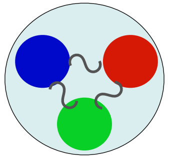
AB INITIO METHODS

Pierre Arthuis

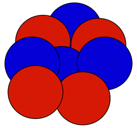
A crash course in nuclear many-body methods

What does ab initio mean for us?



Particle physics

No direct application of
quantum chromodynamics
(Lattice QCD only for few nucleons)



Nuclear theory

Effective Field Theory in the A-body sector

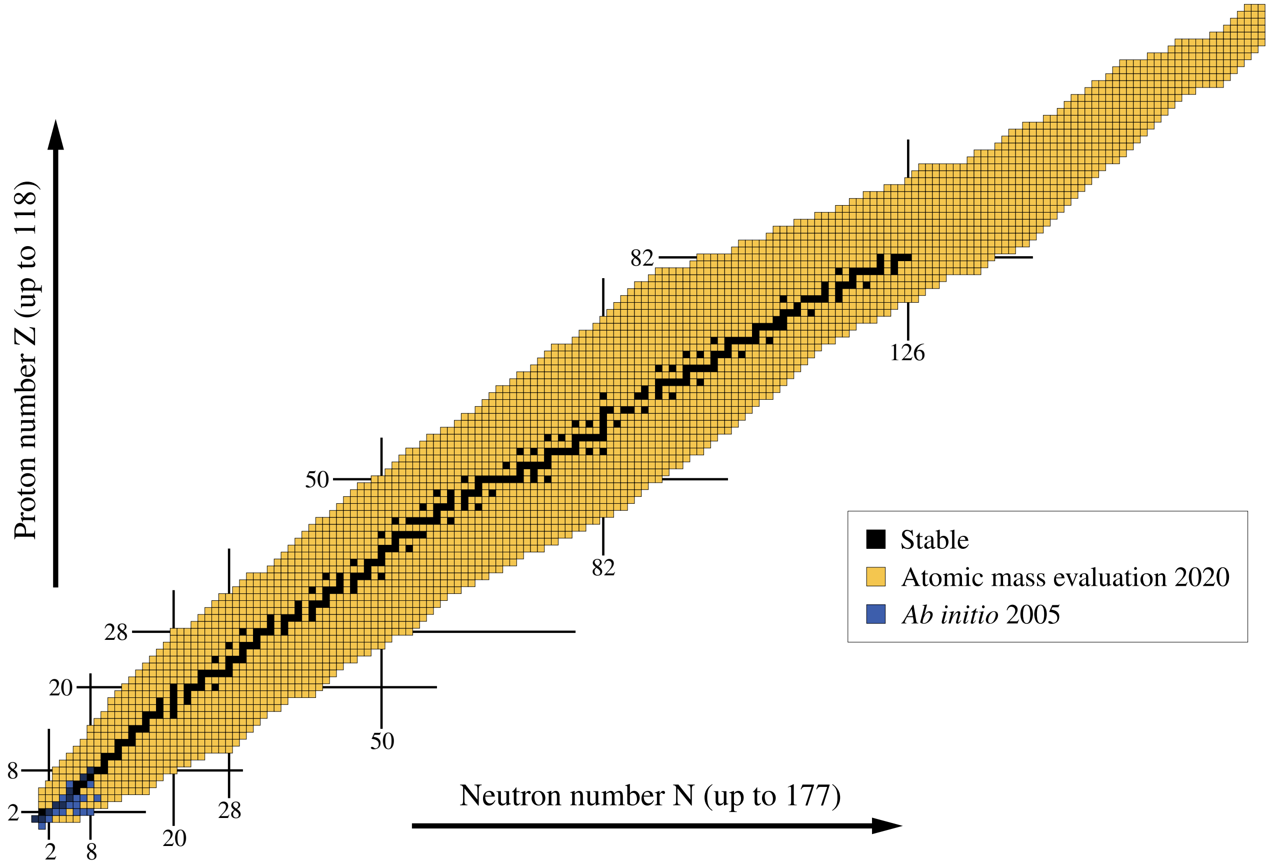
A-body Schrödinger equation

$$H|\Psi^{A}\rangle = E^{A}|\Psi^{A}\rangle$$

Obtain a description that is:

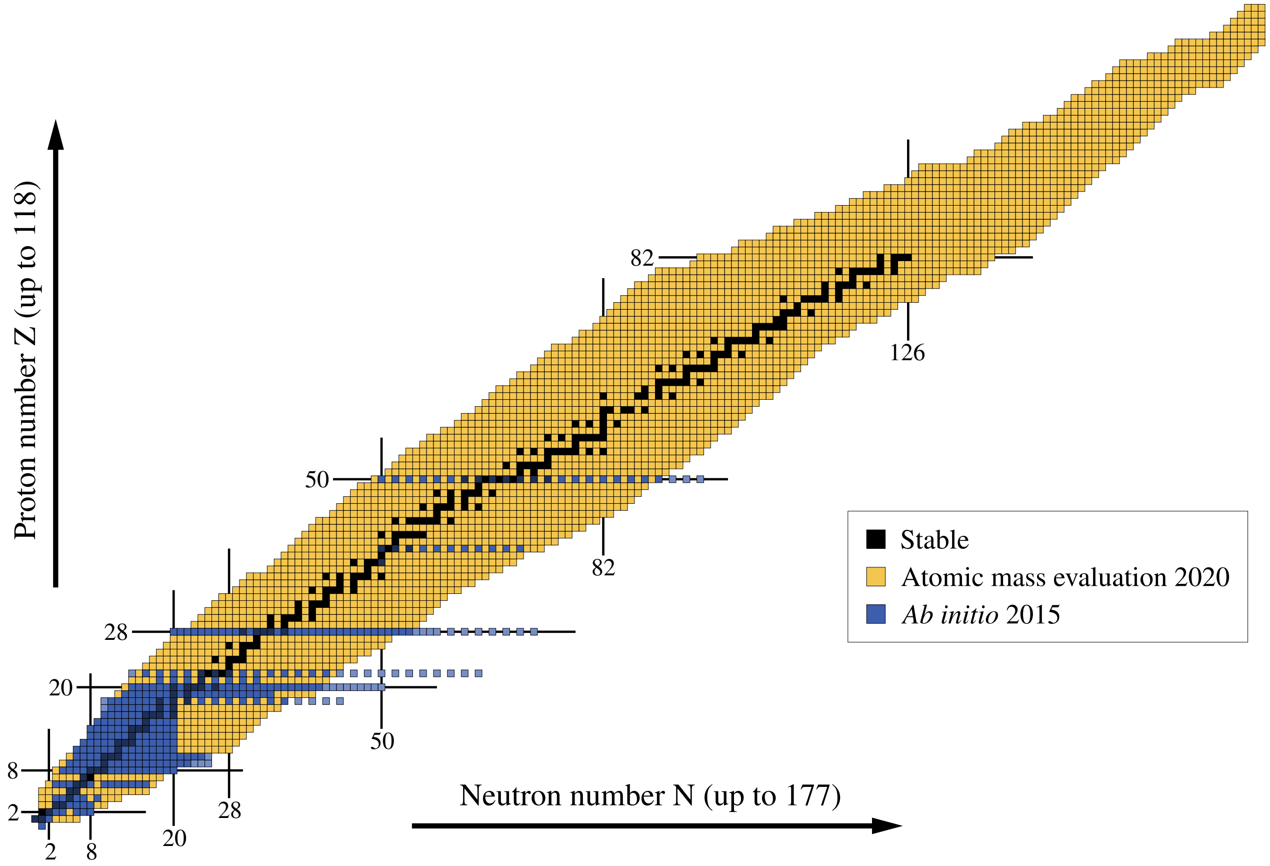
- Consistent
- Systematic
- Accurate enough
- From inter-nucleon interaction
- Rooted in quantum chromodynamics

Ab initio many-body methods range



Adapted from B. Bally

Ab initio many-body methods range



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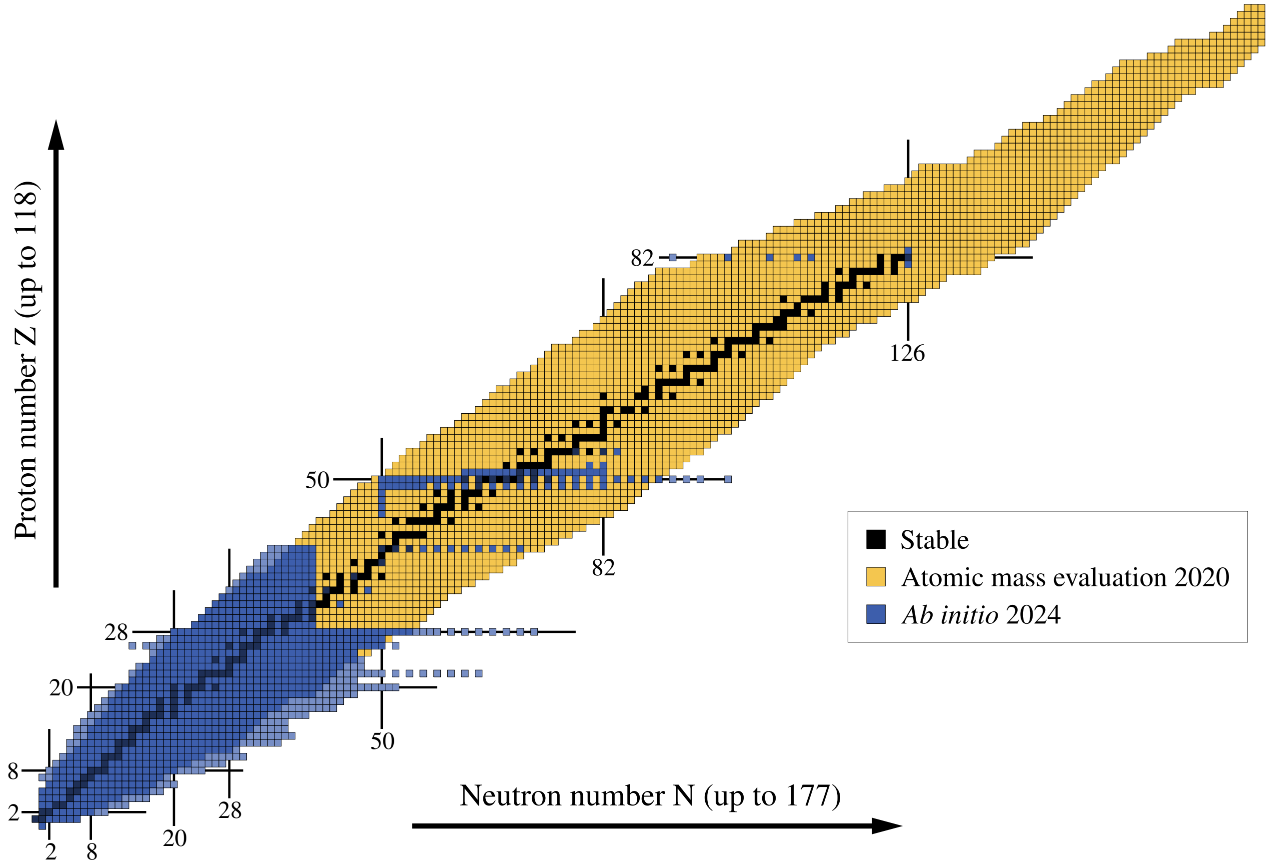

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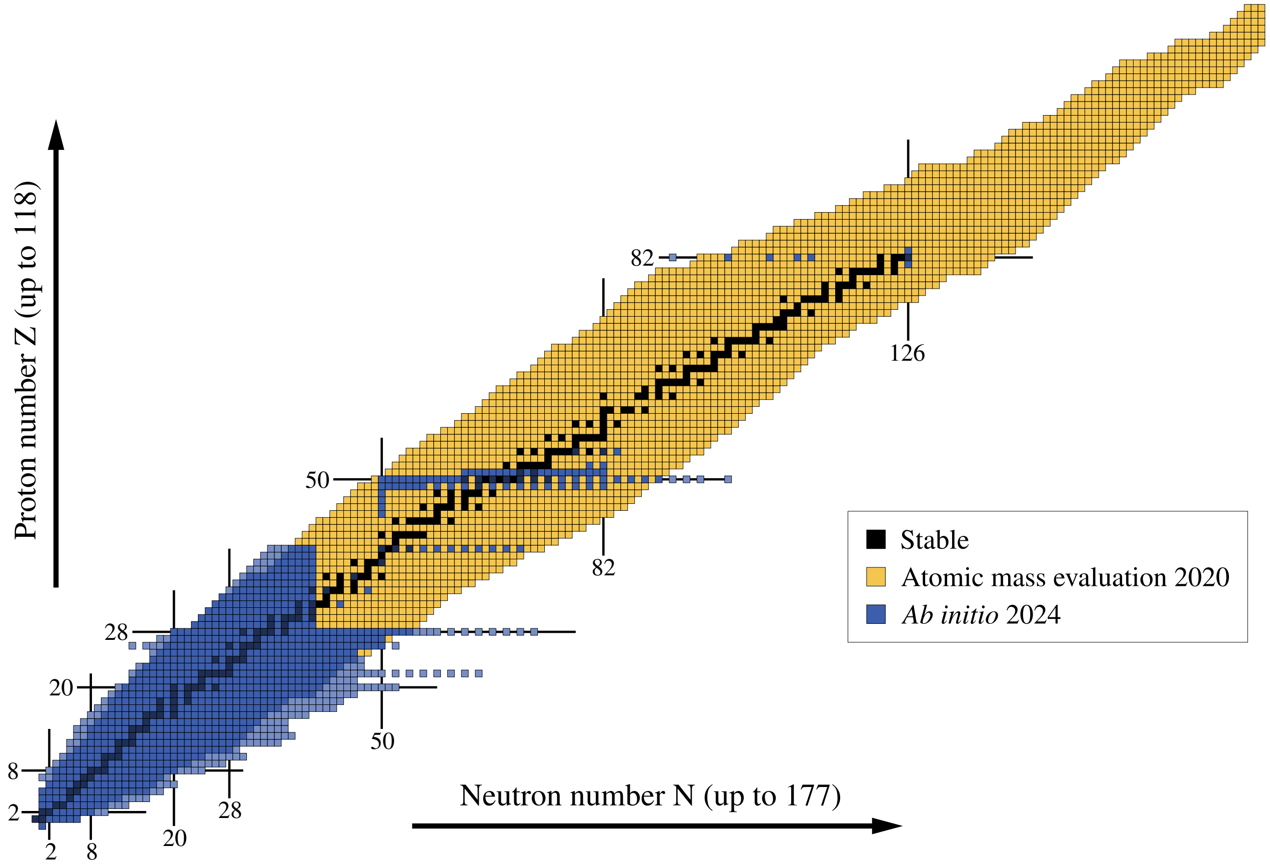

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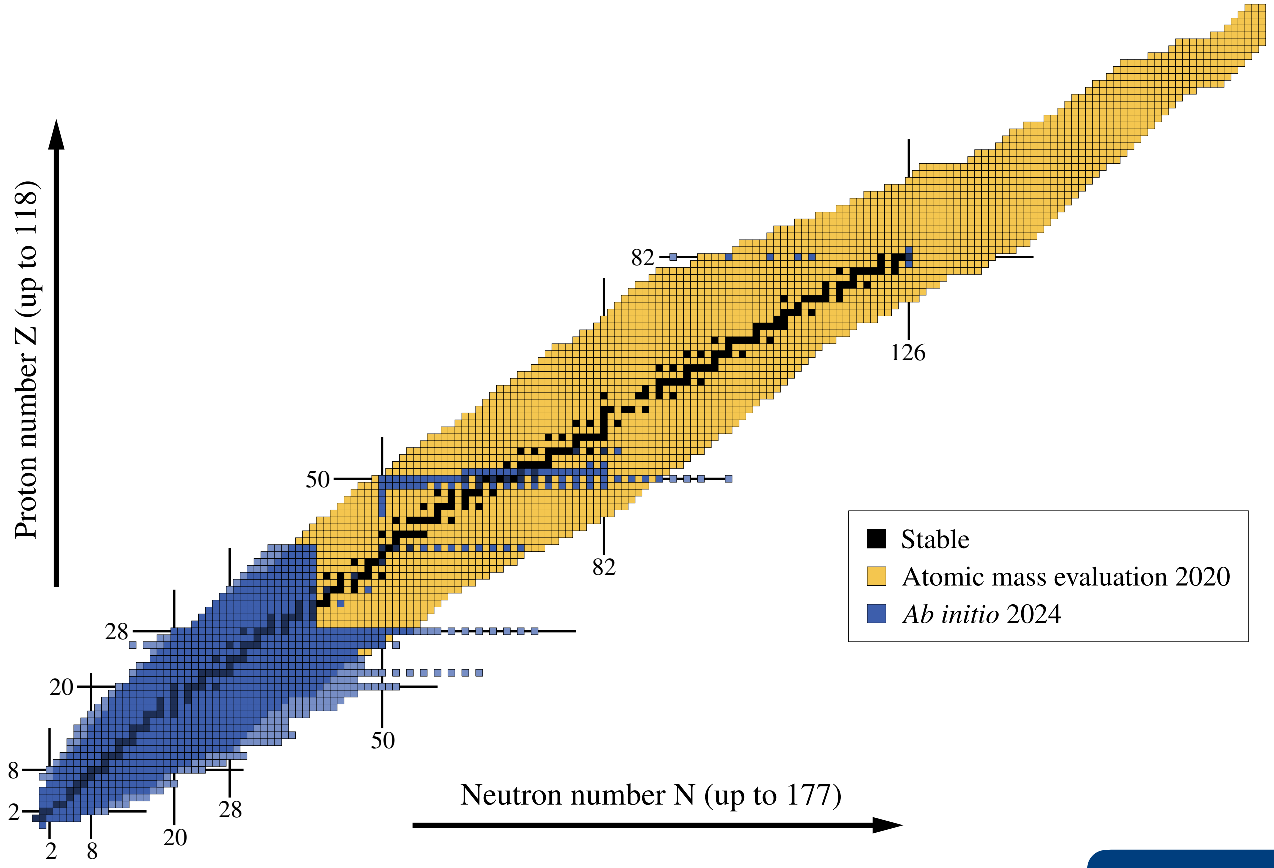
Expansion methods

$$H|\Psi\rangle = U(\infty)|\Phi\rangle$$
$$= (U_1 + U_2 + U_3 + \ldots)|\Phi\rangle$$

- Expand the correlations order by order
- Truncate at desired order
- Estimate uncertainties

Controlled expansion & uncertainty

Moderate cost



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Controlled expansion & uncertainty

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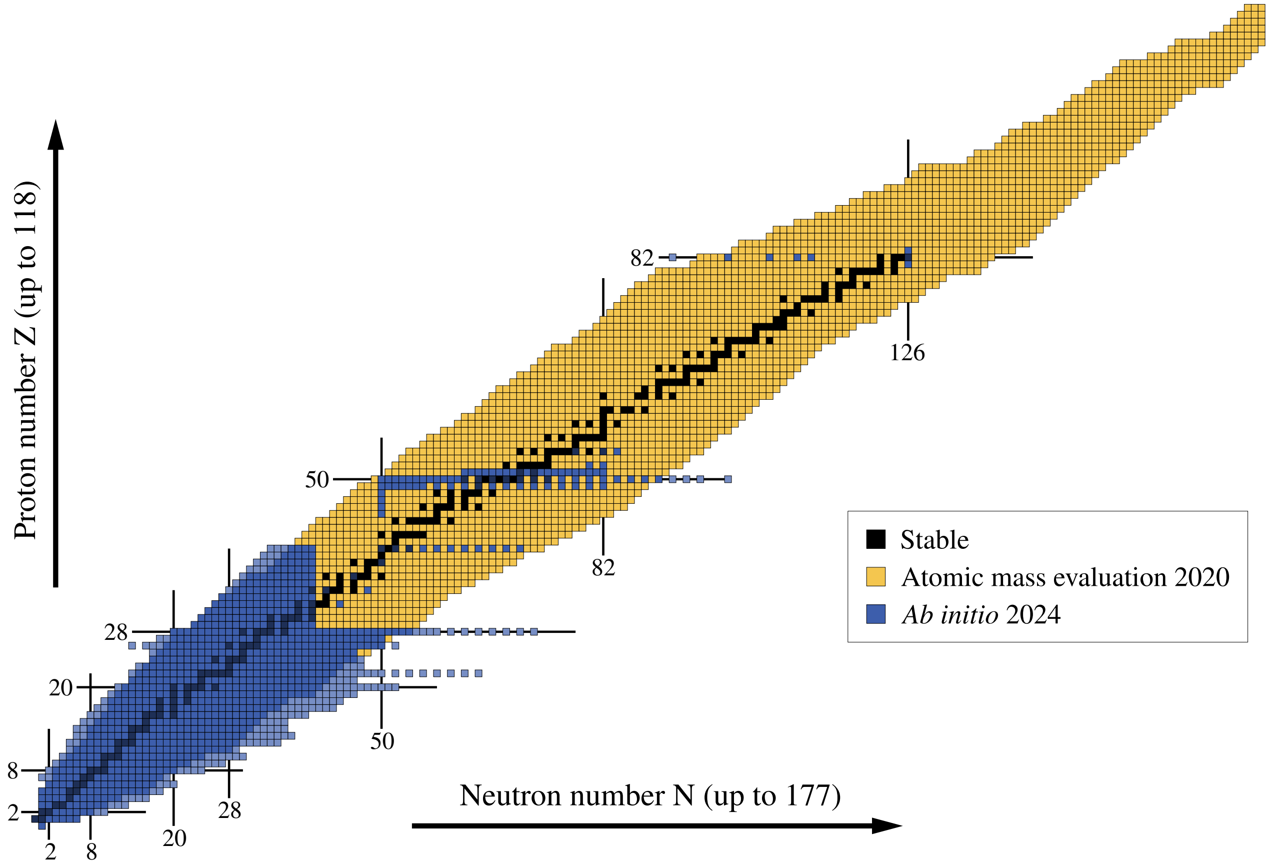
Footnote: Other methods exist for mid-mass (e.g. NLEFT)

A look at experimental facilities



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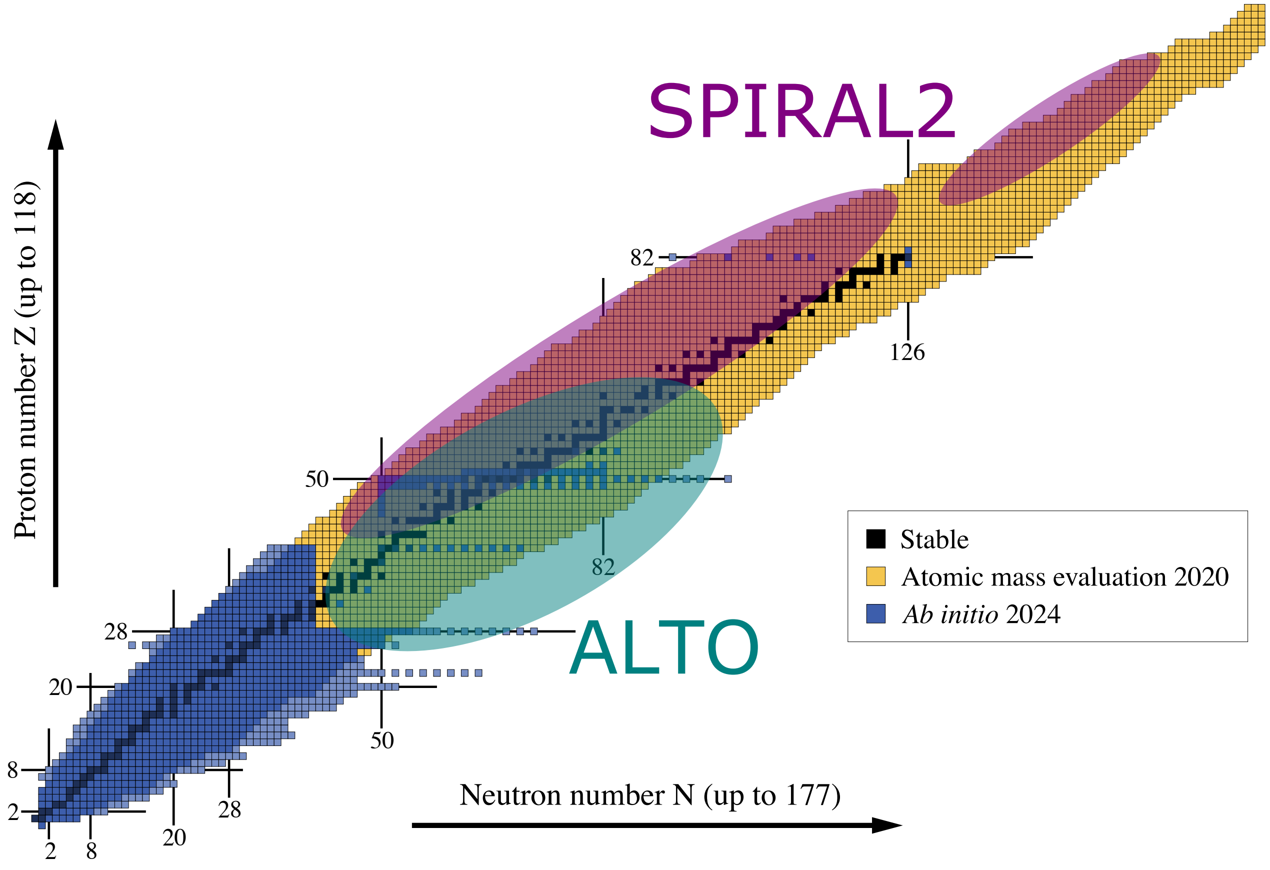

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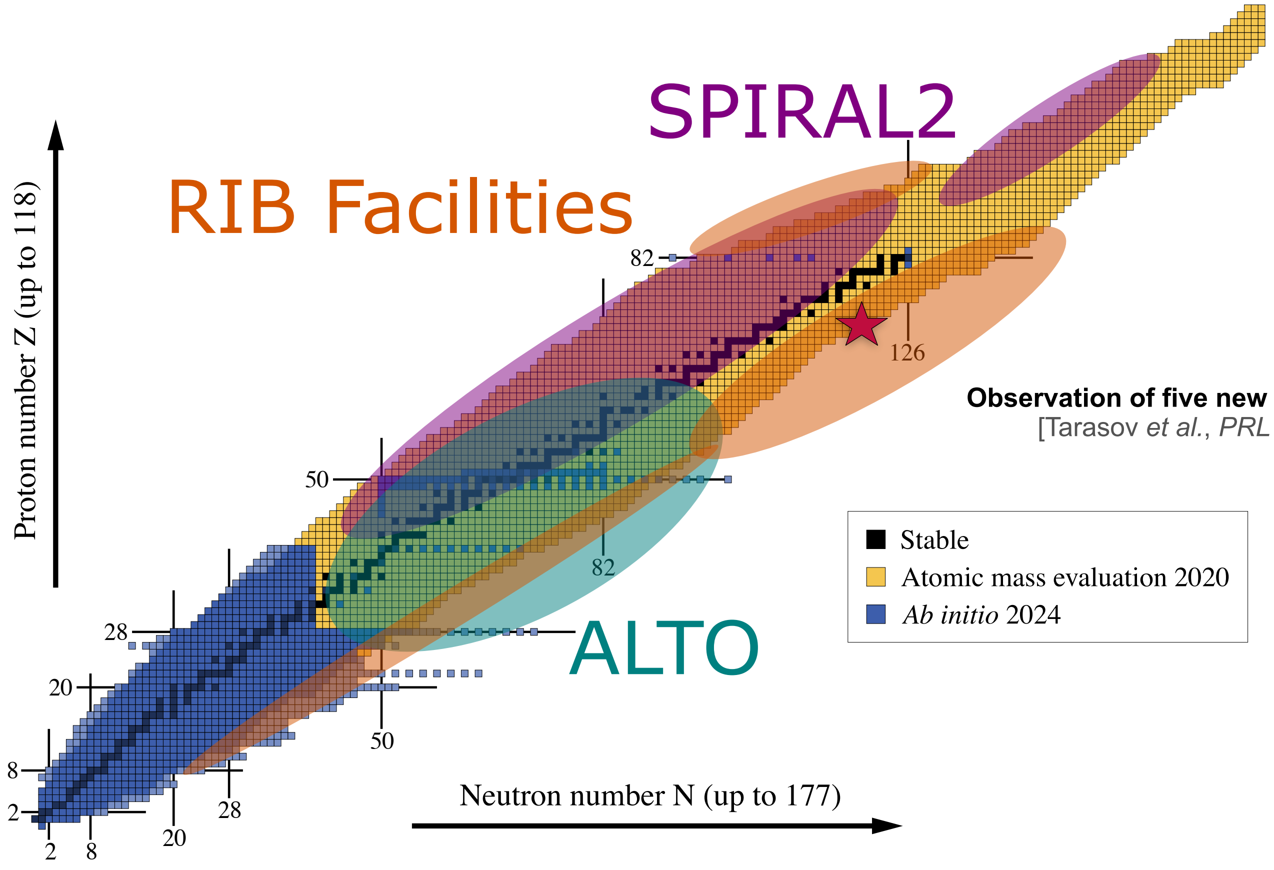
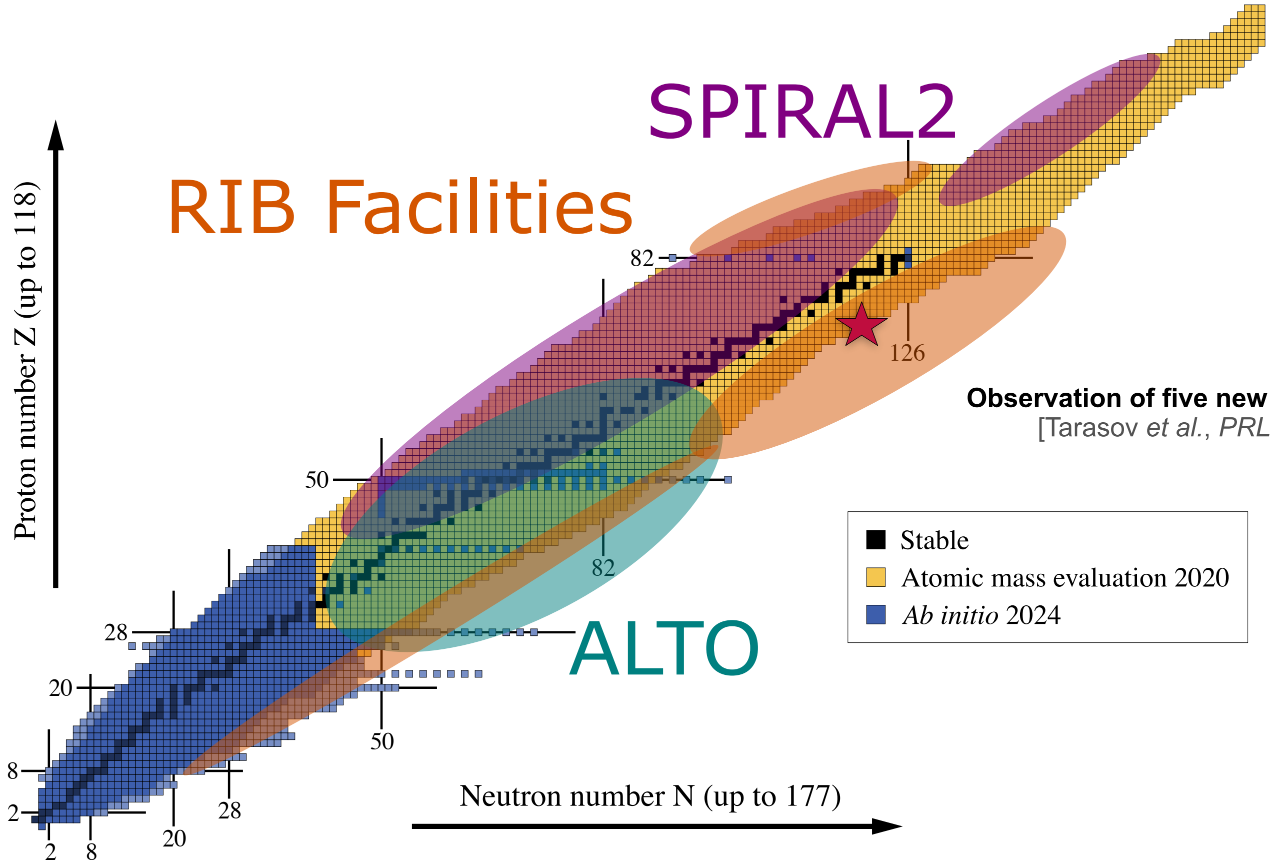


Observation of five new isotopes at FRIB
[Tarasov *et al.*, *PRL* **132** (2024)]

Adapted from B. Bally



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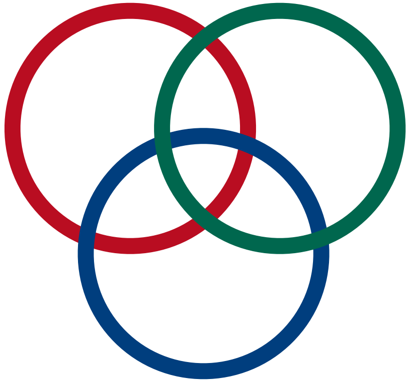
Adapted from B. Bally

New era of shared effort

Heaver nuclei

More exotic nuclei

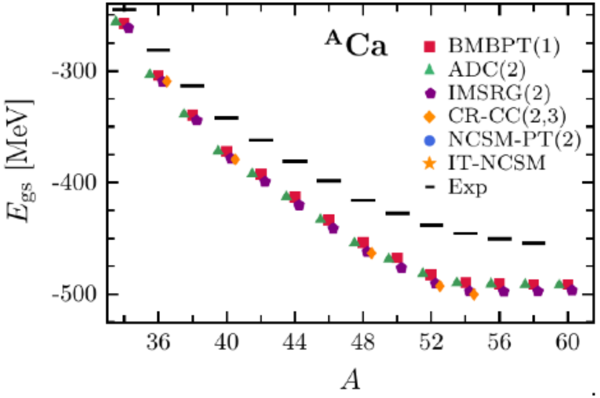
Determine an observable O for a system S with precision η



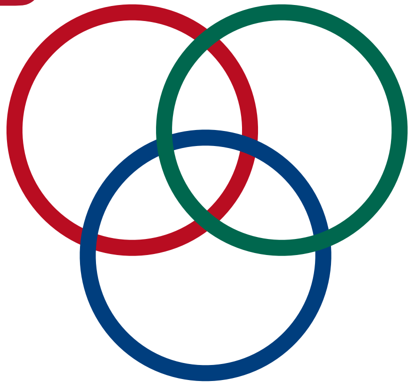
Ab initio challenge(s)

Determine an observable O for a system S with precision η

Nuclear interaction



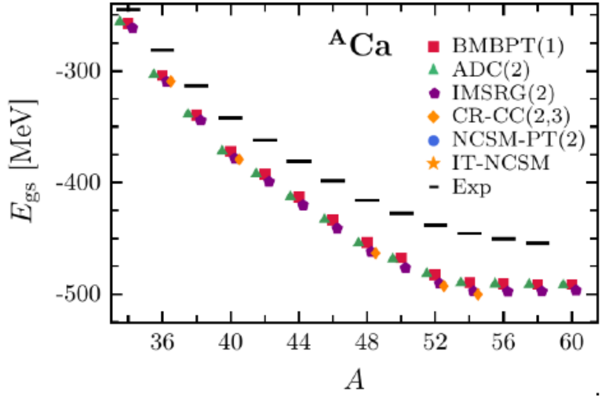
[Tichai, Arthuis *et al.*, *PLB* **786** (2018)]



Determine an observable O for a system S with precision η

Nuclear interaction

Many-body method



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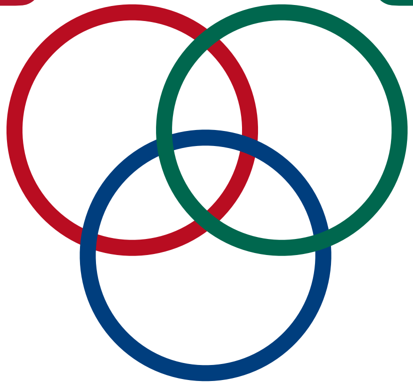

Order	1	2	3	4
# Equations	3	23	396	10 716

[Arthuis *et al.*, *CPC* **240** (2019)]

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Determine an observable O for a system S with precision η

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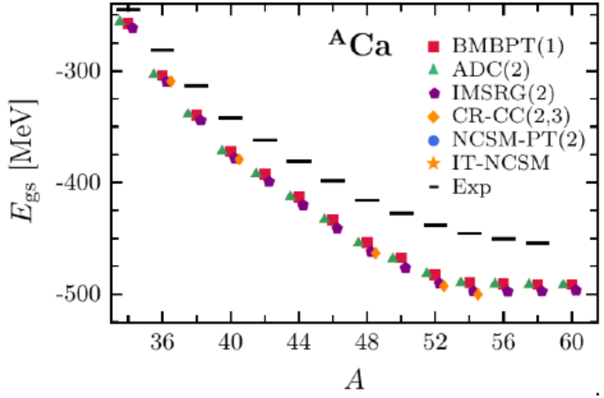

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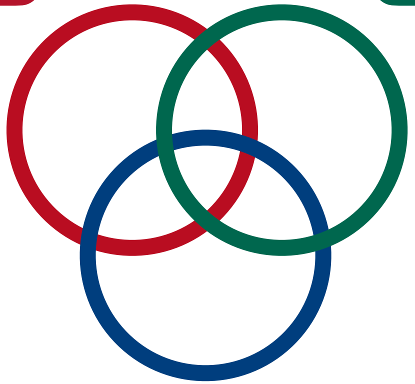

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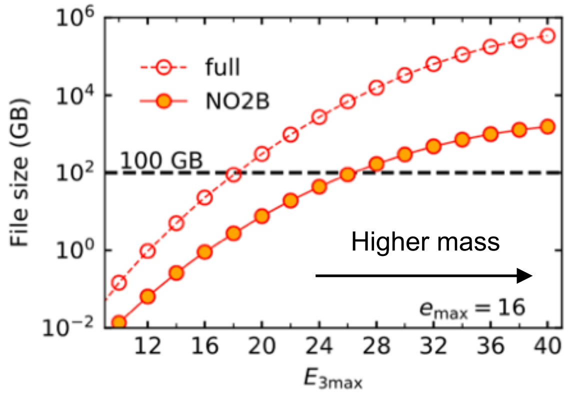
Numerical method

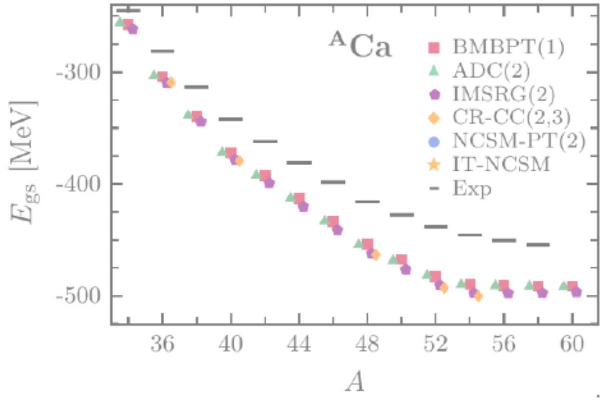


[Miyagi *et al.*, *PRC* **105** (2022)]

Determine an observable O for a system S with precision η

Nuclear interaction

Many-body method



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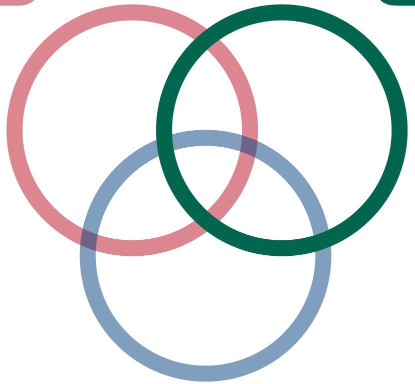

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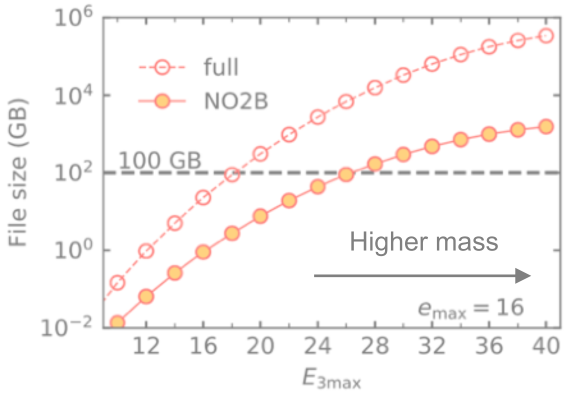
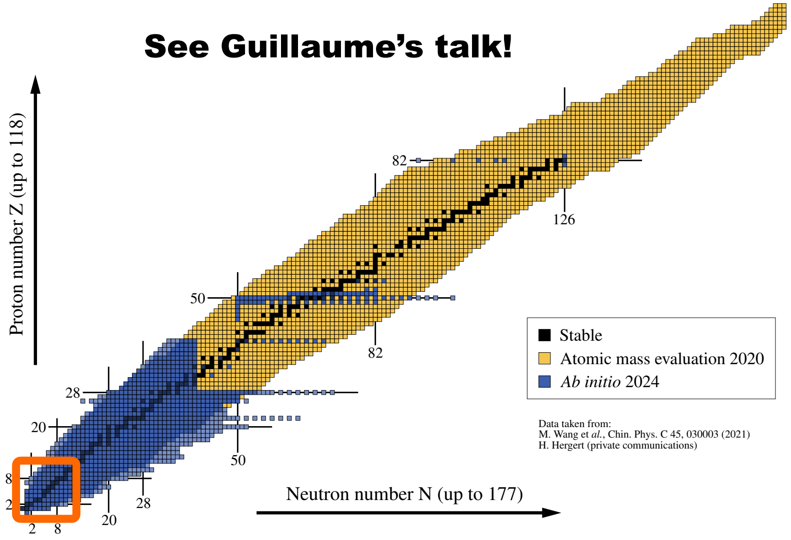


[Miyagi *et al.*, *PRC* **105** (2022)]

A structure and reactions review: [Navrátil *et al.*, *Phys. Scr.* **91** (2016)]

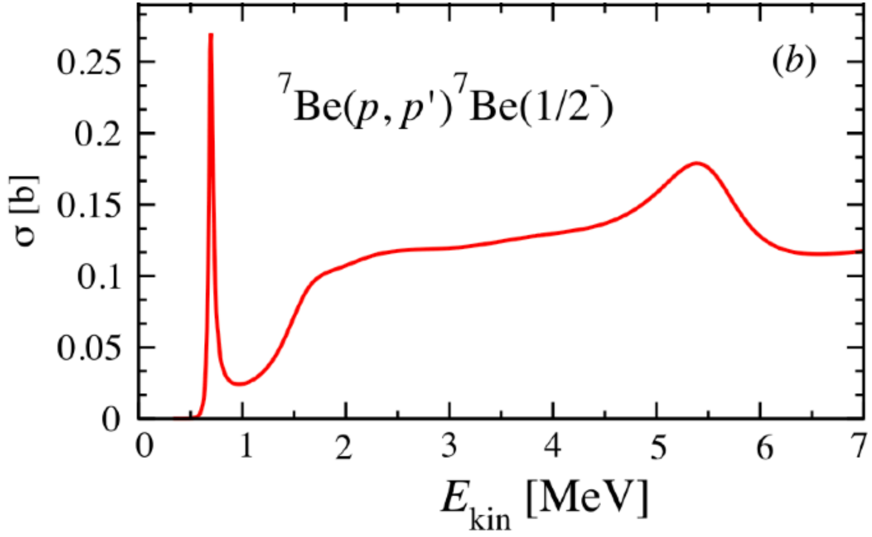
See Guillaume's talk!



Specific case of Configuration-Interaction method

$$|\Psi_n\rangle = \sum_i C_i^{(n)} |\Phi_i\rangle \longleftarrow \textbf{Slater det. basis}$$

See Michael's, Lotta's talks!



[Navrátil et al., *PLB* **704** (2011)]

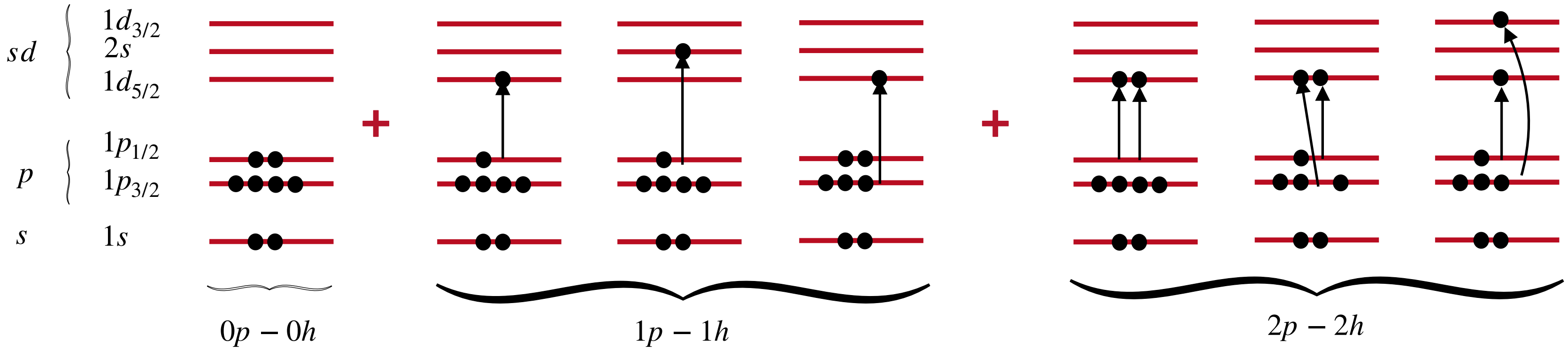
What does it do?

- Full Hamiltonian diagonalisation = matrix eigenvalue problem
- Access to a wide range of observables
- Very computationally costly so limited in range
- Extensions for connections to reactions, continuum
- Symmetry-adapted NCSM (SA-NCSM) for specific, heavier systems

Why this paradigm?

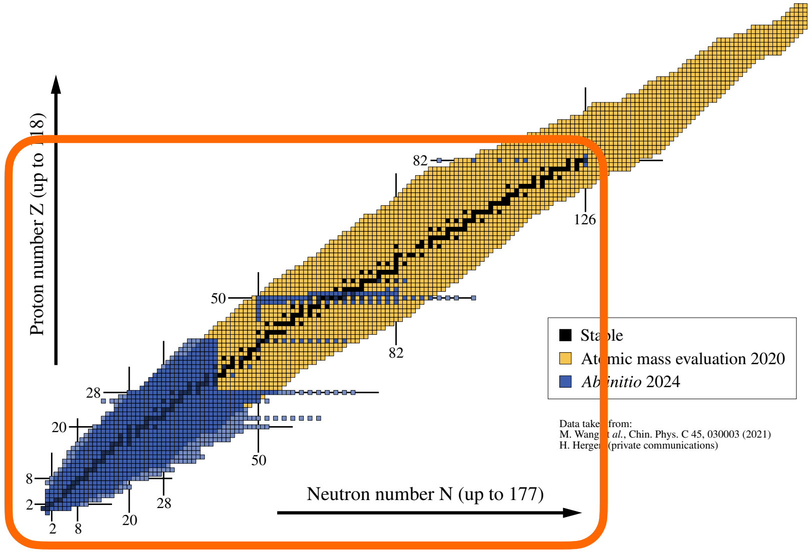
- Intuitive representation starting from the independent shell model
- Emerges naturally from our second quant. representation
- NCSM resums all particle-hole configurations possible
- Other methods expressed in terms of those excitations

$$|\Psi_n\rangle = \sum_i C_i^{(n)} |\Phi_i\rangle$$



Particle states
a,b,c…

Hole states
i,j,k…

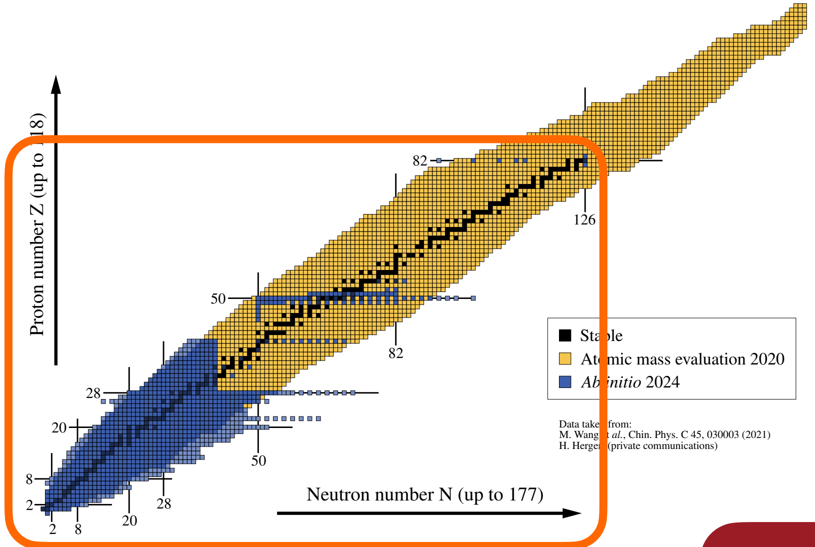


Expansion methods

$$H|\Psi\rangle = U(\infty)|\Phi\rangle$$
$$= (U_1 + U_2 + U_3 + \ldots)|\Phi\rangle$$

Exact result not what we obtain any more!

See Michael's talk for horizontal vs vertical correlations



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$$H|\Psi\rangle = U(\infty)|\Phi\rangle$$
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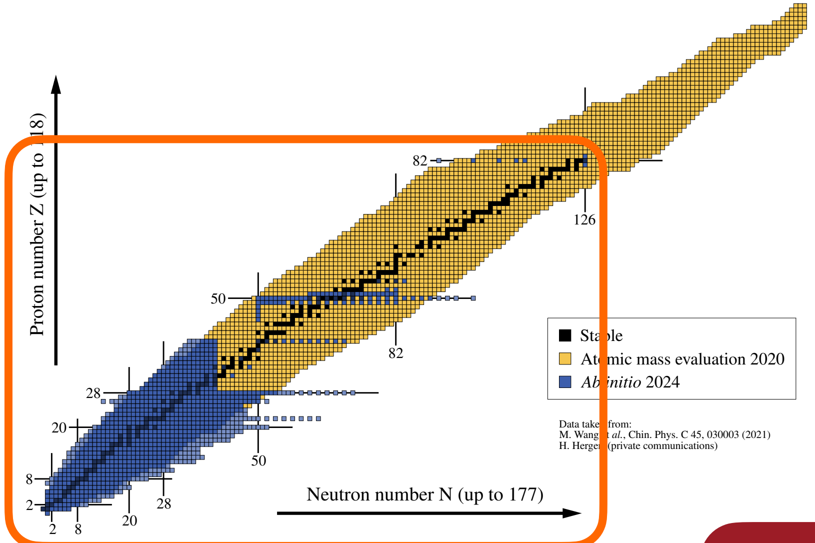
Reference state $|\Phi\rangle$

- Often obtained from Hartree-Fock(-Bogoliubov)
- Can be spherical/deformed…
- Should incorporate *collective* correlations

Horizontal correlations

See Michael's talk for horizontal vs vertical correlations



Vertical correlations

Horizontal correlations

Expansion methods

$$H|\Psi\rangle = U(\infty)|\Phi\rangle$$
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Expansion operator U
- Depends on the many-body method
- Expressed in terms of particle-hole excitations
- Should incorporate *particle-hole* correlations

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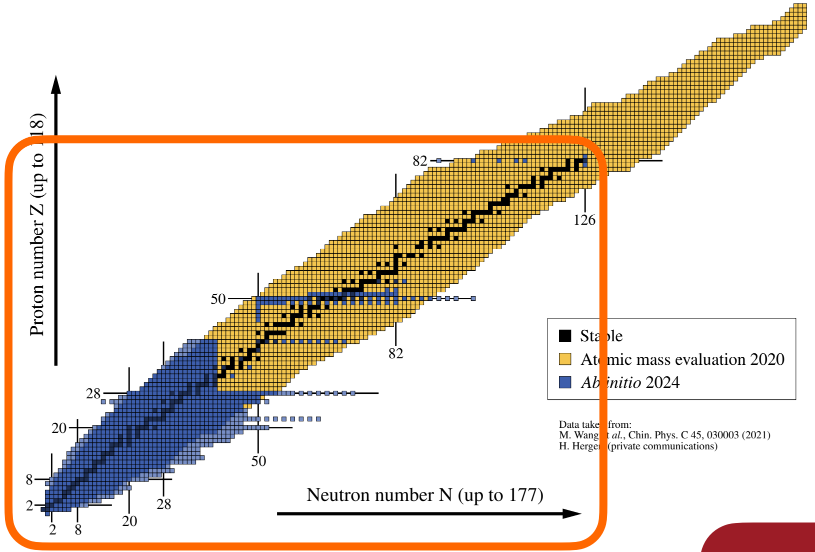

Expansion methods

$$
\begin{aligned}
H|\Psi\rangle &= U(\infty)|\Phi\rangle \\
&= (\boxed{U_1 + U_2 + U_3 + \ldots})\boxed{|\Phi\rangle}
\end{aligned}
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Vertical correlations

Horizontal correlations

Taylor the combination depending on the system

See Michael's talk for horizontal vs vertical correlations

Many-Body Perturbation Theory (MBPT)

Hamiltonian partition

$$H \equiv H_0 + H_1$$

Eigenstates for H_0

$$H_0 |\Phi_k\rangle = E_k^{(0)} |\Phi_k\rangle$$

Expansion series

$$E - E^{(0)} = \sum_{n=2}^{\infty} \langle \Phi | H_1 \left(RH_1\right)^{n-1} | \Phi \rangle$$

with

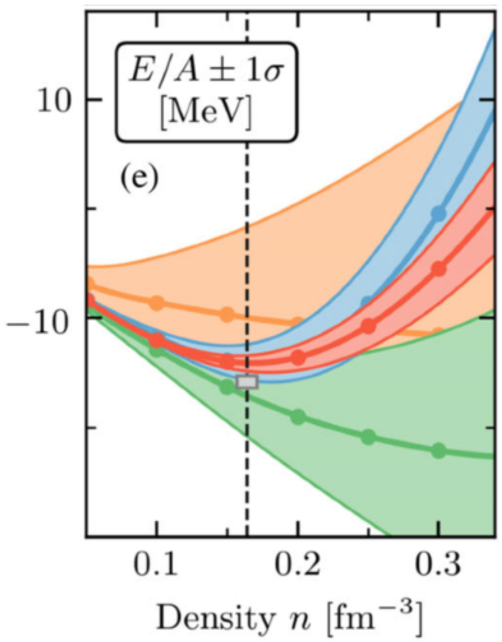
$$R = \sum_k \frac{|\Phi_k\rangle\langle\Phi_k|}{E^0 - E_k^{(0)}}$$

Second-order expansion

$$E^{(2)} = \sum_k \frac{\langle \Phi | H_1 | \Phi_k \rangle \langle \Phi_k | H_1 | \Phi \rangle}{E^0 - E_k^{(0)}}$$

In practice…

$$E^{(2)} = -\frac{1}{4} \sum_{abij} \frac{V_{abij} V_{ijab}}{e_a + e_b - e_i - e_j}$$

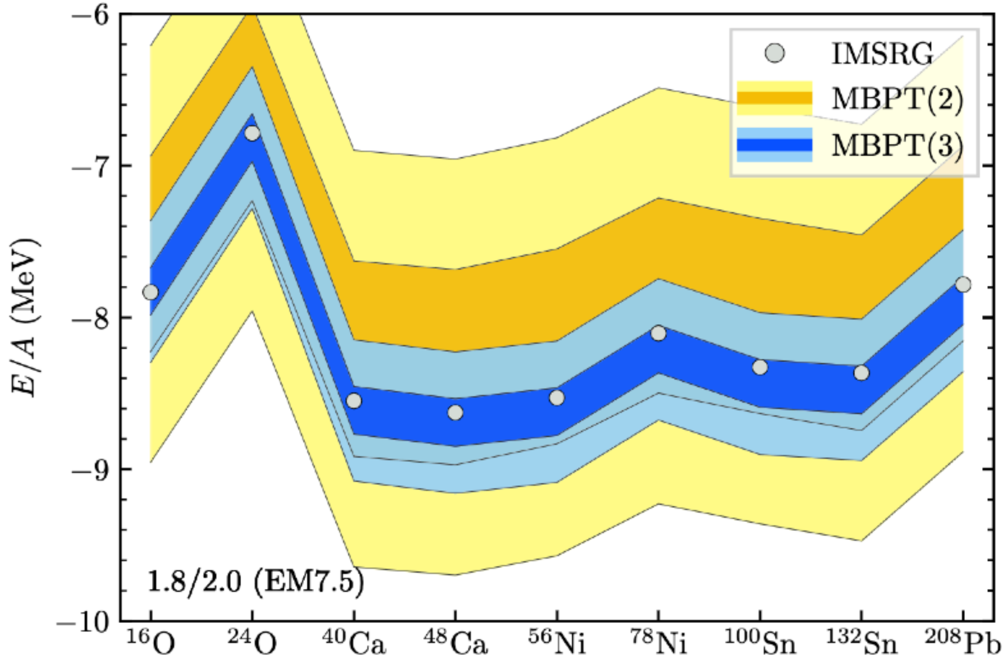


[Drischler et al., *PRL* **125** (2020)]

See Anthea's talk for astro application!

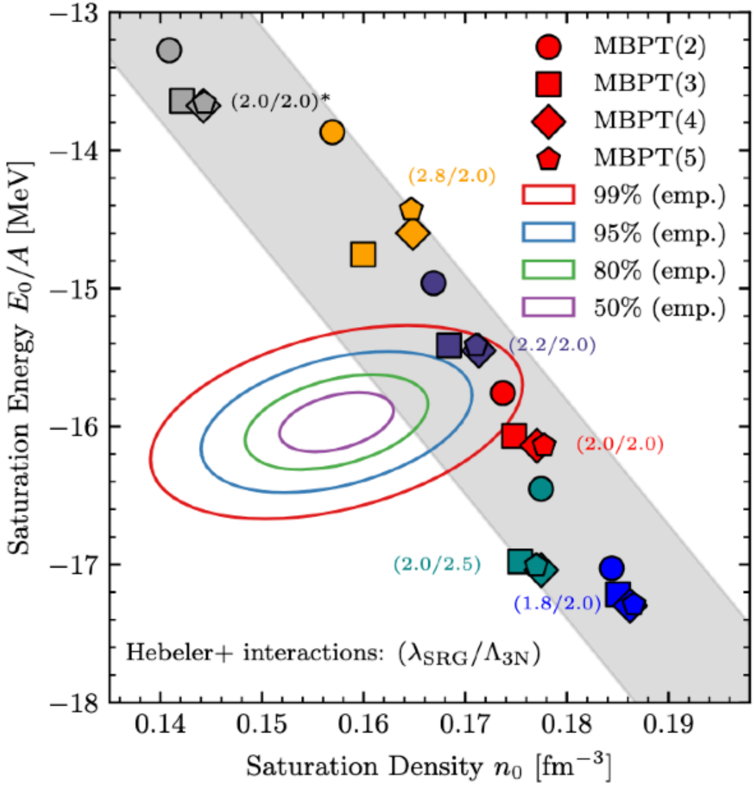
Ab initio MBPT review: [Tichai, Roth, Duguet, *Front. Phys.* **8** (2020)]

Uncertainty quantification in nuclei



[Svensson, Tichai, Hebeler, Schwenk, *PRC* **113** (2026)]

High-order MBPT for infinite matter



[Drischler, McElvain, Arthuis, *PRC* (in press.), arXiv:2603.24532]

A word of caution

Series expansion

Rayleigh-Schrödinger

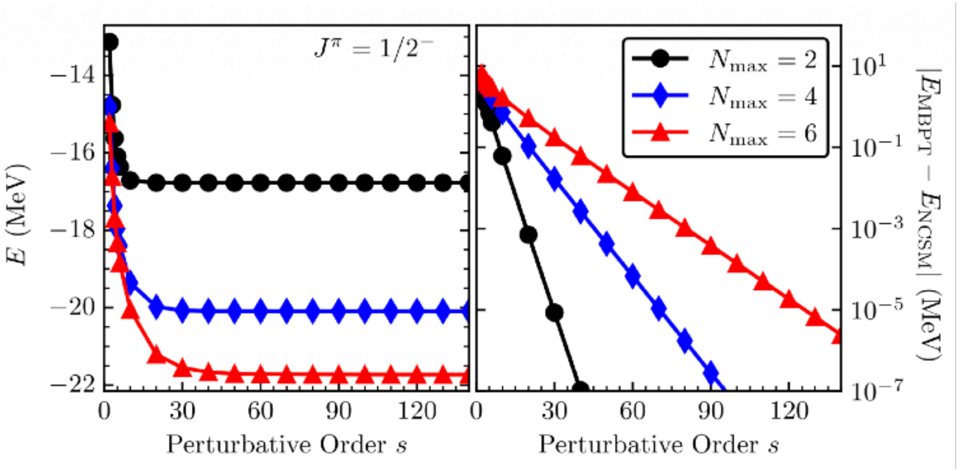
Brillouin-Wigner

Partitioning

Møller-Plesset

Epstein-Nesbet

Some recent Brillouin-Wigner results



[Li, Smirnova, *PRC* **109** (2024)]

Case study A:
Many-body pertubation theories

Expansion methods and symmetry

Operators of interest

- Nuclear Hamiltonian: $H = T + V + W$
- Particle number operator: A
- Grand canonical potential: $\Omega = H - \lambda A$

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A-body eigenvalue problem

$$H\,|\Psi_k^{\mathrm{A}}\rangle = \mathrm{E}_k^{\mathrm{A}}\,|\Psi_k^{\mathrm{A}}\rangle$$

Particle-number conserving

- Split H: $H = H_0 + H_1$

$$[A, H_0] = 0$$

- Introduce reference state

$$|\Psi_0^{\mathrm{A}}\rangle = U^{\mathrm{A}}(\infty)|\Phi^{\mathrm{A}}\rangle$$

Wave operator to be expanded
Reference state sol° of SE

$$H_0|\Psi^{\mathrm{A}}\rangle = \mathrm{E}_0^{\mathrm{A}}|\Phi^{\mathrm{A}}\rangle$$

Symmetry-conserving method
$\rightarrow$ Slater determinant

Operators of interest

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Expansion methods and degenerate systems

- **Basic idea: collect dynamical correlations through ph excitations**

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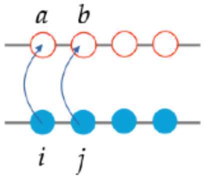
Closed-shell



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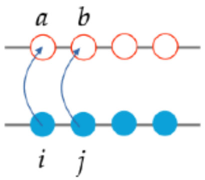

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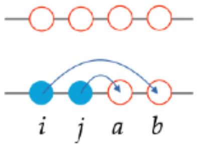

Degeneracy w.r.t ph excitations

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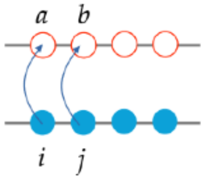

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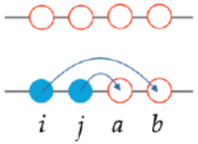

Degeneracy w.r.t ph excitations

- Expansion breakdown signals non-dynamical correlations (superfluidity…)

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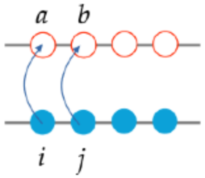

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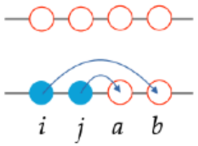

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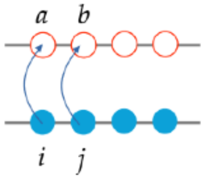

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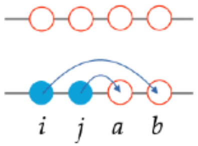

Degeneracy w.r.t ph excitations

- Expansion breakdown signals non-dynamical correlations (superfluidity…)
- Various possible approaches
    - High-order non-perturbative methods (if near-degenerate)

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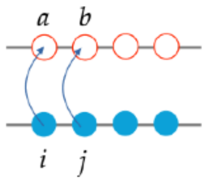

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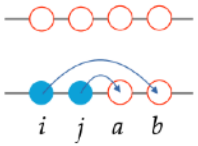

Degeneracy w.r.t ph excitations

- Expansion breakdown signals non-dynamical correlations (superfluidity…)
- Various possible approaches
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    - Multi-reference / configuration methods (MR-MBPT, MR-CC, MCPT, MR-IMSRG…)

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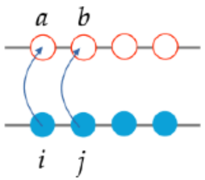
Closed-shell



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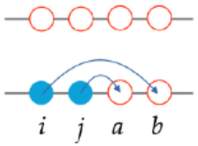

Degeneracy w.r.t ph excitations

- Expansion breakdown signals non-dynamical correlations (superfluidity…)
- Various possible approaches
  - High-order non-perturbative methods (if near-degenerate)
  - Multi-reference / configuration methods (MR-MBPT, MR-CC, MCPT, MR-IMSRG…)
  - Use a symmetry-breaking reference state (BMBPT, BCC, GSCGF, BIMSRG)

Expansion methods and degenerate systems

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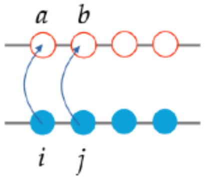
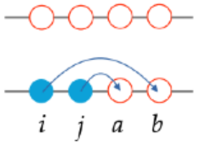


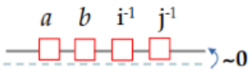
Open-shell



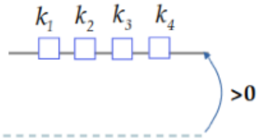
Degeneracy w.r.t ph excitations

- Expansion breakdown signals non-dynamical correlations (superfluidity…)
- Various possible approaches
    - High-order non-perturbative methods (if near-degenerate)
    - Multi-reference / configuration methods (MR-MBPT, MR-CC, MCPT, MR-IMSRG…)
    - Use a symmetry-breaking reference state (BMBPT, BCC, GSCGF, BIMSRG)

Degenerate Slater



Lift the degeneracy



Bogoliubov vacuum

Expansion methods and symmetry

Particle-number conserving

- Split H: $H = H_0 + H_1$

$$[A, H_0] = 0$$

- Introduce reference state

$$|\Psi_0^A\rangle = U^A(\infty)|\Phi^A\rangle$$

Wave operator to be expanded
Reference state sol° of SE

$$H_0|\Psi^A\rangle = E_0^A|\Phi^A\rangle$$

Symmetry-conserving method
$\rightarrow$ Slater determinant

Operators of interest

- Nuclear Hamiltonian: $H = T + V + W$
- Particle number operator: A
- Grand canonical potential: $\Omega = H - \lambda A$

A-body eigenvalue problem

$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$

Particle-number conserving

- Split H: $H = H_0 + H_1$

$$[A, H_0] = 0$$

- Introduce reference state

$$|\Psi_0^{\mathrm{A}}\rangle = U^{\mathrm{A}}(\infty)\,|\Phi^{\mathrm{A}}\rangle$$

Wave operator to be expanded
Reference state sol° of SE

$$H_0\,|\Psi^{\mathrm{A}}\rangle = \mathrm{E}_0^{\mathrm{A}}\,|\Phi^{\mathrm{A}}\rangle$$

Symmetry-conserving method
$\rightarrow$ Slater determinant

Operators of interest

- Nuclear Hamiltonian: $H = T + V + W$
- Particle number operator: A
- Grand canonical potential: $\Omega = H - \lambda A$

A-body eigenvalue problem

$$H\,|\Psi_k^{\mathrm{A}}\rangle = \mathrm{E}_k^{\mathrm{A}}\,|\Psi_k^{\mathrm{A}}\rangle$$

Particle-number breaking

- Split Ω: $\Omega = \Omega_0 + \Omega_1$

$$[A, \Omega_0] \neq 0$$

- Introduce reference state

$$|\Psi_0^{\mathrm{A}}\rangle = U(\infty)\,|\Phi\rangle$$

Wave operator to be expanded
Reference state sol° of SE

$$\Omega_0\,|\Phi\rangle = \mathrm{E}_0\,|\Phi\rangle$$

Symmetry-breaking method
$\rightarrow$ Bogoliubov ref. state

Particle-number projected BMBPT formalism

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Exact diagrammatic expansion with symmetry breaking and restoration

[Duguet and Signoracci, J. Phys. G 44, 015103 (2017)]

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Formalism actualisation

Particle-number projected BMBPT formalism

Exact diagrammatic expansion with symmetry breaking and restoration

[Duguet and Signoracci, J. Phys. G 44, 015103 (2017)]

Formalism actualisation

Expand off-diagonal kernels

$$\langle \Psi | H | \Phi(\phi) \rangle \quad ; \quad \langle \Psi | \Phi(\phi) \rangle$$

Symmetry restoration

Particle-number projected BMBPT formalism

Exact diagrammatic expansion with symmetry breaking and restoration

[Duguet and Signoracci, J. Phys. G 44, 015103 (2017)]

Formalism actualisation

Expand off-diagonal kernels

$$\langle \Psi | H | \Phi(\phi) \rangle \quad ; \quad \langle \Psi | \Phi(\phi) \rangle$$

Symmetry restoration

Diagonal reduction

$$\langle \Psi | H | \Phi \rangle \quad ; \quad \langle \Psi | \Phi \rangle$$

No symmetry restoration

Bogoliubov reference state

Bogoliubov reference state

Bogoliubov vacuum $|\Phi\rangle$: $\beta_k|\Phi\rangle = 0 \forall k$

$$\beta_p^\dagger \equiv \sum_k U_{pk} c_k^\dagger + V_{pk} c_k$$

$$\beta_p \equiv \sum_k U_{pk}^* c_k + V_{pk}^* c_k^\dagger$$

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$$A|\Phi\rangle \neq |\Phi\rangle$$

Breaks U(1) symmetry

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Particle-number breaking

$$A|\Phi\rangle \neq |\Phi\rangle$$

Breaks U(1) symmetry

$$H \Rightarrow \Omega = H - \lambda A$$

Grand potential Ω in qp basis, normal-ordered w.r.t. $|\Phi\rangle$:

$$\Omega = \Omega^{00} + \frac{1}{1!}\sum_{k_1k_2}\Omega^{11}_{k_1k_2}\beta^\dagger_{k_1}\beta_{k_2} + \frac{1}{2!}\sum_{k_1k_2}\left\{\Omega^{20}_{k_1k_2}\beta^\dagger_{k_1}\beta^\dagger_{k_2} + \Omega^{02}_{k_1k_2}\beta_{k_2}\beta_{k_1}\right\}$$
$$+ \frac{1}{(2!)^2}\sum_{k_1k_2k_3k_4}\Omega^{22}_{k_1k_2k_3k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta_{k_4}\beta_{k_3} + \frac{1}{3!}\sum_{k_1k_2k_3k_4}\left\{\Omega^{31}_{k_1k_2k_3k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta^\dagger_{k_3}\beta_{k_4} + \Omega^{13}_{k_1k_2k_3k_4}\beta^\dagger_{k_1}\beta_{k_4}\beta_{k_3}\beta_{k_2}\right\}$$
$$+ \frac{1}{4!}\sum_{k_1k_2k_3k_4}\left\{\Omega^{40}_{k_1k_2k_3k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta^\dagger_{k_3}\beta^\dagger_{k_4} + \Omega^{04}_{k_1k_2k_3k_4}\beta_{k_4}\beta_{k_3}\beta_{k_2}\beta_{k_1}\right\} + \ldots$$

Time-dependent BMBPT

Grand potential partitioning:

$$\Omega_0 = \Omega^{00} + \bar{\Omega}^{11} = \Omega^{00} + \sum_k E_k \beta_k^\dagger \beta_k$$

$$\Omega_1 = \breve{\Omega}^{11} + \Omega^{20} + \Omega^{02} + \Omega^{[4]} + \Omega^{[6]}$$

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Time-evolved state

$$\begin{aligned} |\Psi(\tau)\rangle &\equiv \mathscr{U}(\tau)|\Phi\rangle \\ &= e^{-\tau\Omega_0} T e^{-\int_0^\tau d\tau \Omega_1(\tau)} |\Phi\rangle \end{aligned}$$

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Ground-state energy of an open-shell nucleus

$$\mathrm{E}_0^{\mathrm{A}} - \lambda \mathrm{A} = \langle \Psi_0^{\mathrm{A}} | \Omega | \Phi \rangle_c = \lim_{\tau \to \infty} \langle \Phi | T e^{-\int_0^\tau d\tau_1 \Omega_1(\tau)} \Omega | \Phi \rangle_c$$

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Propagators:

$$G_{k_1k_2}^{+-(0)}(\tau_1, \tau_2) = \frac{\langle \Phi | T[\beta_{k_1}^\dagger(\tau_1)\beta_{k_2}(\tau_2)] | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

$$G_{k_1k_2}^{-+(0)}(\tau_1, \tau_2) = \frac{\langle \Phi | T[\beta_{k_1}(\tau_1)\beta_{k_2}^\dagger(\tau_2)] | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

$$G_{k_1k_2}^{+-(0)}(\tau_1, \tau_2) = -G_{k_2k_1}^{-+(0)}(\tau_2, \tau_1)$$

Time-dependent BMBPT

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$$\Omega_0 = \Omega^{00} + \bar{\Omega}^{11} = \Omega^{00} + \sum_k E_k \beta_k^\dagger \beta_k$$

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Ground-state energy of an open-shell nucleus

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Propagators:

$$G^{+-(0)}_{k_1 k_2}(\tau_1, \tau_2) = \frac{\langle \Phi | T[\beta^\dagger_{k_1}(\tau_1)\beta_{k_2}(\tau_2)] | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

$$G^{-+(0)}_{k_1 k_2}(\tau_1, \tau_2) = \frac{\langle \Phi | T[\beta_{k_1}(\tau_1)\beta^\dagger_{k_2}(\tau_2)] | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

$$G^{+-(0)}_{k_1 k_2}(\tau_1, \tau_2) = -\,G^{-+(0)}_{k_2 k_1}(\tau_2, \tau_1)$$

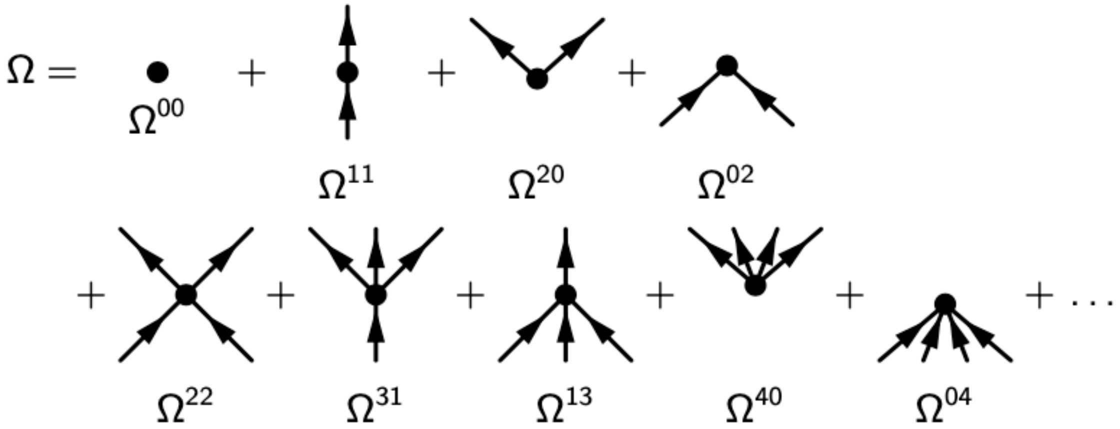
Perturbative expansion of g.s. energy:

$$\mathrm{E}_0^{\mathrm{A}} - \lambda \mathrm{A} = \langle \Phi | \{ \Omega(0) - \int_0^\infty d\tau_1 T[\Omega_1(\tau_1)\Omega(0)] + \frac{1}{2!}\int_0^\infty d\tau_1 d\tau_2 T[\Omega_1(\tau_1)\Omega_1(\tau_2)\Omega(0)] \ldots \} | \Phi \rangle_c$$

Building blocks of the diagrammatic

Building blocks of the diagrammatic

Normal-ordered form of Ω with respect to $|\Phi\rangle$



Building blocks of the diagrammatic

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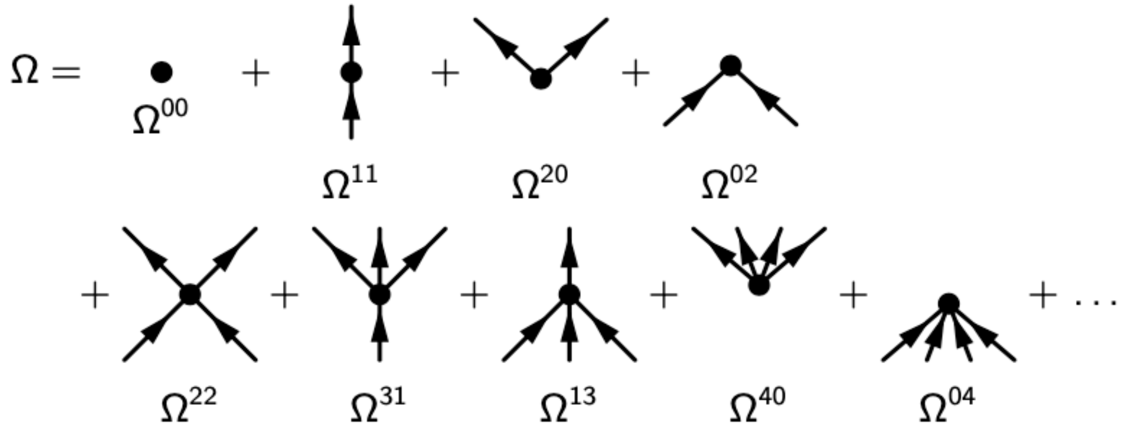
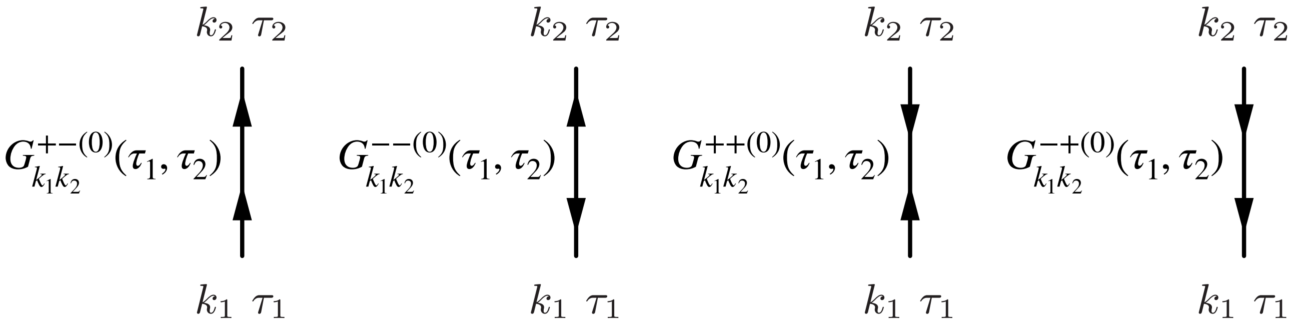
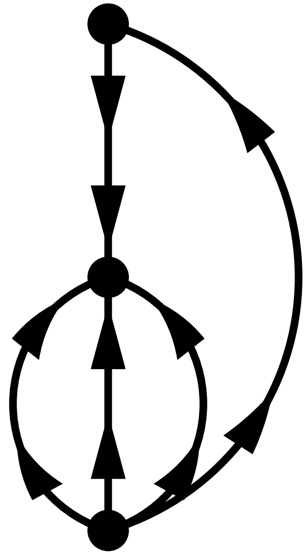


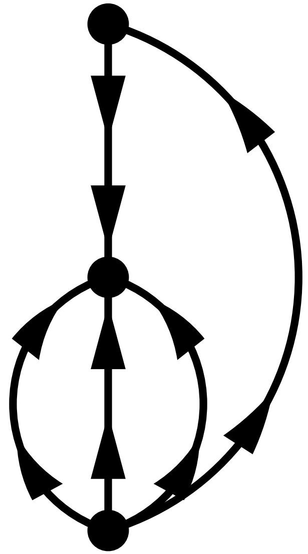
Quasiparticle propagators





I. Topological rules

- No external legs
- No oriented loop between vertices
- No self-contraction
- Propagators go out of the Ω vertex at time 0

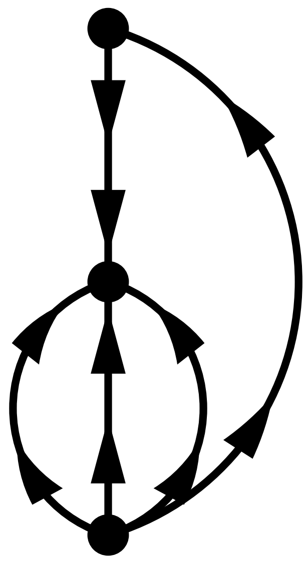


I. Topological rules

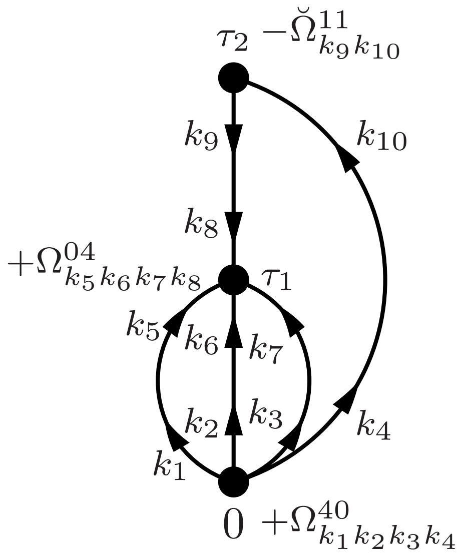
- No external legs
- No oriented loop between vertices
- No self-contraction
- Propagators go out of the Ω vertex at time 0

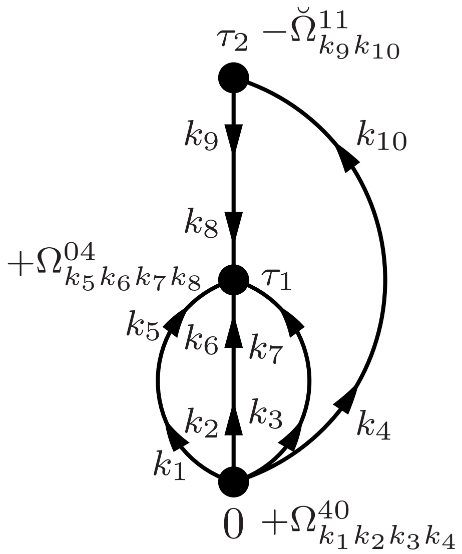
II. Algebraic rules

- Vertex, propagators labelling
- Sign factor for crossing lines
- Symmetry factor for equivalent lines, vertex exchange
- Sum over all q.p. states, integrate over all time labels



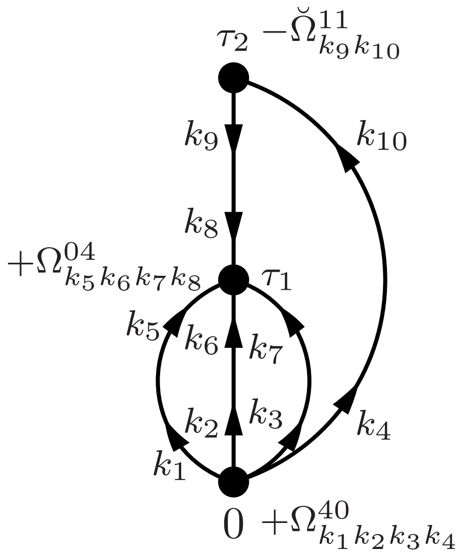
Derivation of a second-order diagram





Convention

Order p ⇔ Order p+1 in standard counting



Convention

Order p ⇔ Order p+1 in standard counting

Time-dependent and time-integrated expressions:

$$P\Omega 2.6 = -\frac{1}{3!}\sum_{k_1k_2k_3k_4k_8} \Omega^{40}_{k_1k_2k_3k_4}\Omega^{04}_{k_1k_2k_3k_8}\breve{\Omega}^{11}_{k_8k_4}\int_0^{\infty} d\tau_1 d\tau_2 \theta(\tau_1-\tau_2) e^{-\tau_1(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_8})} e^{\tau_2(E_{k_8}-E_{k_4})}$$

$$= -\frac{1}{3!}\sum_{k_1k_2k_3k_4k_8} \Omega^{40}_{k_1k_2k_3k_4}\Omega^{04}_{k_1k_2k_3k_8}\breve{\Omega}^{11}_{k_8k_4}\frac{1}{(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4})(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_8})}$$

How to build an automated framework

Technical goal

Technical goal

Challenges

How to build an automated framework

Technical goal

Challenges

Tools

How to build an automated framework

Technical goal

Challenges

Tools

End product

Technical goal

p-order diagram production

Challenges

Tools

End product

How to build an automated framework

Technical goal

p-order diagram production

p-order diagram evaluation

Challenges

Tools

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How to build an automated framework

Technical goal

p-order diagram production

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Challenges

Handling complexity of diagrams

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How to build an automated framework

Technical goal

p-order diagram production

p-order diagram evaluation

Challenges

Handling complexity of diagrams

Perform p-tuple time integral

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End product

How to build an automated framework

Technical goal

p-order diagram production	p-order diagram evaluation

Challenges

Handling complexity of diagrams	Perform p-tuple time integral

Tools

Adjacency matrices

End product

How to build an automated framework

Technical goal

p-order diagram production

p-order diagram evaluation

Challenges

Handling complexity of diagrams

Perform p-tuple time integral

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Time-structure diagrams

End product

How to build an automated framework

Technical goal

p-order diagram production | **p-order diagram evaluation**

Challenges

Handling complexity of diagrams | **Perform p-tuple time integral**

Tools

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End product

Open-source computer code

How to build an automated framework

Technical goal

p-order diagram production

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Automatic generation of diagrams

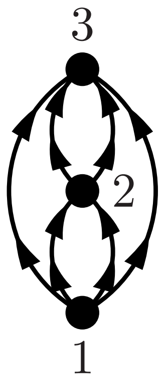
Oriented adjacency matrix from graph theory

Automatic generation of diagrams

Oriented adjacency matrix from graph theory

Topological rules constraining the matrices

- Upper triangular
- Zeros on the diagonal
- Cannot be recast as block-diagonal
- For each vertex i, $\sum_j (a_{ij} + a_{ji})$ is 2, 4 or 6



$$\longleftrightarrow \begin{pmatrix} 0 & 2 & 2 \\ 0 & 0 & 2 \\ 0 & 0 & 0 \end{pmatrix}$$

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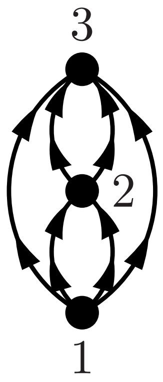

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Generation of BMBPT diagrams at order p

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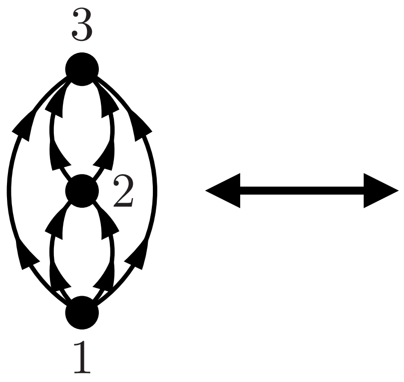

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Generation of BMBPT diagrams at order p

Algorithm

- Generate all $(p+1) \times (p+1)$ matrices
  - Fill them 'vertex-wise' with all allowed integers
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- Discard matrices leading to topologically identical diagrams
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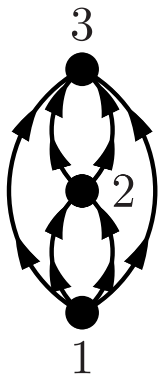

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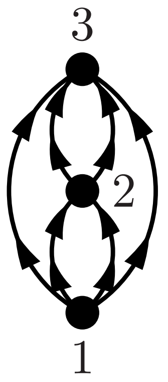

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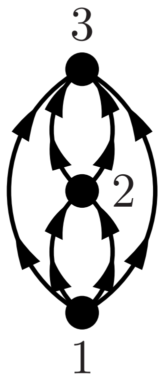

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$$\begin{pmatrix} 0 & 2 & 2 \\ 0 & 0 & {\color{red}2} \\ 0 & 0 & 0 \end{pmatrix}$$

Automatic generation of diagrams

Automatic generation of diagrams

3rd-order BMBPT diagrams for vertices with 2, 4 and 6 legs…

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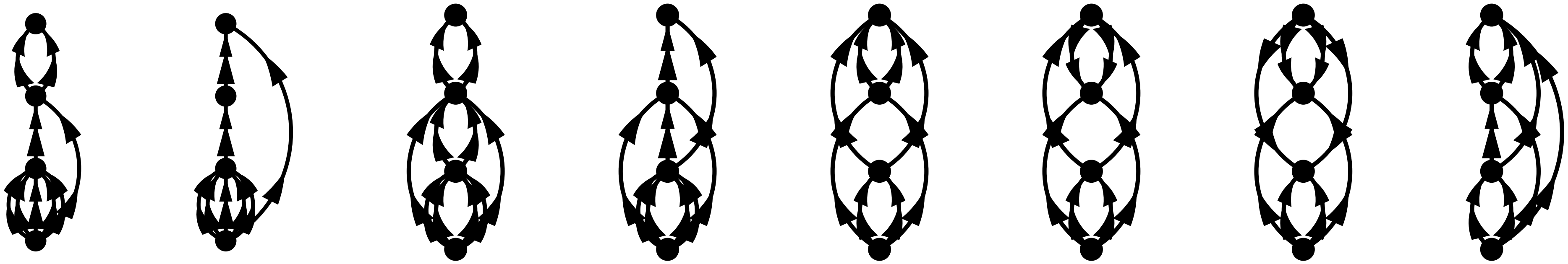
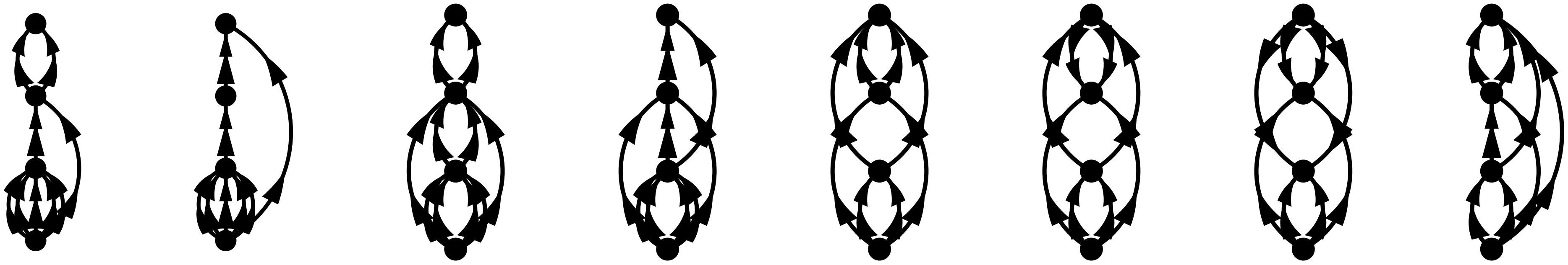
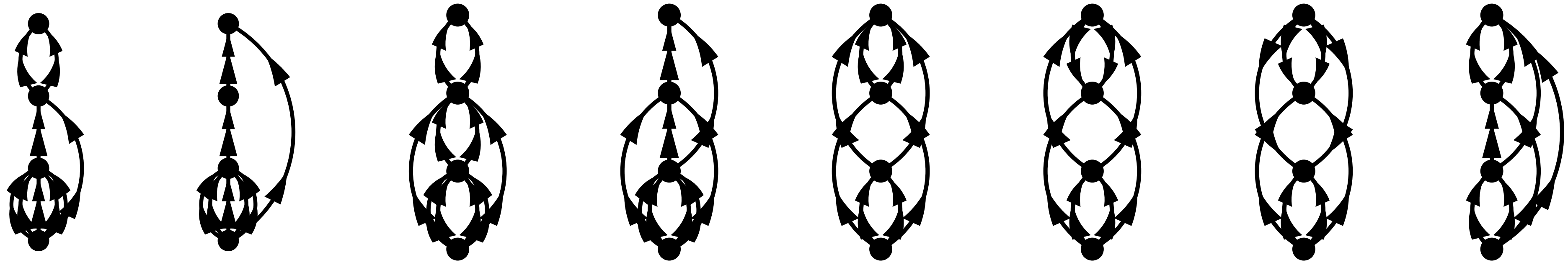


3rd-order BMBPT diagrams for vertices with 2, 4 and 6 legs…



+ 388 others!

3rd-order BMBPT diagrams for vertices with 2, 4 and 6 legs…



+ 388 others!

Systematic combinatoric

Order		0	1	2	3	4	5
Rank 4	General case	1	2	8	59	568	6 805
	HFB vacuum	1	1	1	10	82	938
Rank 6	General case	1	3	23	396	10 716	100 000+
	HFB vacuum	1	2	8	77	5 055	100 000+

How to build an automated framework

Technical goal

p-order diagram production | p-order diagram evaluation

Challenges

Handling complexity of diagrams | Perform p-tuple time integral

Tools

Adjacency matrices | Time-structure diagrams

End product

Open-source computer code

Time-structure diagrams

Time-structure diagrams

Integrand of p-tuple time integral governed by time structure of the diagram

$$TSD = \lim_{\tau \to \infty} \int_0^{\tau} \mathrm{d}\tau_1 \ldots \mathrm{d}\tau_p \, \theta(\tau_q - \tau_r) \ldots \theta(\tau_u - \tau_v) e^{-a_1 \tau_1} \ldots e^{-a_p \tau_p}$$

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Time-structure diagram extraction:

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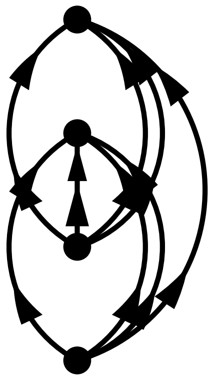
Time-structure diagram extraction:



Time-structure diagrams

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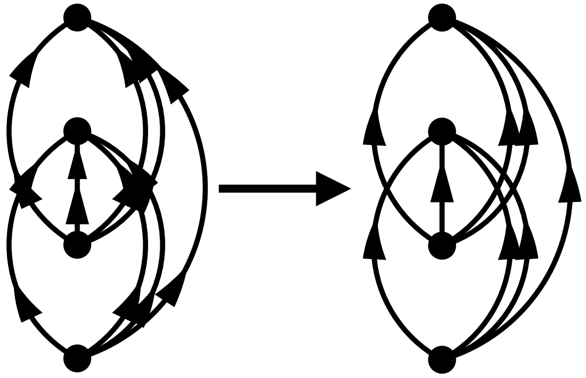

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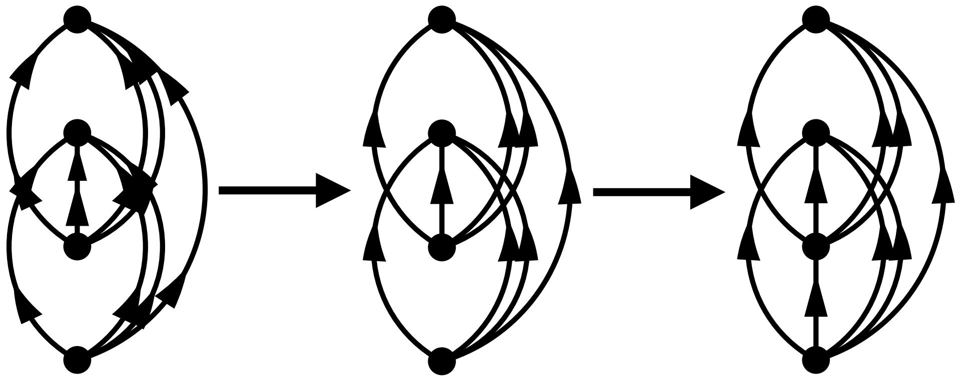

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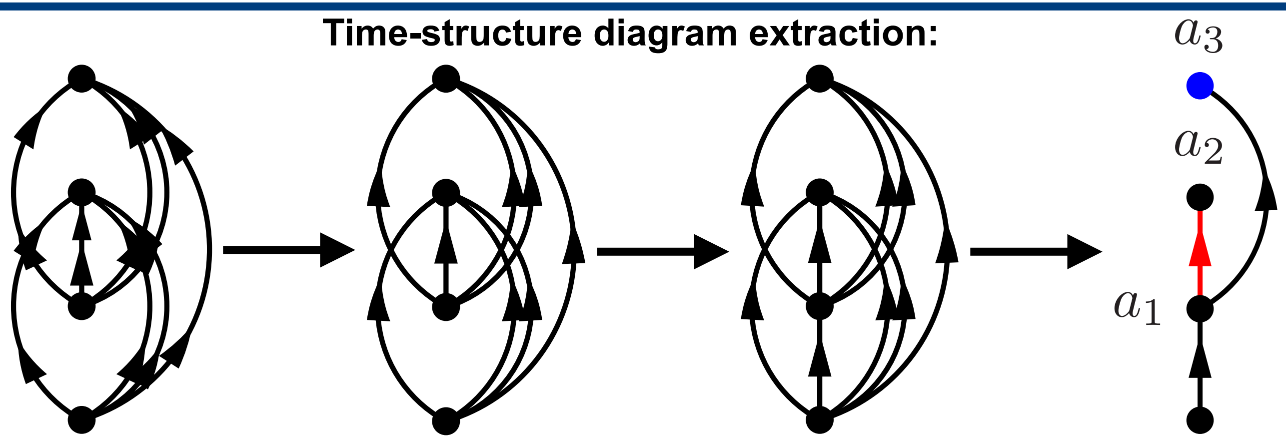

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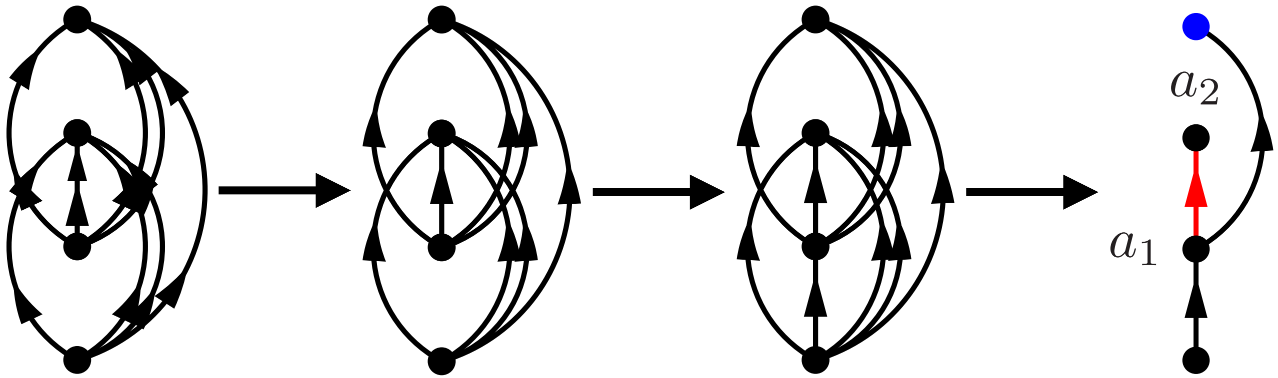

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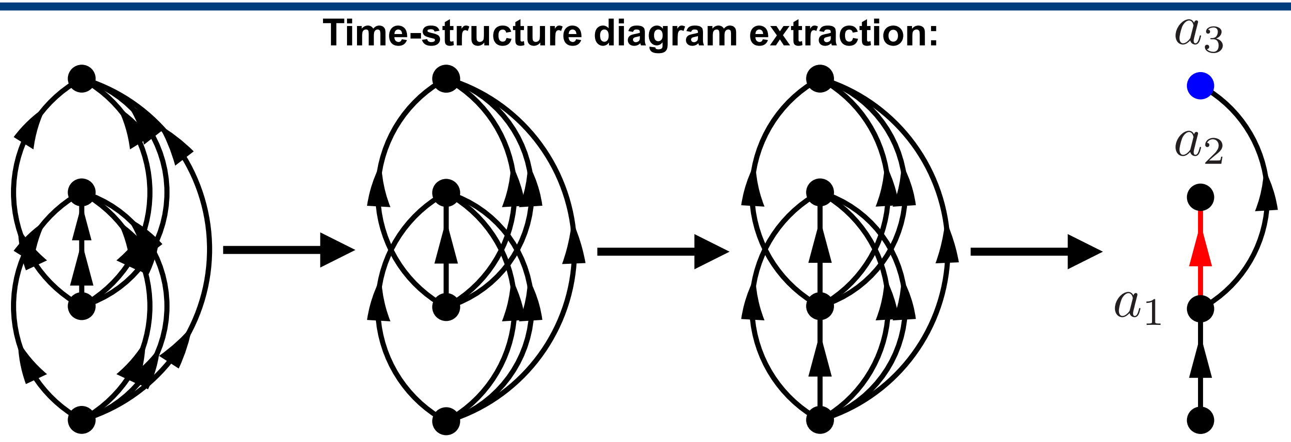

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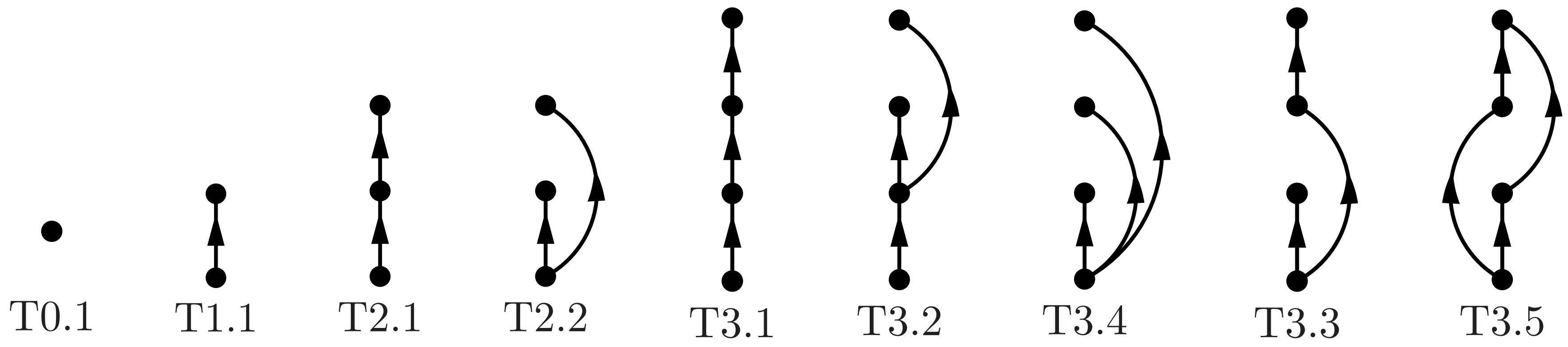
- Several BMBPT diagrams may have same TSD
- Replace a_i with appropriate q.p. energy sum for final expression

TSD topology crucial for result extraction



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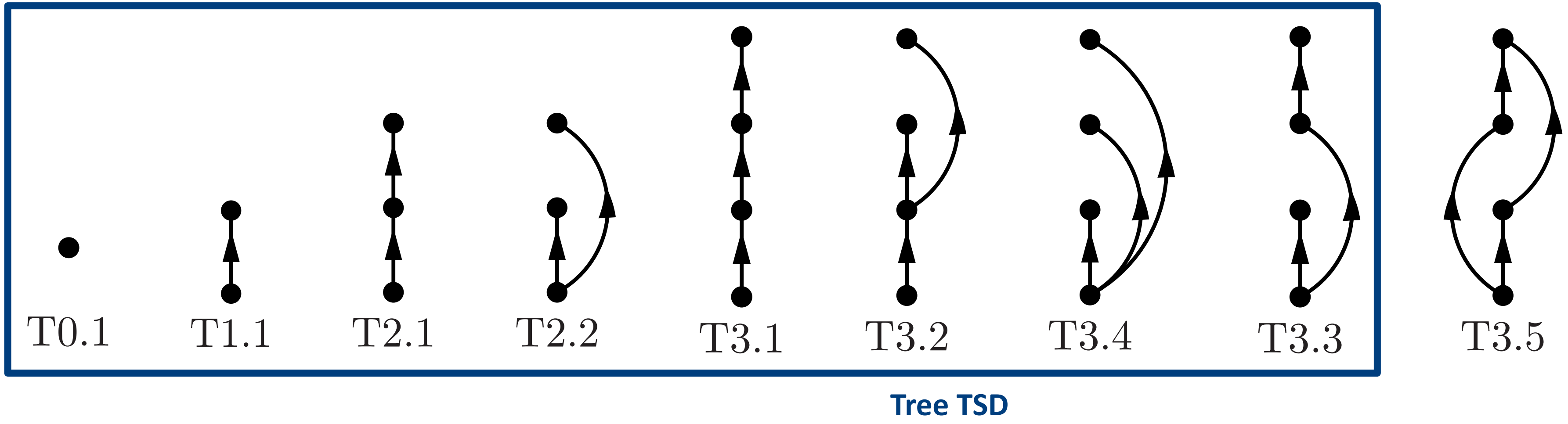

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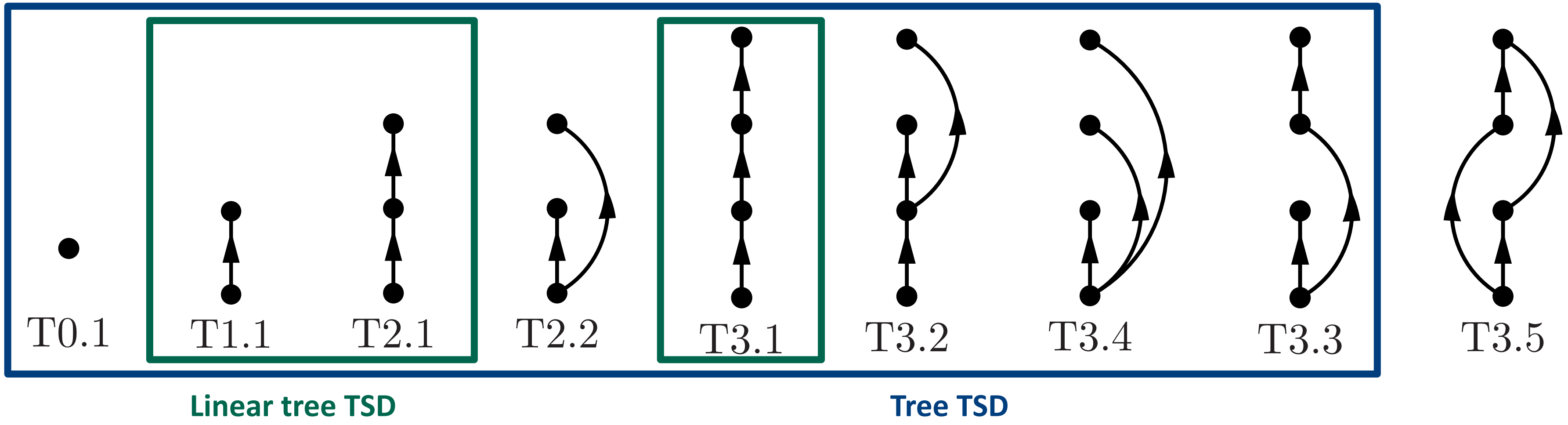

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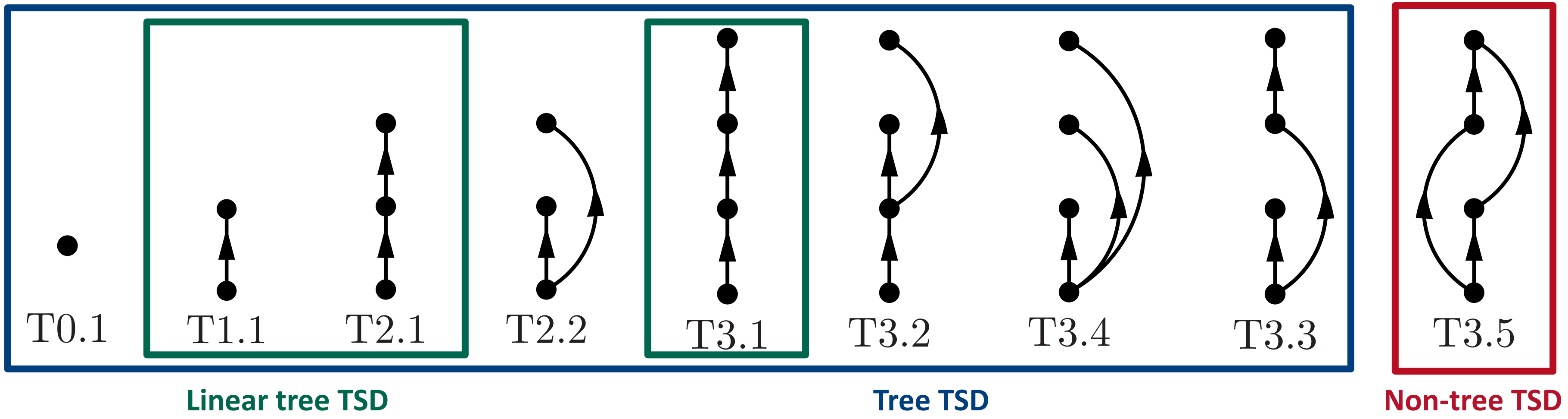
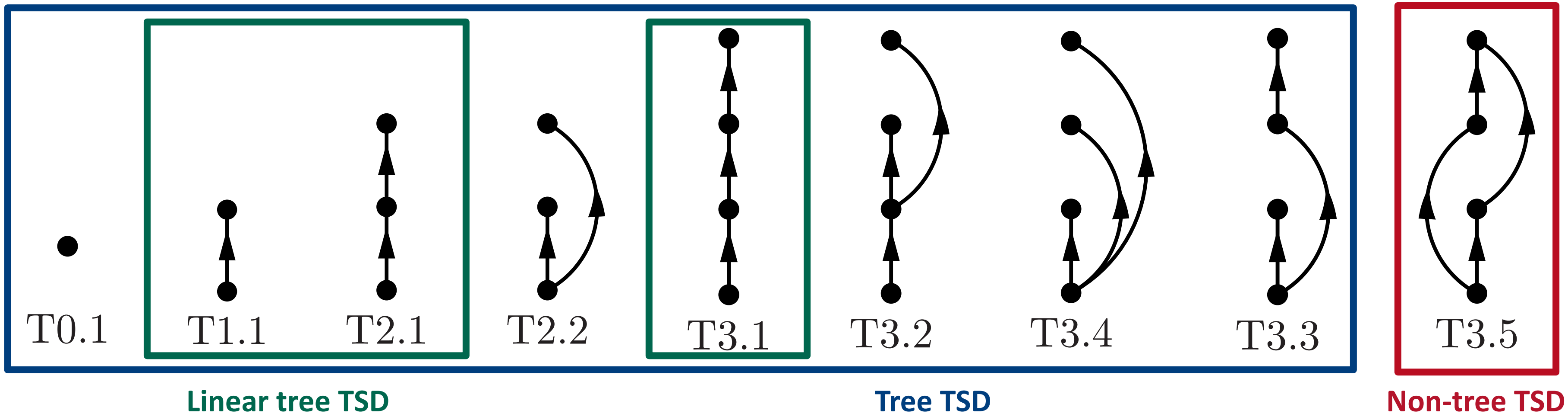


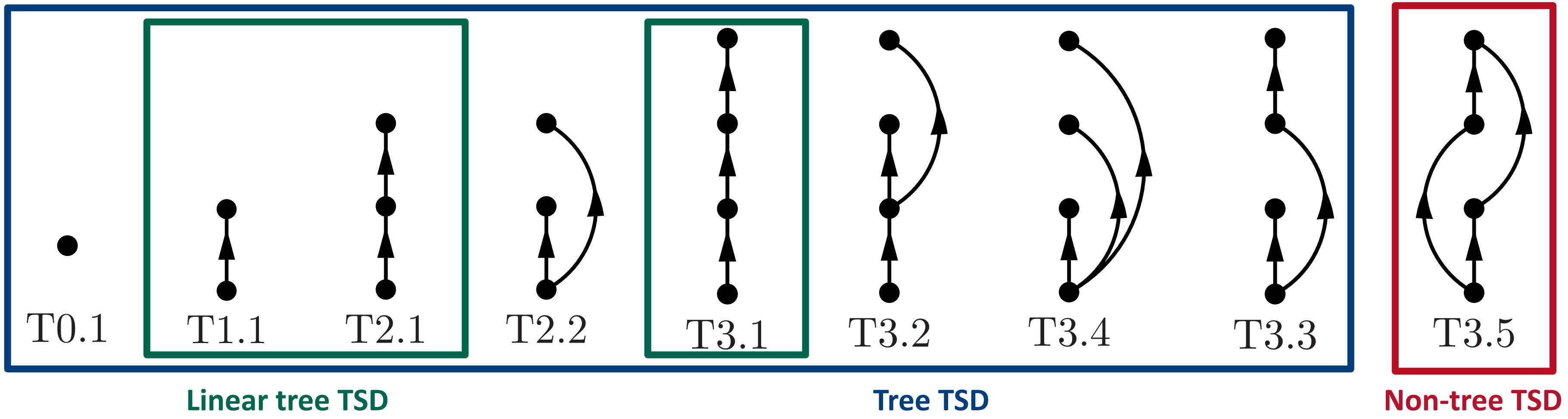
Topologies of time-structure diagrams

TSD topology crucial for result extraction



Extraction of time-integrated expressions depends on tree/non-tree

TSD topology crucial for result extraction



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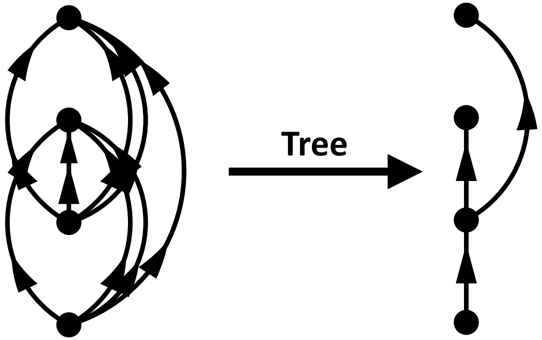
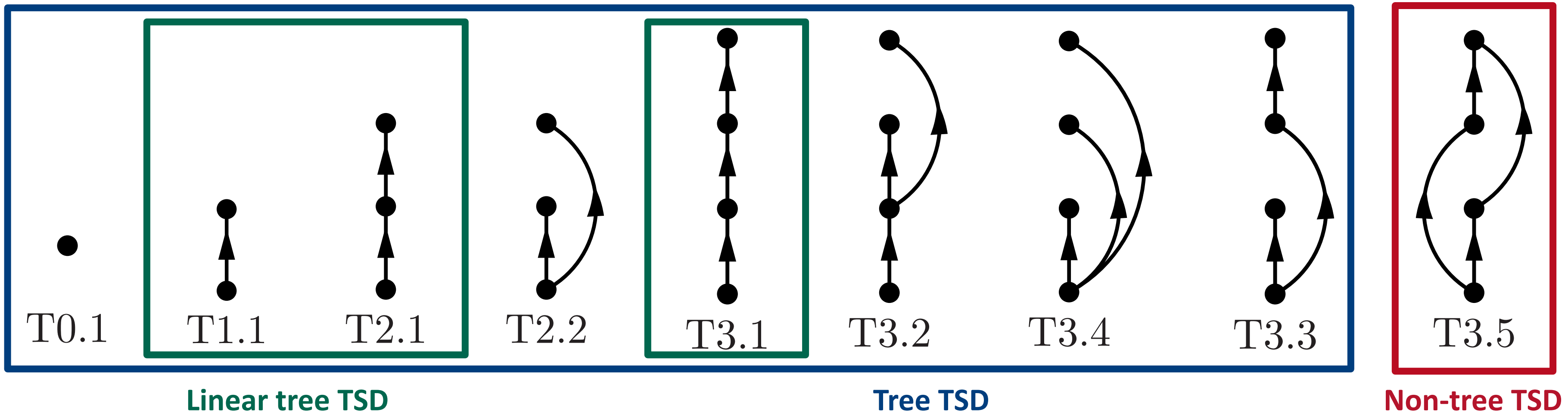


TSD topology crucial for result extraction



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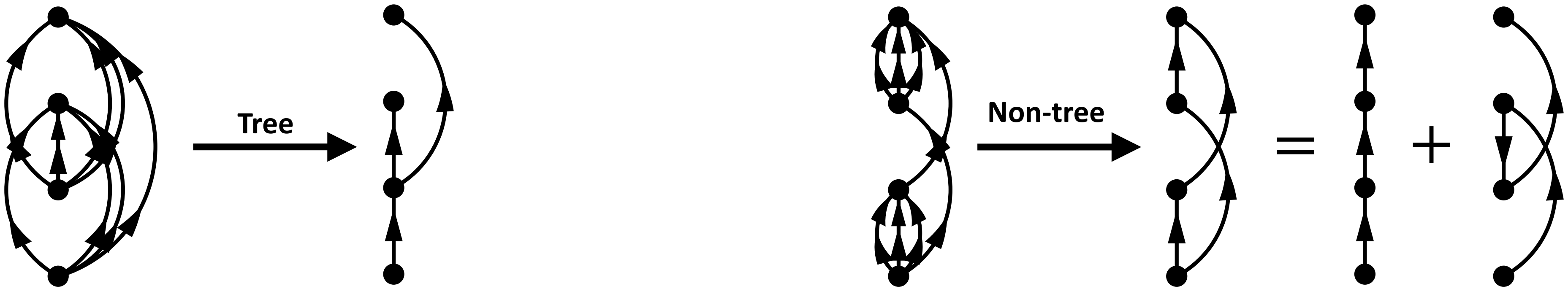

Denominator extraction and integral structure

Denominator extraction and integral structure

Why a so simple structure for all trees?

Link between tree TSD structure and time integrals structure

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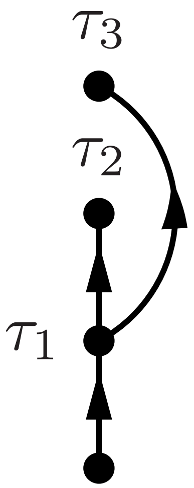

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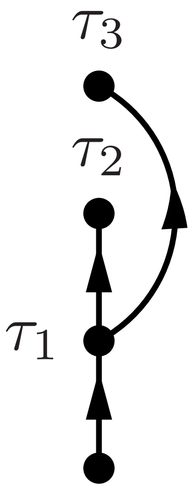

$$
\begin{aligned}
D &= \lim_{\tau\to\infty} \int_0^{\tau} d\tau_1 d\tau_2 d\tau_3 \theta(\tau_3 - \tau_1)\theta(\tau_2 - \tau_1) e^{a\tau_1} e^{b\tau_2} e^{c\tau_3} \\
&= \lim_{\tau\to\infty} \int_0^{\tau} d\tau_1 e^{a\tau_1} \int_0^{\tau_1} d\tau_2 e^{b\tau_2} \int_0^{\tau_1} d\tau_3 e^{c\tau_3} \\
&= \lim_{\tau\to\infty} \frac{1}{bc} \int_0^{\tau} d\tau_1 e^{a\tau_1} \left(e^{b\tau} - e^{b\tau_1}\right)\left(e^{c\tau} - e^{c\tau_1}\right) \\
&= \frac{1}{bc(a+b+c)}
\end{aligned}
$$

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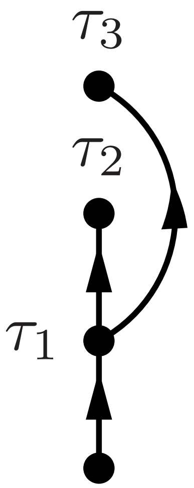

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&= \frac{1}{bc(a+b+c)}
\end{aligned}
$$

- Integrate from the leaves first
- Go down each branch
- Each vertes depends on the vertices above

New diagrammatic rule

New diagrammatic rule

Direct time-integrated expression extraction from time-unordered diagrams

New diagrammatic rule

Direct time-integrated expression extraction from time-unordered diagrams

For each perturbation vertex in a diagram associated to a tree TSD:

- Determine all its descendants using the TSD
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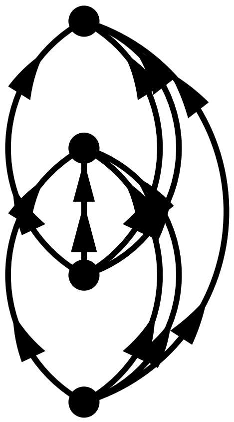

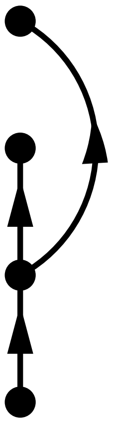

$$\frac{1}{\epsilon_{k_1k_2k_3k_4}\epsilon_{k_1k_2k_3k_5}\epsilon_{k_4k_6k_7k_8}} = \frac{1}{(a_1 + a_2 + a_3)a_2a_3}$$

New diagrammatic rule

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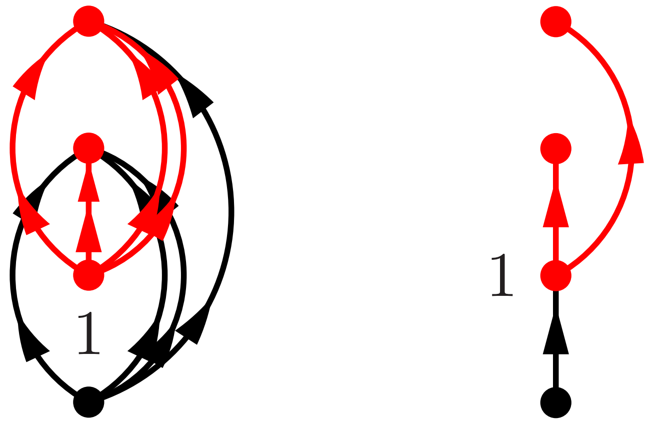

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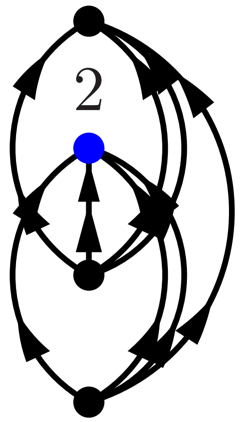

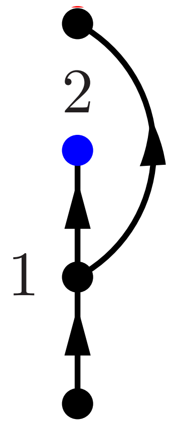

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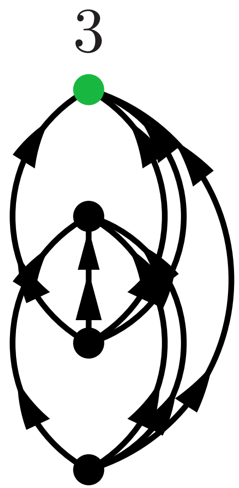

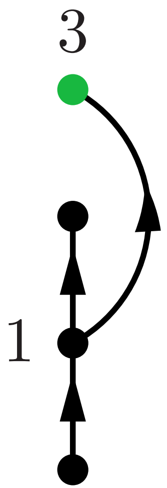

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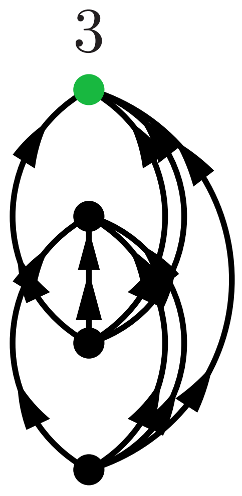

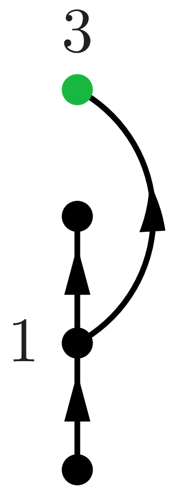

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New rule yields double, not quadruple

Physics of whole topology captured at once

New diagrammatic rule

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Direct time-integrated expression extraction from time-unordered diagrams

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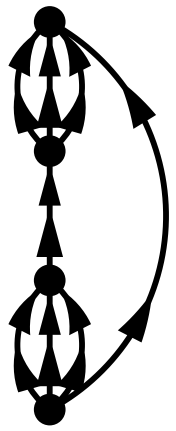

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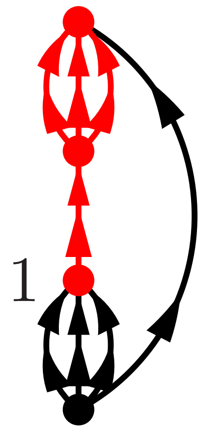

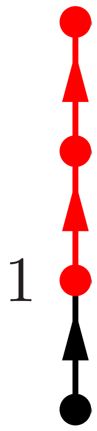

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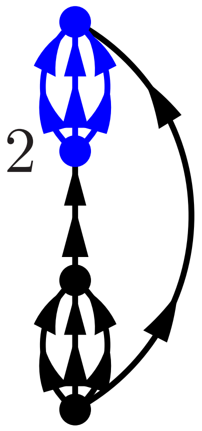

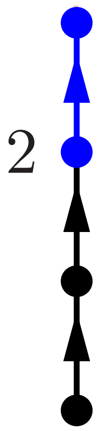

$$\frac{1}{\epsilon_{k_1k_2k_3k_4}{\color{blue}\epsilon_{k_5k_4}}\epsilon_{k_4k_6k_7k_8}} = \frac{1}{(a_1+a_2+a_3){\color{blue}(a_2+a_3)}a_3}$$

New diagrammatic rule

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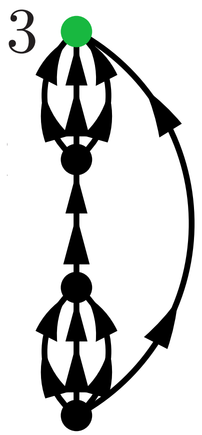

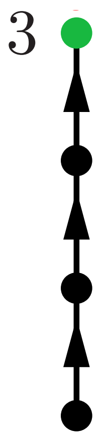

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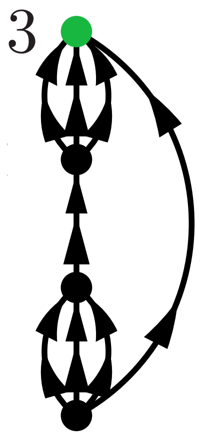

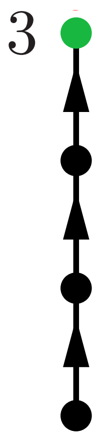

New rule reduces to resolvent rule for time-ordered diagrams

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Denominator extraction: Non-tree case

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If the associated TSD is not a tree:

- Separate the TSD into a sum of tree TSDs
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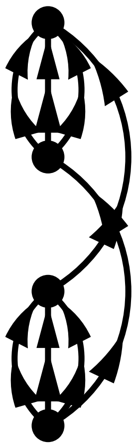

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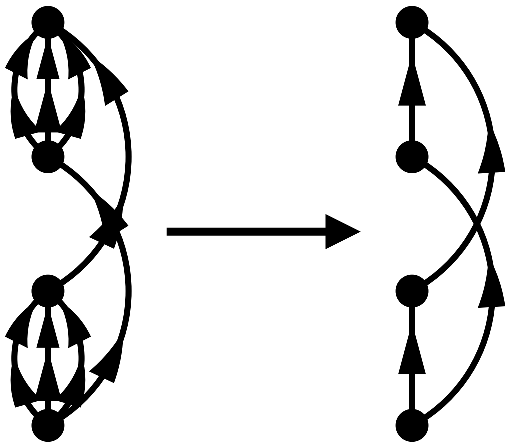

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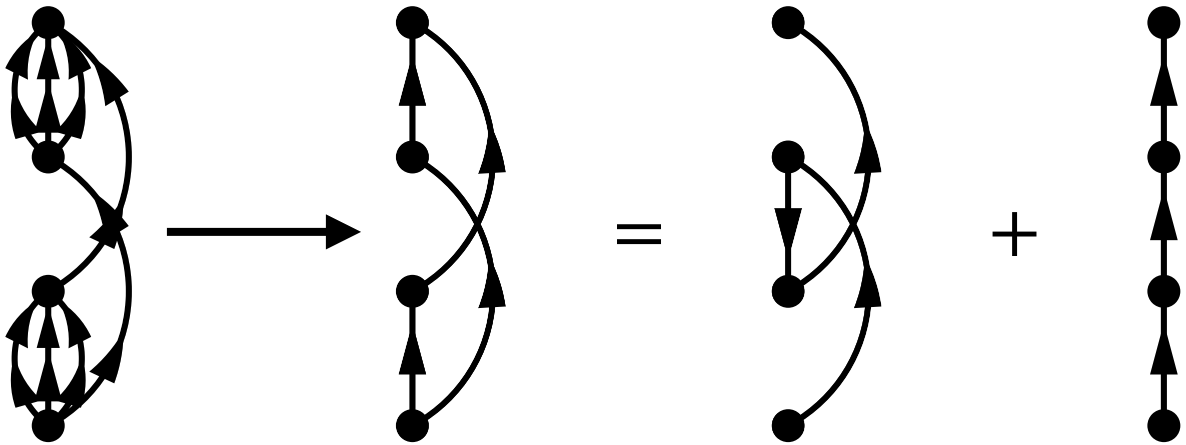

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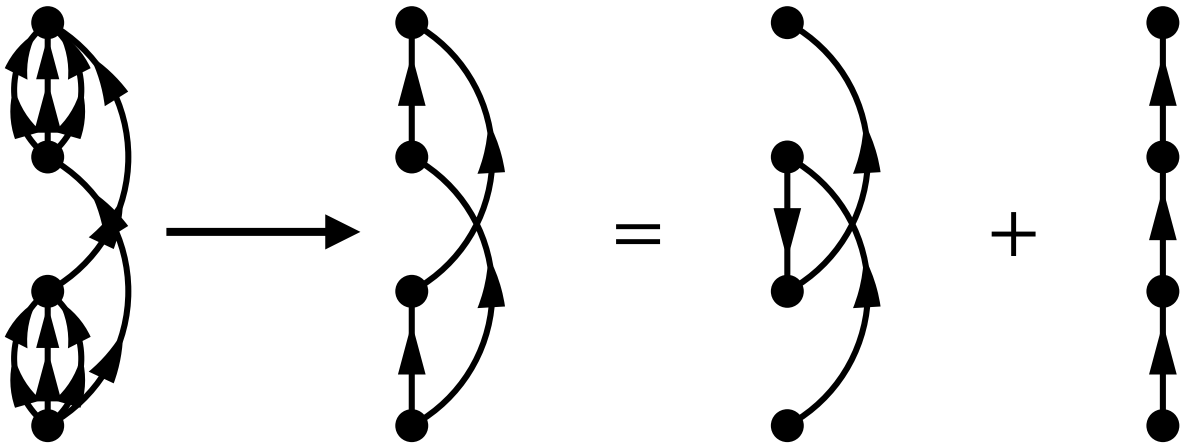

$$\frac{-(-1)^3}{(3!)^2}\sum_{k_i}\Omega^{40}_{k_1k_2k_3k_4}\Omega^{13}_{k_5k_1k_2k_3}\Omega^{31}_{k_6k_7k_8k_4}\Omega^{04}_{k_6k_7k_8k_5}\Big[\frac{1}{(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_6}+E_{k_7}+E_{k_8})(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4})(E_{k_5}+E_{k_6}+E_{k_7}+E_{k_8})}$$

$$+\frac{1}{(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4})(E_{k_4}+E_{k_5})(E_{k_5}+E_{k_6}+E_{k_7}+E_{k_8})}\Big]$$

How to build an automated framework

Technical goal

p-order diagram production

p-order diagram evaluation

Challenges

Handling complexity of diagrams

Perform p-tuple time integral

Tools

Adjacency matrices

Time-structure diagrams

End product

Open-source computer code

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Open-source computer code → Arbitrary order expressions

Time-unordered vs time-ordered diagrammatics

34

Time-dependent perturbation theory = Time-unordered diagrams

Time-independent perturbation theory = Time-ordered diagrams

34

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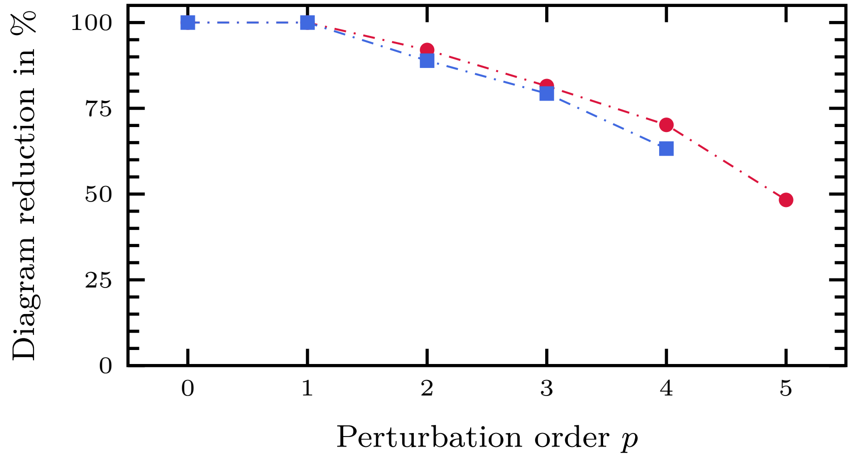
- A single time-unordered diagram may resum several time-ordered one
- Treatment of cycles ↔ Partial explicit reordering
- Less diagrams to deal with due to new diagrammatic method



34

Time-unordered vs time-ordered diagrammatics

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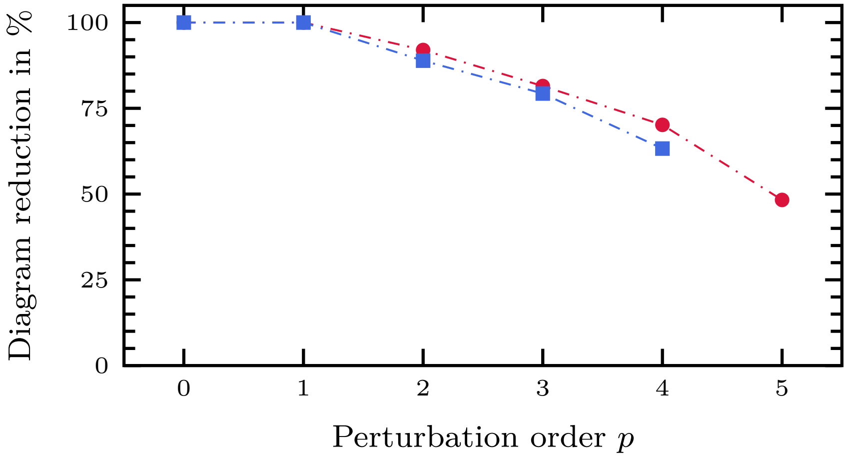

Maximum number of time-ordered diagrams resumed into a tree time-unordered diagram

Order	0	1	2	3	4	5	6	7
Rank 4	1	1	2	3	8	30	90	420
Rank 6	1	1	2	6	12	40	180	1008
p!	1	1	2	6	24	120	720	4040

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Towards projected BMBPT

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Projected PBMBPT as the next step:

- Symmetry restoration at arbitrary order
- Formalism was already available
- More complex diagrammatic structure departing from known cases

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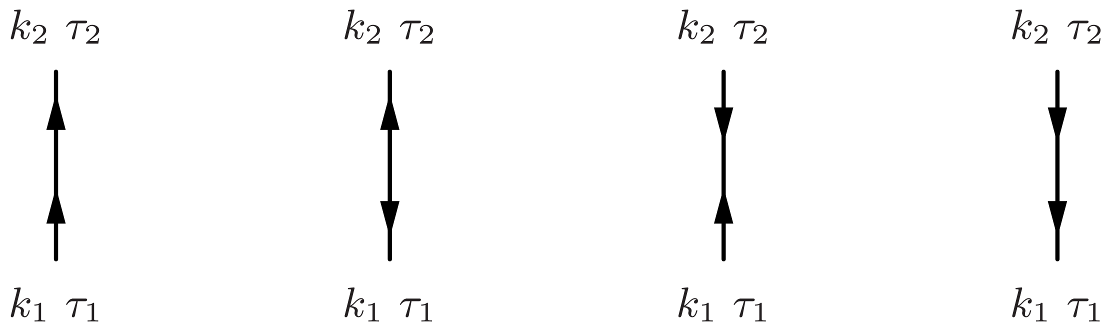
More refined formalism:

- Introduction of the anomalous contractions
- Introduction of self-contractions
- Tremendous increase in diagrams numbers
- Need to reduce complexity as much as feasible

More propagators?



$G^{+-(0)}_{k_1k_2}(\tau_1,\tau_2)$ $G^{--(0)}_{k_1k_2}(\tau_1,\tau_2)$ $G^{++(0)}_{k_1k_2}(\tau_1,\tau_2)$ $G^{-+(0)}_{k_1k_2}(\tau_1,\tau_2)$

$$G^{+-(0)}_{k_1k_2}(\tau_1,\tau_2) \equiv \frac{\langle \Phi | \mathrm{T}[\beta^\dagger_{k_1}(\tau_1)\beta_{k_2}(\tau_2)] | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

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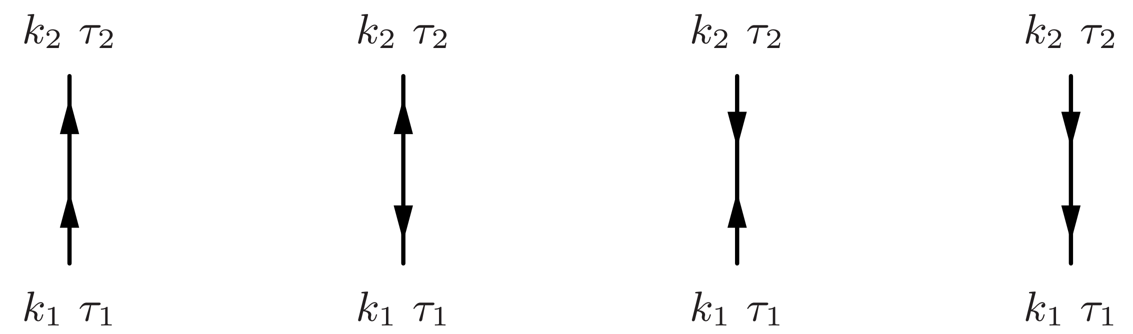
$$G^{+-(0)}_{k_1k_2}(\tau_1,\tau_2) = -\,G^{-+(0)}_{k_2k_1}(\tau_2,\tau_1)$$

$$G^{++(0)}_{k_1k_2}(\tau_1,\tau_2) = 0$$



$G^{+-(0)}_{k_1k_2}(\tau_1, \tau_2)$ $\quad$ $G^{--(0)}_{k_1k_2}(\tau_1, \tau_2)$ $\quad$ $G^{++(0)}_{k_1k_2}(\tau_1, \tau_2)$ $\quad$ $G^{-+(0)}_{k_1k_2}(\tau_1, \tau_2)$

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Only one more

How to produce an off-diagonal PBMBPT diagram?

How to produce an off-diagonal PBMBPT diagram?

Naive algorithm:

- Start from an existing diagonal diagram, i.e. normal BMBPT ones
- Turn normal propagators anomalous via all possible combinations (unchanged interaction rank)
- All self-contraction on vertices via all possible combinations (increase interaction rank)

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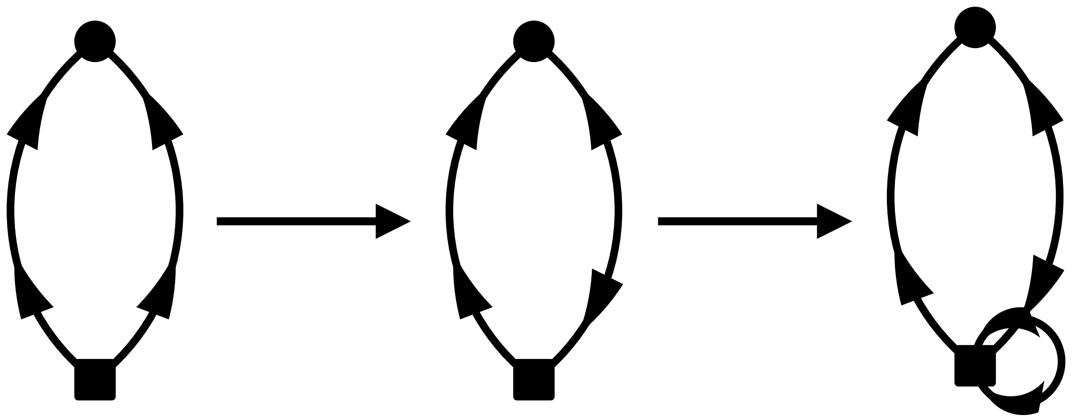

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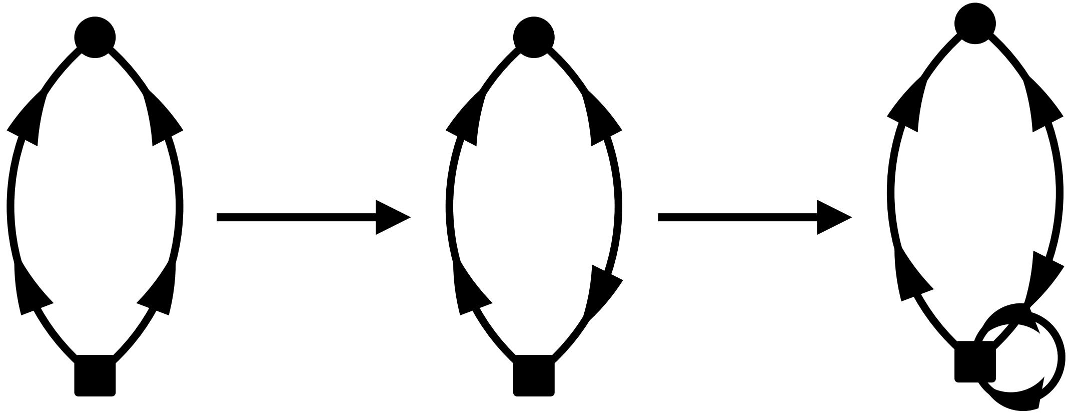
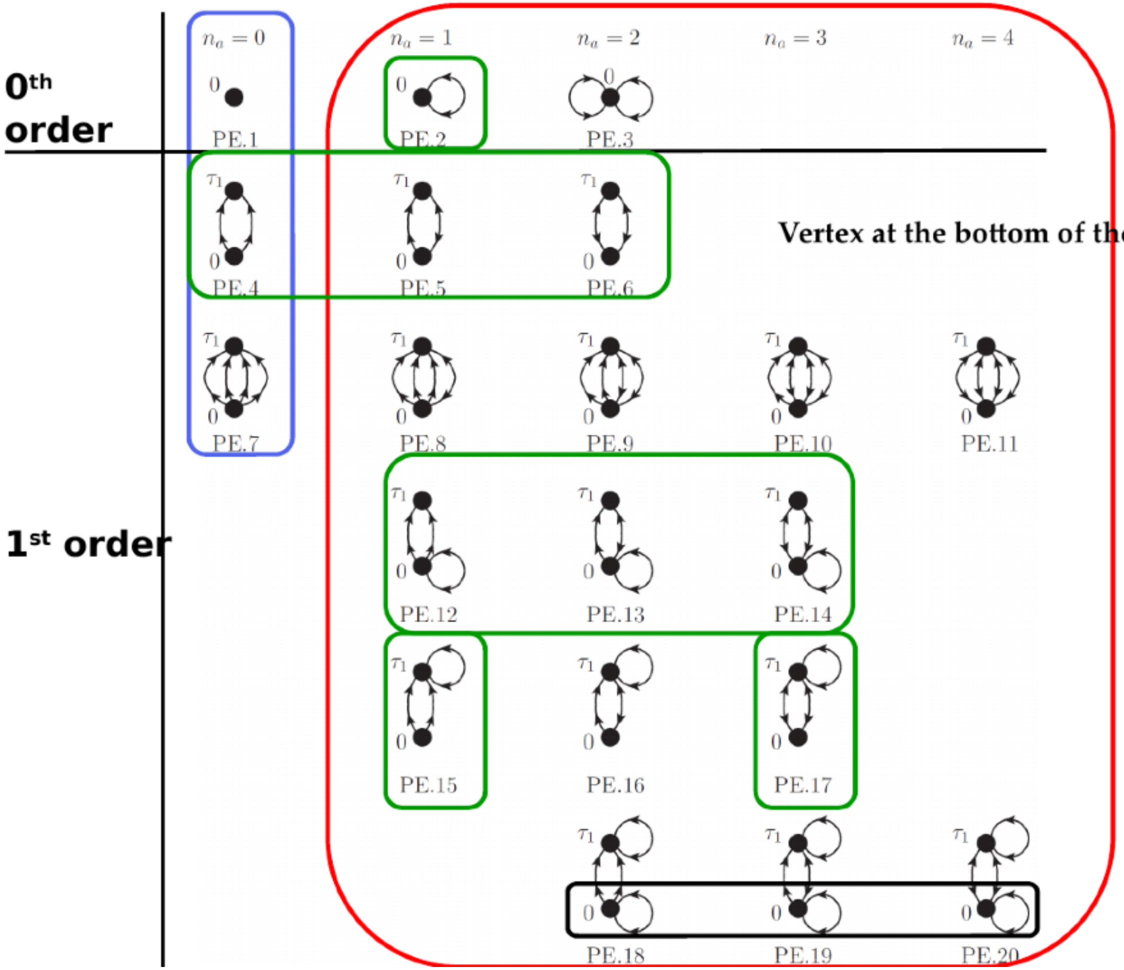


The combinatorics is not looking good...

A naive representation of PBMBPT diagrams



20 diagrams
3 diagrams
17 diagrams
9 diagrams

Vertex at the bottom of the diagrams at fixed time 0

Only contributions to $\varphi = 0$

Carry the φ dependence

Null for HFB reference state

Factorising complexity

39

Focusing on the effect of anomalous diagrams

- Anomalous propagators do not carry time dependency
- Time structure left unchanged if they apply to the operator vertex
- Refactor anomalous contributions on the operator vertex

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Similarity transformation

$$\tilde{O}(\varphi) \equiv e^{-Z(\varphi)} O e^{-Z(\varphi)}$$

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Reduction in the number of diagrams:

- Previous 20 diagrams reduce to only 4
- Overall scaling unaffected: other anomalous contractions remain

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How to produce all PBMBPT diagrams?

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Diagram generation:

- Reuse naive algorithm apart from operator vertex
- Avoid producing topologically equivalent diagrams in advance
- Eliminate leftover topologically equivalent diagrams on-the-fly

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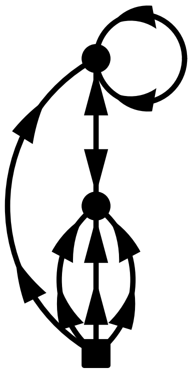
Generated diagrams

Order	0	1	2	3	4
BMBPT (rank 4)	1	2	8	59	568
BMBPT (rank 6)	1	3	23	396	10 716
PBMBPT (rank 4)	1	3	33	602	14 977
PBMBPT (rank 6)	1	6	189	13 046	…

Extend on diagonal BMBPT rules:

- Adjustment for symmetry factors
- Anomalous propagators give different q.p.e.s with respect to time labels τ
- Additional R^{--} factors for anomalous propagators
- Time-independent expressions need deeper extensions



$$\mathrm{PO2.3.3} = \lim_{\tau\to\infty} \frac{(-1)^2}{(3\,!)} \sum_{k_i} \tilde{O}^{40}_{k_1k_2k_3k_4}(\varphi)\Omega^{04}_{k_1k_2k_3k_5}\Omega^{04}_{k_6k_4k_7k_8}R^{--}_{k_6k_5}(\varphi)R^{--}_{k_8k_7}(\varphi)$$

$$\times \int_0^\tau \mathrm{d}\tau_1\mathrm{d}\tau_2\theta(\tau_2-\tau_1)\theta(\tau_2-\tau_2)e^{-\tau_1\epsilon_{k_1k_2k_3k_6}}e^{-\tau_2\epsilon_{k_4k_5k_7k_8}}$$

Extending the TSD rules by leaving them unchanged

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Remove all anomalous lines then proceed as before

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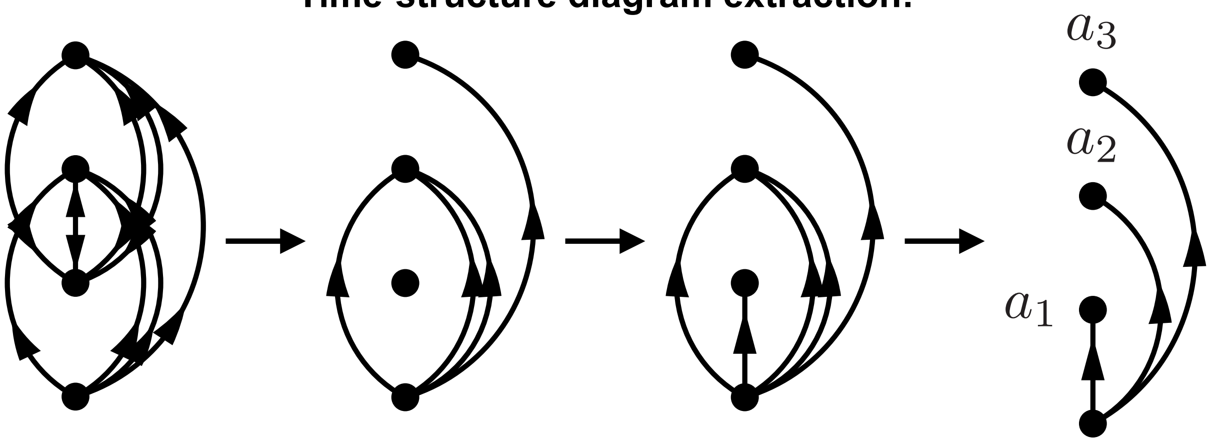
Time-structure diagram extraction:



$$TSD = \lim_{\tau\to\infty} \int_0^\tau \mathrm{d}\tau_1 \mathrm{d}\tau_2 \mathrm{d}\tau_3 \, e^{-a_1\tau_1} e^{-a_2\tau_2} e^{-a_3\tau_3}$$

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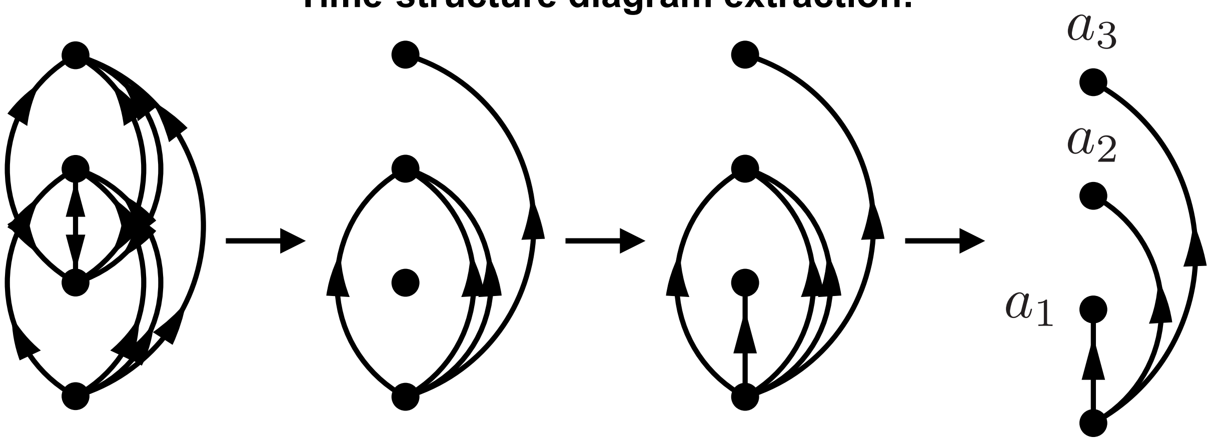

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End result will differ from the diagonal BMBPT one:

- TSD might be different from the one of the original BMBPT diagram
- Apparition of TSDs arising from more complex diagonal topologies

Extension of the denominator extraction rule

Extension of the denominator extraction rule

For each perturbation vertex in a diagram associated to a tree TSD:

- Determine all its descendants using the TSD
- Form a subgraph of **normal propagators** using the vertex and its descendants
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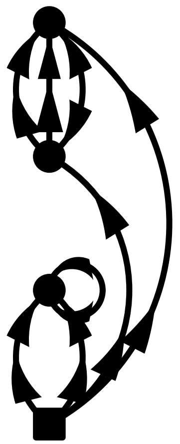

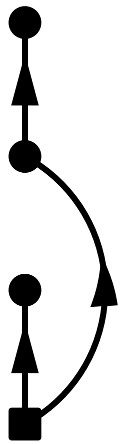

$$\frac{1}{\epsilon_{k_1k_2k_6k_5}\ \epsilon_{k_3k_4k_9k_{10}}\ \epsilon_{k_4k_7k_8k_{10}}} = \frac{1}{a_1(a_2+a_3)a_3}$$

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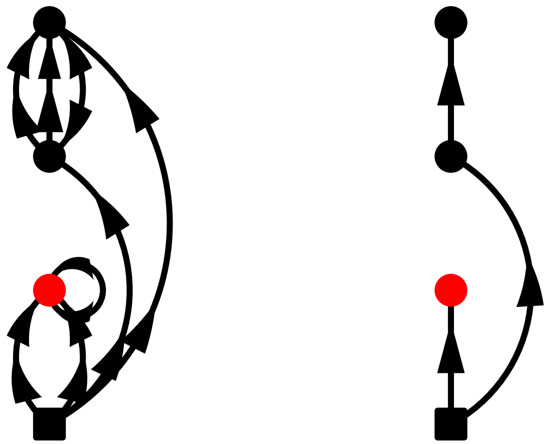

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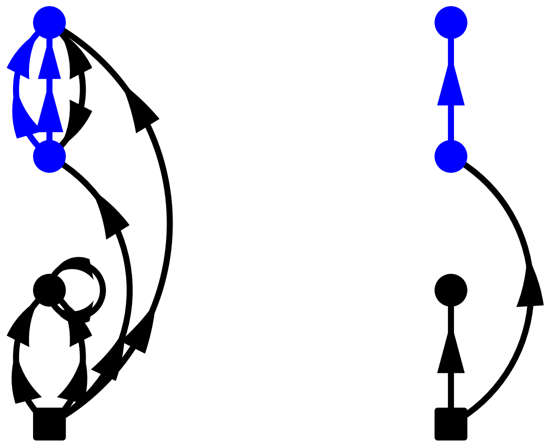

$$\frac{1}{\epsilon_{k_1k_2k_6k_5}\ \color{blue}{\epsilon_{k_3k_4k_9k_{10}}}\ \epsilon_{k_4k_7k_8k_{10}}} = \frac{1}{a_1\color{blue}{(a_2+a_3)}a_3}$$

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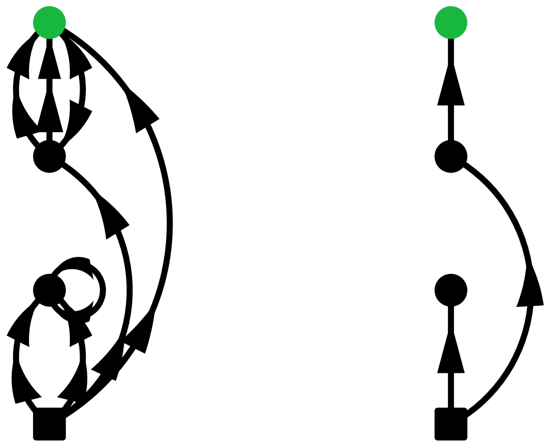

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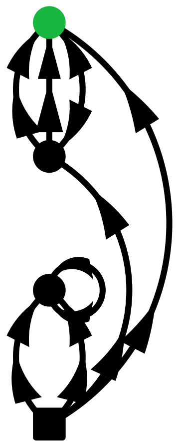

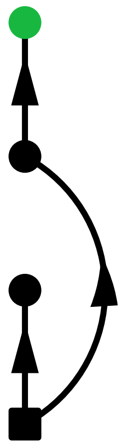

$$\frac{1}{\epsilon_{k_1k_2k_6k_5}\ \epsilon_{k_3k_4k_9k_{10}}\ \epsilon_{k_4k_7k_8k_{10}}} = \frac{1}{a_1(a_2+a_3)a_3}$$

Anomalous propagators contribute as separate q.p.e.

Case study B:
Bogoliubov In-Medium SRG

Continuous unitary transformation acting on operators

$$H(s) = U(s)H(0)U^\dagger(s)$$

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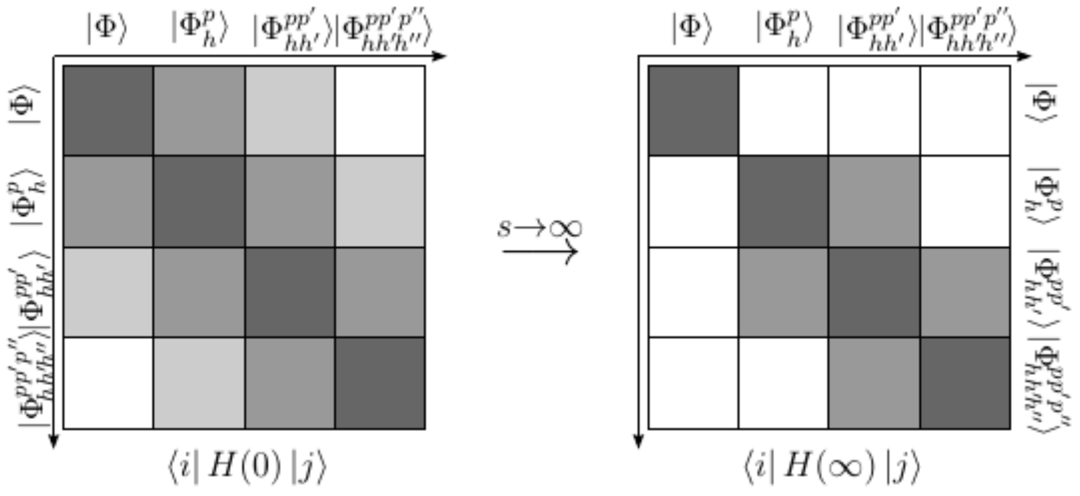
IMSRG flow equation

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



[Hergert *et al.*, J.Phys.Conf.Ser. 1041 (2018)]

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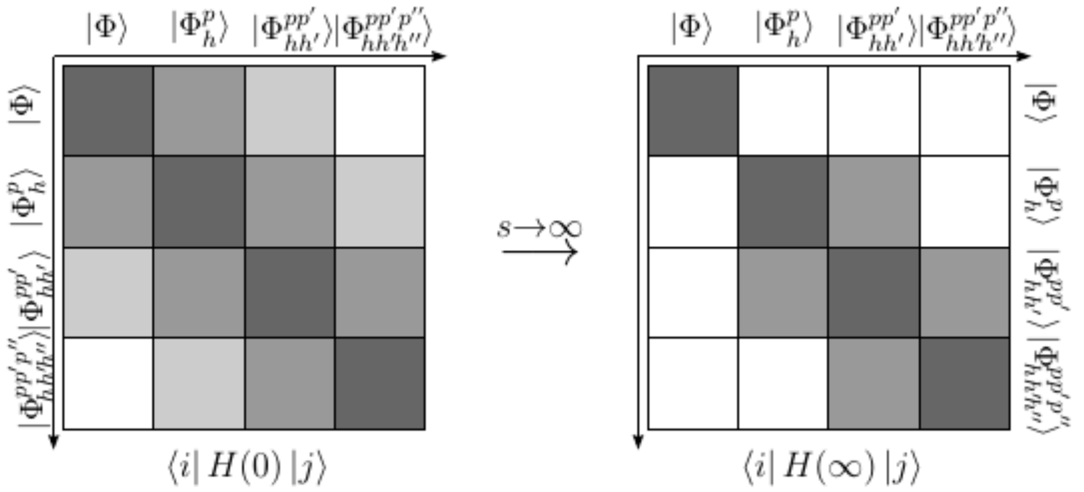
Decouple reference state from excitations



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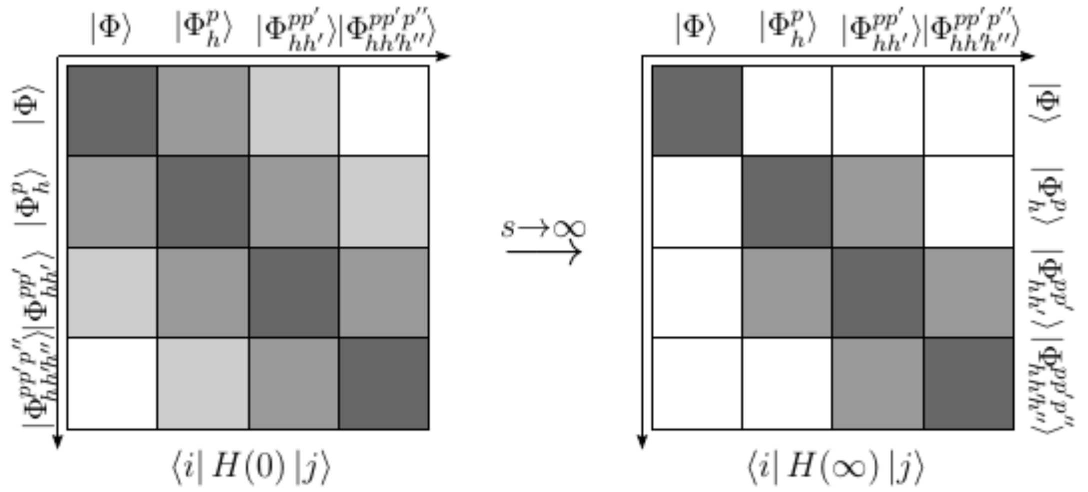

[Hergert *et al.*, J.Phys.Conf.Ser. 1041 (2018)]

Decouple reference state from excitations

Can we formulate an open-shell, single-reference version?

Bogoliubov IMSRG flow equation

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

Bogoliubov IMSRG flow equation

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Zero- and one-body contributions at BIMSRG(2):

$$\frac{\mathrm{d}}{\mathrm{d}s}\Omega^{00} = \frac{1}{2}\sum_{pq}\eta^{02}_{pq}\Omega^{20}_{pq} + \frac{1}{4!}\sum_{pqrs}\eta^{04}_{pqrs}\Omega^{40}_{pqrs} - [\eta \leftrightarrow \Omega]$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\Omega^{20}_{k_1k_2} = P(k_1/k_2)\sum_{p}\eta^{11}_{k_2p}\Omega^{20}_{k_1p} + \frac{1}{2}\sum_{pq}\eta^{22}_{k_1k_2pq}\Omega^{20}_{pq} + \frac{1}{2}\sum_{pq}\eta^{02}_{pq}\Omega^{40}_{k_1k_2pq} + P(k_1/k_2)\frac{1}{3!}\sum_{pqr}\eta^{13}_{k_2pqr}\Omega^{40}_{k_1pqr} - [\eta \leftrightarrow \Omega]$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\Omega^{11}_{k_1k_2} = \sum_{p}\eta^{11}_{k_1p}\Omega^{11}_{pk_2} + \sum_{p}\eta^{02}_{k_2p}\Omega^{20}_{pk_1} + \frac{1}{2}\sum_{pq}\eta^{13}_{k_1k_2pq}\Omega^{20}pq$$
$$+ \frac{1}{2}\sum_{pq}\eta^{02}_{pq}\Omega^{31}_{pqk_1k_2} + \frac{1}{3!}\sum_{pqr}\eta^{04}_{k_2pqr}\Omega^{40}_{pqrk_1} + \frac{1}{3!}\sum_{pqr}\eta^{13}_{k_1pqr}\Omega^{31}_{pqrk_2} - [\eta \leftrightarrow \Omega]$$

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$$\frac{\mathrm{d}}{\mathrm{d}s}\Omega^{11}_{k_1k_2} = \sum_{p}\eta^{11}_{k_1p}\Omega^{11}_{pk_2} + \sum_{p}\eta^{02}_{k_2p}\Omega^{20}_{pk_1} + \frac{1}{2}\sum_{pq}\eta^{13}_{k_1k_2pq}\Omega^{20}pq$$
$$+ \frac{1}{2}\sum_{pq}\eta^{02}_{pq}\Omega^{31}_{pqk_1k_2} + \frac{1}{3!}\sum_{pqr}\eta^{04}_{k_2pqr}\Omega^{40}_{pqrk_1} + \frac{1}{3!}\sum_{pqr}\eta^{13}_{k_1pqr}\Omega^{31}_{pqrk_2} - [\eta \leftrightarrow \Omega]$$

Plus $\frac{\mathrm{d}}{\mathrm{d}s}\Omega^{02}_{k_1k_2}$ **from Hermiticity, plus two-body…**

Bogoliubov IMSRG flow equation

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

BIMSRG(n)

=

Operators up to n-body

Zero- and one-body contributions at BIMSRG(2):

$$\frac{\mathrm{d}}{\mathrm{d}s}\Omega^{00} = \frac{1}{2}\sum_{pq}\eta^{02}_{pq}\Omega^{20}_{pq} + \frac{1}{4!}\sum_{pqrs}\eta^{04}_{pqrs}\Omega^{40}_{pqrs} - [\eta \leftrightarrow \Omega]$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\Omega^{20}_{k_1k_2} = P(k_1/k_2)\sum_{p}\eta^{11}_{k_2p}\Omega^{20}_{k_1p} + \frac{1}{2}\sum_{pq}\eta^{22}_{k_1k_2pq}\Omega^{20}_{pq} + \frac{1}{2}\sum_{pq}\eta^{02}_{pq}\Omega^{40}_{k_1k_2pq} + P(k_1/k_2)\frac{1}{3!}\sum_{pqr}\eta^{13}_{k_2pqr}\Omega^{40}_{k_1pqr} - [\eta \leftrightarrow \Omega]$$

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Only two operators A and B:

- Some contractions between A and B
- External legs corresponding to indices of C

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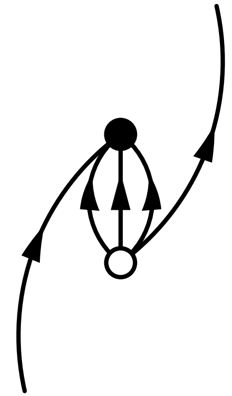

$C^{11}(04, 40)$

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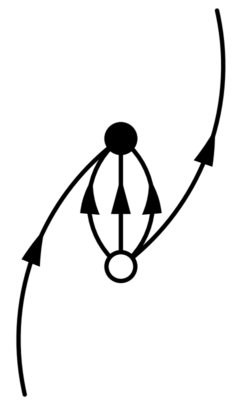

$C^{11}(04, 40)$

That makes for an easy automation!

Constraining matrices from the diagrams

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Open diagrams: top/bottom considered as vertices

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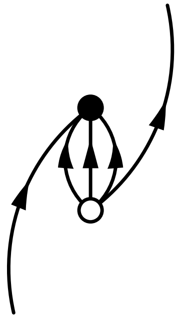

$C^{11}(04, 40)$

$\longleftrightarrow$

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 3 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

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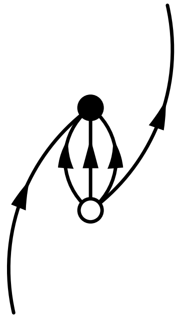

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Diagrammatic constraints

All lines go up
No self-contractions
All lines connected to a vertex

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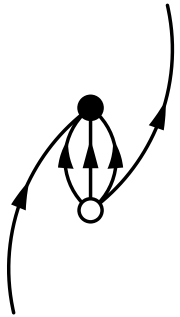

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Diagrammatic constraints

All lines go up
No self-contractions
All lines connected to a vertex

Matrices constraints

Upper triangular
Empty diagonal
$a_{14} = 0$

Generating matrices automatically

Select A or B as the top operator
Not relevant for the matrix but its treatment

$$\begin{pmatrix} 0 & ? & ? & 0 \\ 0 & 0 & ? & ? \\ 0 & 0 & 0 & ? \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

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Not relevant for the matrix but its treatment

Select a valid vertex degree for C: $d_C \in \{2,4,6,\ldots\}$

$$\begin{pmatrix} 0 & ? & ? & 0 \\ 0 & 0 & ? & ? \\ 0 & 0 & 0 & ? \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

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Select a valid vertex degree for C: $d_C \in \{2{,}4{,}6{,}\ldots\}$

Partition between incoming and outgoing legs
$a_{12} + a_{13} + a_{24} + a_{34} = d_C$

$$\begin{pmatrix} 0 & ? & ? & 0 \\ 0 & 0 & ? & ? \\ 0 & 0 & 0 & ? \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

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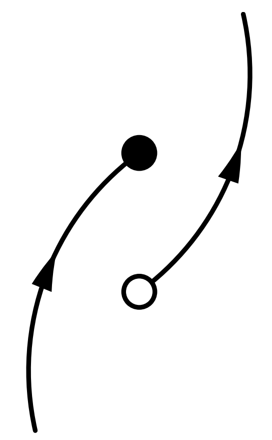
Connect them to A and B
A and B must have same parity



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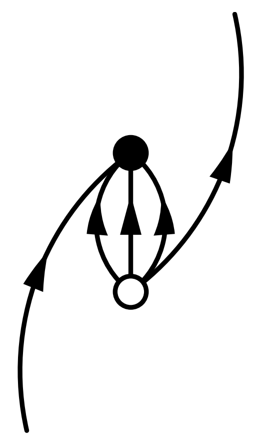
Contract A and B up to a valid vertex degree



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Generating BIMSRG diagrams

Generated diagrams up to BIMSRG(2)

Includes a diagram that was missed by hand

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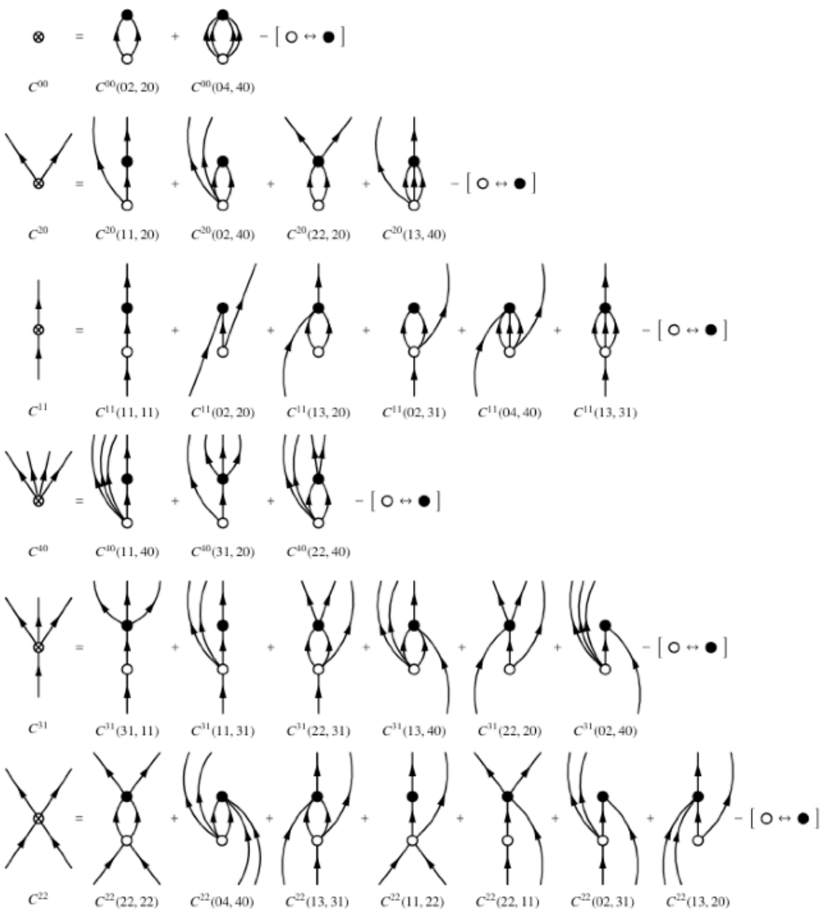


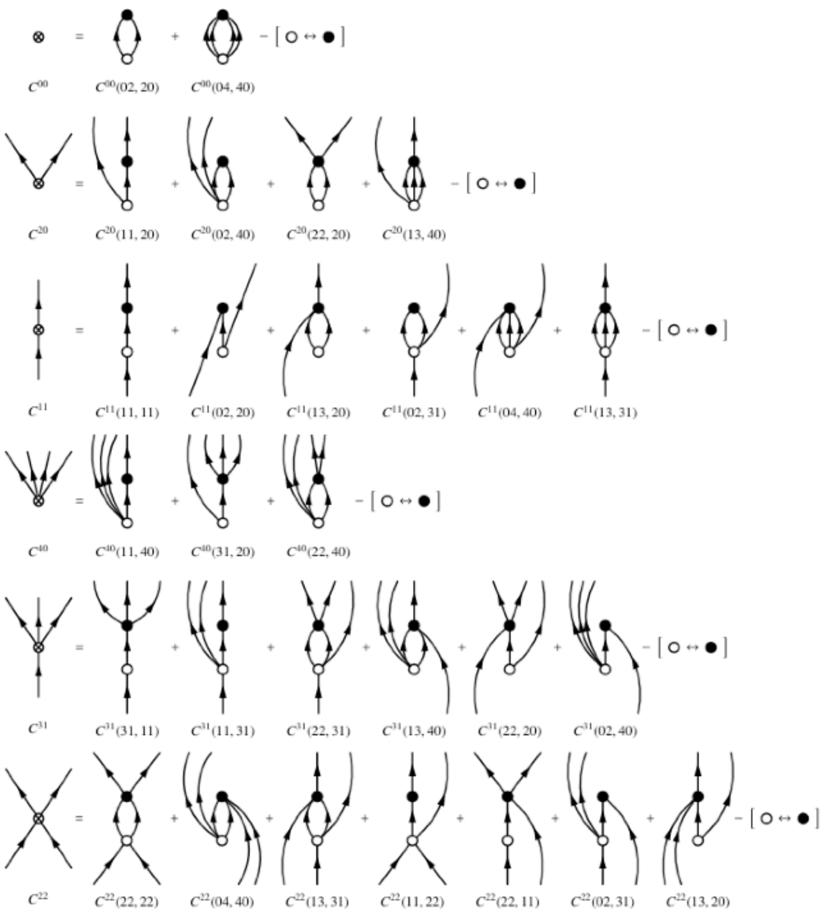
Fig. 6 Diagrams contributing to the (2, 2; 2) commutator under the hypothesis that C is Hermitian or anti-Hermitian, i.e., only the subset $\{C^{ij}, i \geq j\}$ is explicitly computed.

Generated diagrams up to BIMSRG(2)

Includes a diagram that was missed by hand

Moving to higher orders

# diagrams	1	2	3	4	5	6	7	8	9
Naive counting	10	72	264	700	1550	2930	5152	8424	13046
Using Hermiticit	4	24	82	208	452	830	1436	2320	3558



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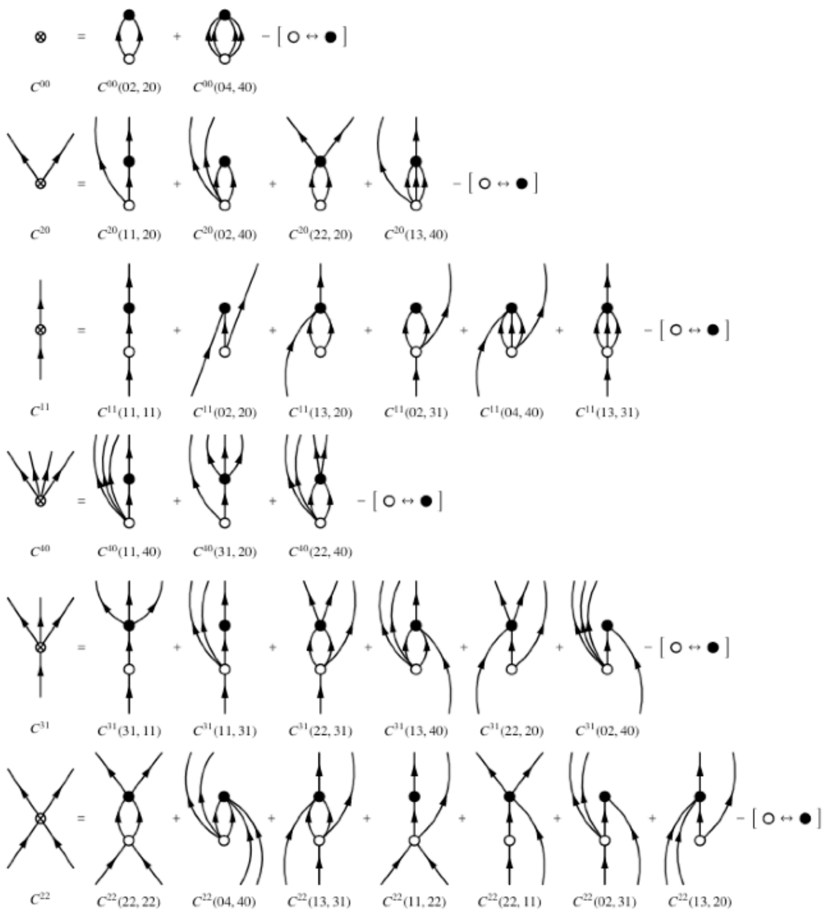
Formalism is complete to order N within three months of work!



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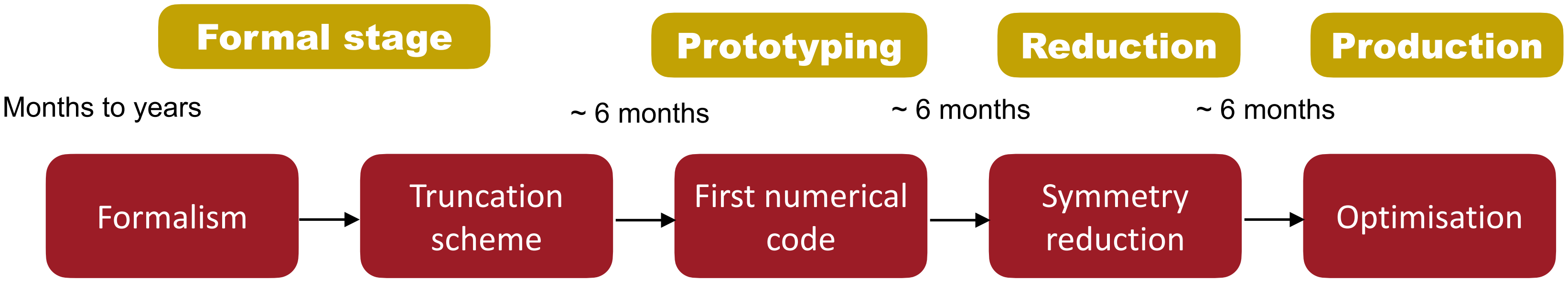
Automated methods tools in nuclear physics

Automated nuclear Many-body methods



Automated nuclear Many-body methods

Formal stage — Months to years

Prototyping — ~ 6 months

Reduction — ~ 6 months

Production — ~ 6 months

Formalism → Truncation scheme → First numerical code → Symmetry reduction → Optimisation

Wick theorem + diagrammatic representation

Automated nuclear Many-body methods

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+
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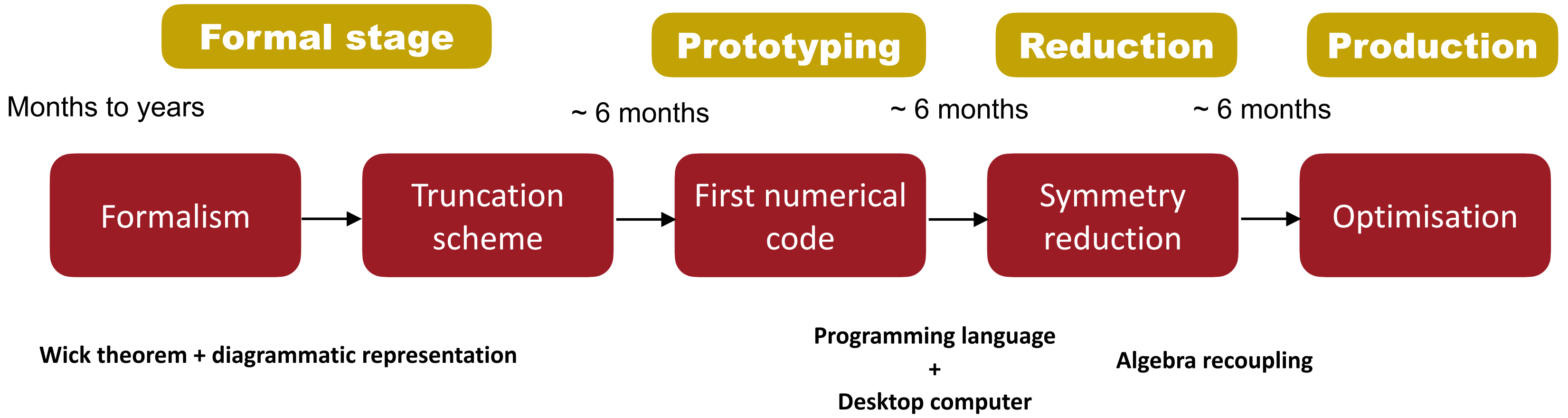
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Arthuis, Tichai, Ripoche, Duguet, *CPC* **261** (2021)
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Angular Momentum Coupling
Tichai, Wirth, Ripoche, Duguet, *EPJA* **56** (2020)

https://github.com/adgproject/adg

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Faster and safer with automation
- Graph theory methods & open-source libraries
- Gain formal and numerical insights

Thank your for your attention!

T. Duguet
J.-P. Ebran
V. Somà

A. Tichai

H. Hergert

C. Drischler

K. McElvain