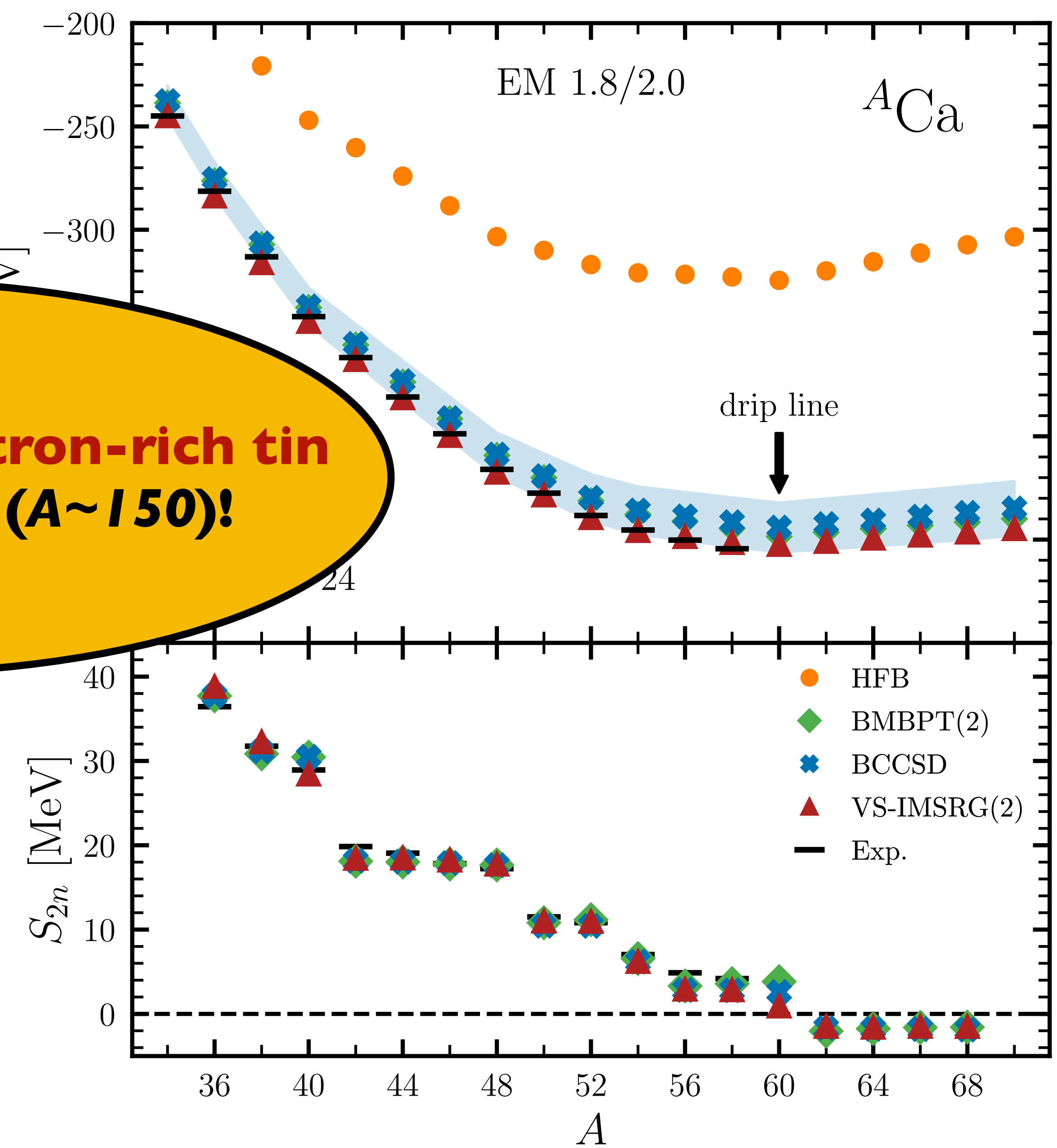
- **Cluster operator** in B

$$\mathcal{T}_n = \frac{1}{(2n)!} \sum_{k_1 \ldots k_{2n}} t_{k_1 \ldots k_{2n}} \beta^\dagger_{k_1} \cdots \beta^\dagger_{k_{2n}}$$

- **Open-shell nuclei** at (rather) low cost by exploiting rotational invariance

- Many-body **uncertainty estimate** due to missing triples correlations

Calculations for neutron-rich tin isotopes ongoing (*A*~*150*)!



Tichai, Demol, Duguet (in preparation, 2023)

Conclusion and outlook

<< pip3 install amc

Things to remember

- Symmetry-adaption may provide significant computational gains
- SU(2)-reduction is an extremely tedious and error-prone task
- Automated AMC tool condenses months of derivation in a second

Ongoing developments

- Extension to quasi-particle-based many-body frameworks (P. Demol)
- Transfer to CC codes in atomic physics (see talk by Reitsma/Chamorro Mena)
- Systematic understanding of *'best coupling order'* for higher-body operators

Final remark for discussion

- **Nuclear physics:** a lot progress on automated derivation and symmetry reduction
- Missing link: automated code generation of many-body tensor networks
- Solution: generic tensor-contraction library for block-sparse storage formats

So far we only have hand-optimized code with limited scalability!

What are existing technologies in other communities?

How can we leverage GPU acceleration?

Can we easily implement abelian symmetries?

How can we account for decomposed tensors (RI/DF techniques)