Helmholtz Forschungsakademie Hessen für FAIR

TECHNISCHE UNIVERSITÄT DARMSTADT

SFB 1245

AUTOMATED GENERATION AND EVALUATION OF DIAGRAMS AT PLAY IN VARIOUS MANY-BODY METHODS

Pierre Arthuis

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AUTOMATED GENERATION AND EVALUATION OF DIAGRAMS

A CRASH COURSE IN LOW-ENERGY NUCLEAR MANY-BODY METHODS

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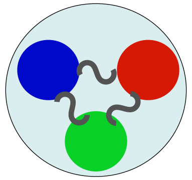
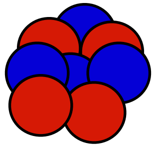
WHAT DOES AB INITIO MEAN FOR US?



Particle physics

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



Nuclear theory

Effective Field Theory in the A-body sector

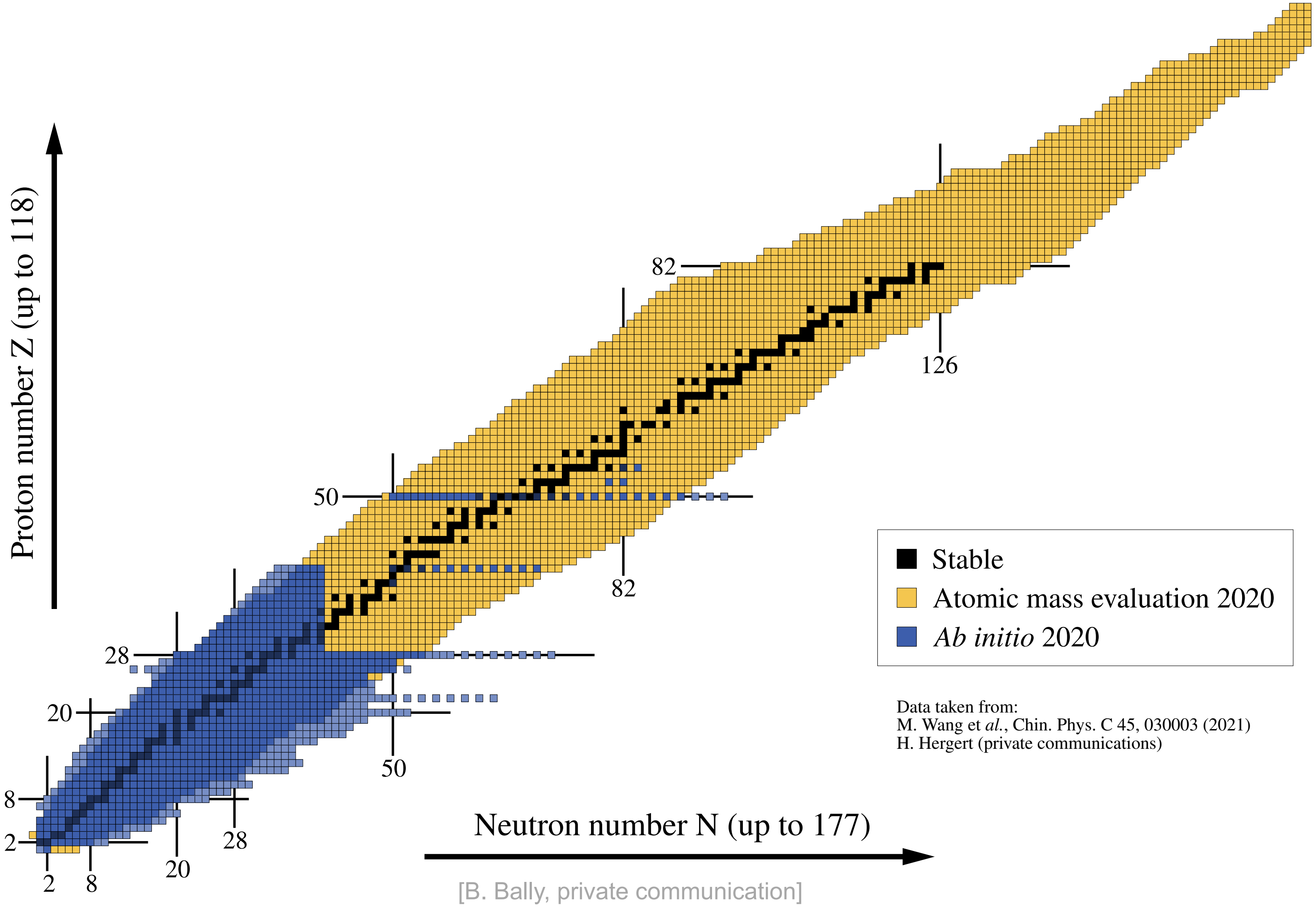
A-body Schrödinger equation

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

Obtain a description that is:

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

FROM THE LIGHTEST NUCLEI…



[B. Bally, private communication]

« Exact » methods (80's)

- GFMC, NCSM, FY, HH

Closed-shell methods (00's)

- CC, DSCGF, IMSRG, MBPT

Open-shell methods (10's)

- BCC, GSCGF, MR-IMSRG, BMBPT

***Ab initio* shell model (2014)**

- SM with interaction from CC, IMSRG

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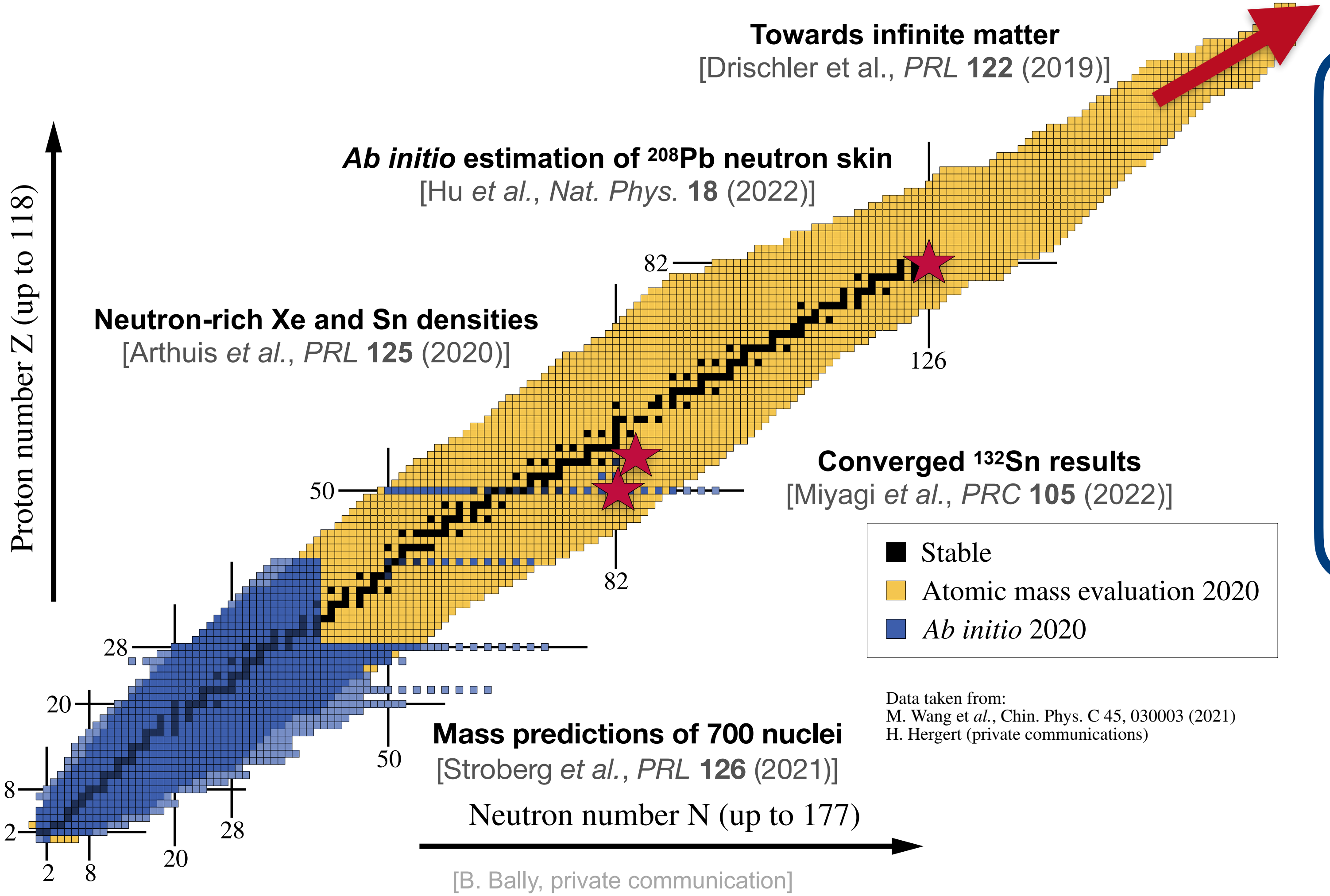
…TOWARDS MEDIUM- AND HEAVY-MASS SYSTEMS



[B. Bally, private communication]

Expansion methods

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

- Build from a simple reference state $|\Phi\rangle$
- Add the correlations on top order by order
- Truncate at the desired order
- Estimate uncertainties from the truncated terms

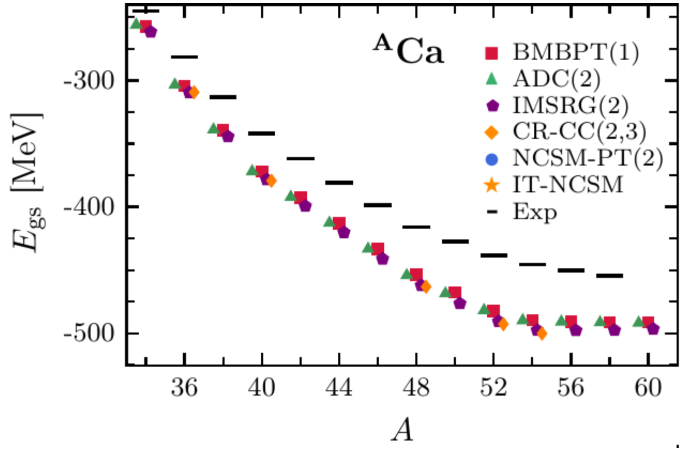
Controlled expansion & uncertainty

Polynomial cost

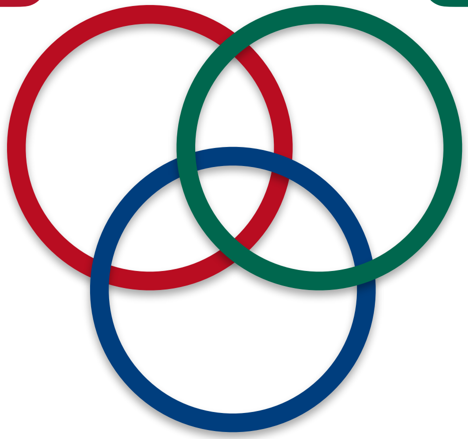
AB INITIO CHALLENGE(S)

Determine an observable $\mathcal{O}$ for a system $\mathcal{S}$ with precision η

Nuclear interaction



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

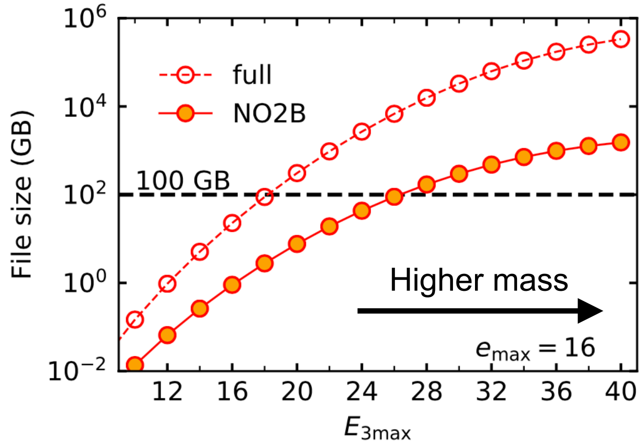


Many-body method

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

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

Numerical method



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

AUTOMATED GENERATION AND EVALUATION OF DIAGRAMS

AUTOMATED METHODS TOOLS IN NUCLEAR PHYSICS

AUTOMATED NUCLEAR MANY-BODY METHODS

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Formal stage		Prototyping	Reduction	Production
Months to years		~ 6 months	~ 6 months	~ 6 months
Formalism →	Truncation scheme →	First numerical code →	Symmetry reduction →	Optimisation
Wick theorem + diagrammatic representation		Programming language + Desktop computer	Algebra recoupling	Programming language + HPC cluster

Automated Diagram Generator
Arthuis, Duguet, Tichai, Lasseri, Ebran, *CPC* **240** (2019)
Arthuis, Tichai, Ripoche, Duguet, *CPC* **261** (2021)
Tichai, Arthuis, Hergert, Duguet, *EPJA* **58** (2022)

`https://github.com/adgproject/adg`

Angular Momentum Coupling
Tichai, Wirth, Ripoche, Duguet, *EPJA* **56** (2020)

See Alex' talk!

Automated Code Generation
Drischler, Hebeler, Schwenk, *PRL* **122** (2019)

See Christian's talk!

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

AUTOMATED GENERATION AND EVALUATION OF DIAGRAMS

CASE STUDY A: MANY-BODY PERTURBATION THEORIES

[Arthuis, Duguet, Tihai, Lasseri, Ebran, CPC 240 (2019), Arthuis, Tichai, Ripoche, Duguet, CPC 261 (2021)]

EXPANSION METHODS AND SYMMETRY

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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
→ 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

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

EXPANSION METHODS AND DEGENERATE SYSTEMS

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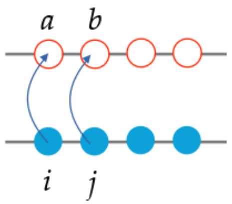
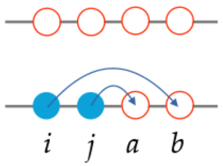
Basic idea: collect dynamical correlations through ph excitations

Closed-shell



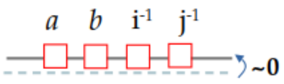
Open-shell



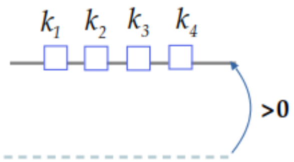
Degeneracy w.r.t ph excitations

- 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

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Particle-number conserving

- Split H: $H = H_0 + H_1$

$$[A, H_0] = 0$$

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Wave operator to be expanded
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→ 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 breaking

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

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

- Introduce reference state

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

Wave operator to be expanded
Reference state sol° of SE

$$\Omega_0|\Phi\rangle = E_0|\Phi\rangle$$

Symmetry-breaking method
→ Bogoliubov ref. state

BOGOLIUBOV MANY-BODY PERTURBATION THEORY

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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

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

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

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

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.** $|\Phi\rangle$:

$$\Omega = \Omega^{00} + \frac{1}{1!} \sum_{k_1 k_2} \Omega^{11}_{k_1 k_2} \beta^\dagger_{k_1} \beta_{k_2} + \frac{1}{2!} \sum_{k_1 k_2} \left\{ \Omega^{20}_{k_1 k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2} + \Omega^{02}_{k_1 k_2} \beta_{k_2} \beta_{k_1} \right\}$$

$$+ \frac{1}{(2!)^2} \sum_{k_1 k_2 k_3 k_4} \Omega^{22}_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta_{k_4} \beta_{k_3} + \frac{1}{3!} \sum_{k_1 k_2 k_3 k_4} \left\{ \Omega^{31}_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta_{k_4} + \Omega^{13}_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta_{k_4} \beta_{k_3} \beta_{k_2} \right\}$$

$$+ \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} \left\{ \Omega^{40}_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4} + \Omega^{04}_{k_1 k_2 k_3 k_4} \beta_{k_4} \beta_{k_3} \beta_{k_2} \beta_{k_1} \right\} + \ldots$$

TIME-DEPENDENT BMBPT

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Grand potential partitioning:

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

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

Time-evolved state

$$|\Psi(\tau)\rangle \equiv \mathcal{U}(\tau)|\Phi\rangle = e^{-\tau\Omega_0} T e^{-\int_0^\tau d\tau \Omega_1(\tau)} |\Phi\rangle$$

Ground-state energy of an open-shell nucleus

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

Propagators:

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

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

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

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

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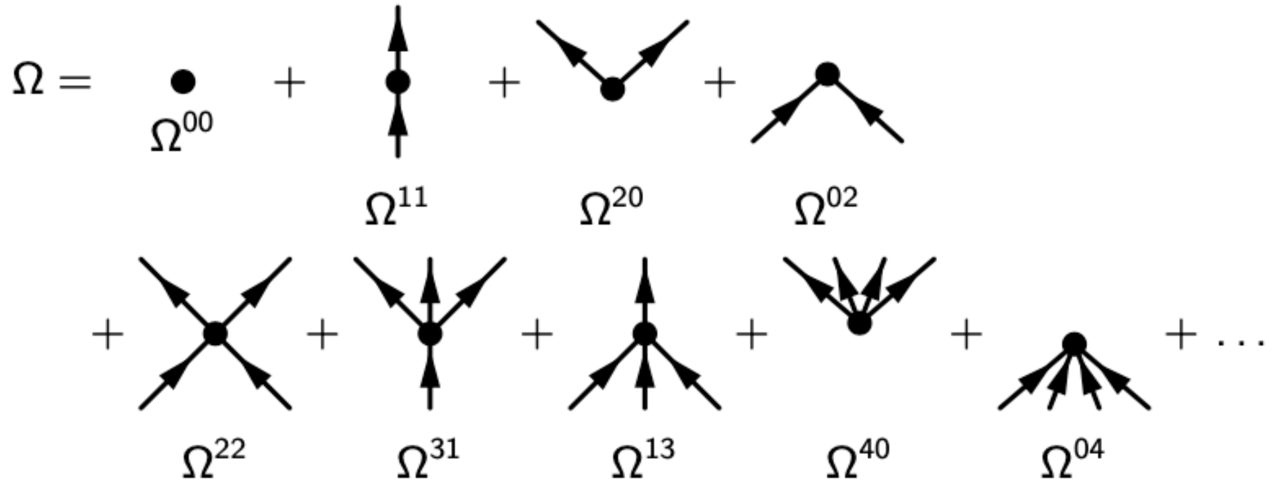
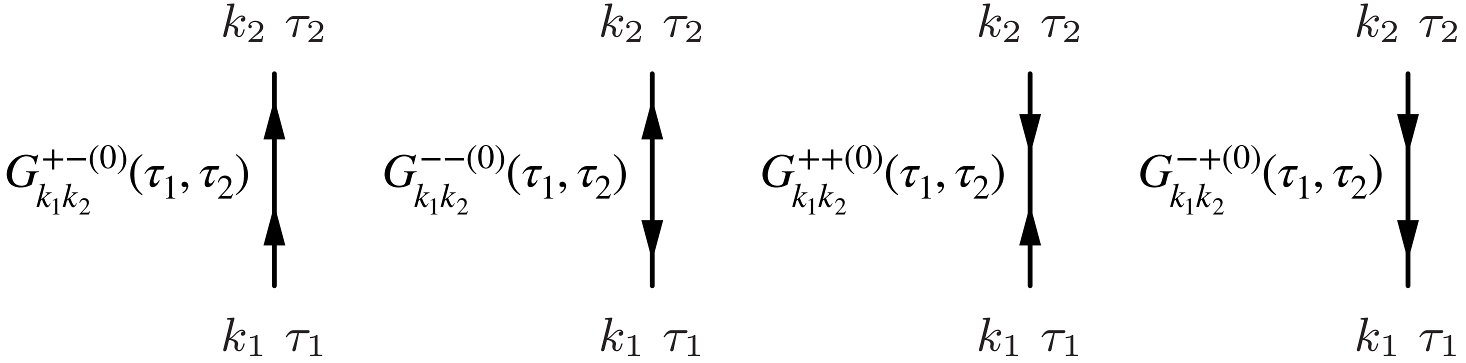
Normal-ordered form of Ω with respect to $|\Phi\rangle$



Quasiparticle propagators



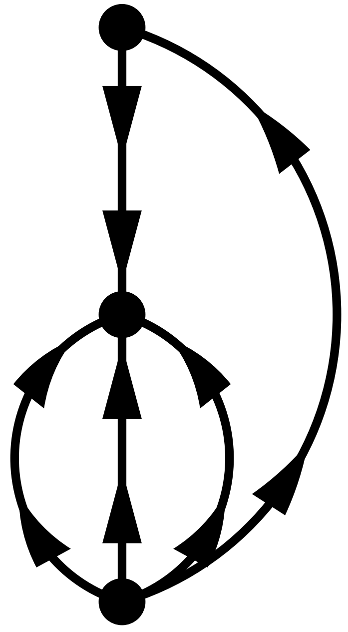
DIAGRAMMATIC RULES FOR GROUND-STATE ENERGY

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

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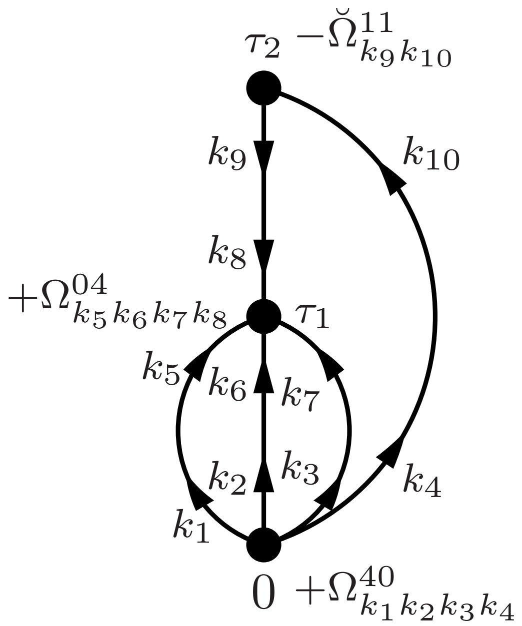

Convention

Order p ⇔ Order p+1 in standard counting

Time-dependent and time-integrated expressions:

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

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

HOW TO BUILD AN AUTOMATED FRAMEWORK

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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

AUTOMATIC GENERATION OF DIAGRAMS

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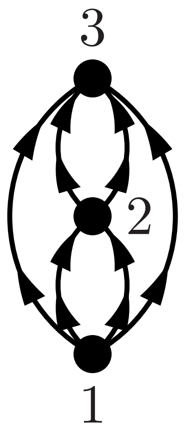
Oriented adjacency matrix from graph theory

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



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

Generation of BMBPT diagrams at order p

Algorithm

- Generate all $(p+1) \times (p+1)$ matrices
  - Fill them 'vertex-wise' with all allowed integers
  - Check the degree of each vertex before moving on
- Discard matrices leading to topologically identical diagrams
- Translate the matrix into drawing instructions

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

AUTOMATIC GENERATION OF DIAGRAMS

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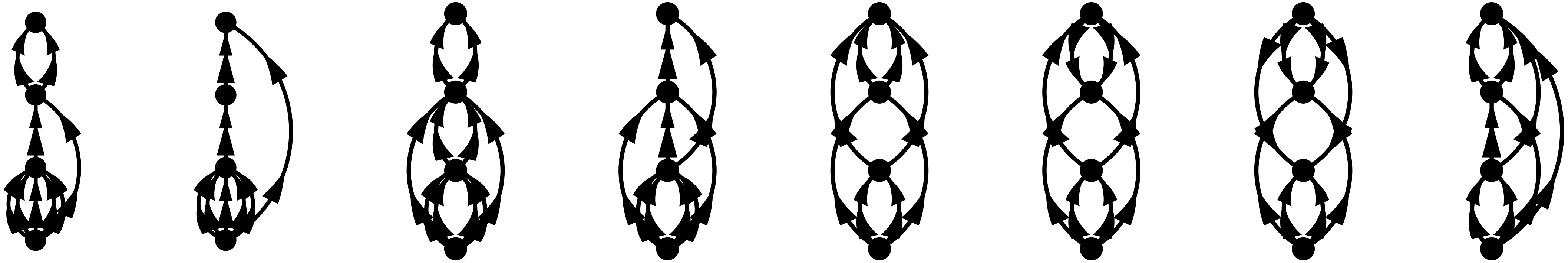
3rd-order BMBPT diagrams for vertices with 2, 4 and 6 legs…



+ 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

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TIME-STRUCTURE DIAGRAMS

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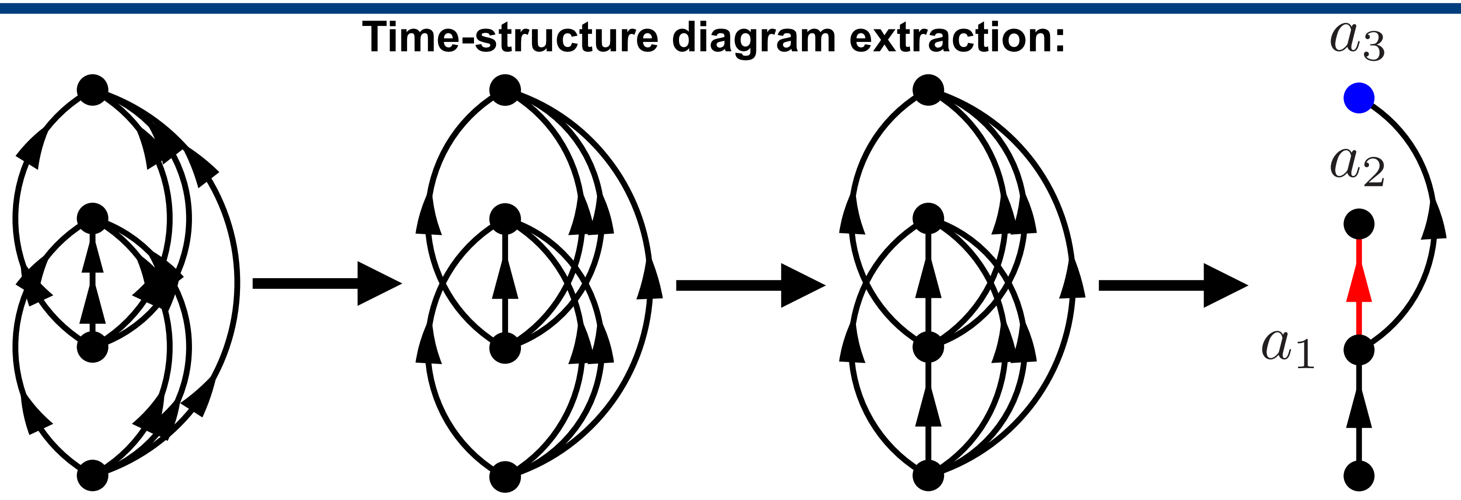
Integrand of p-tuple time integral governed by time structure of the diagram

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

Time-structure diagram extraction:

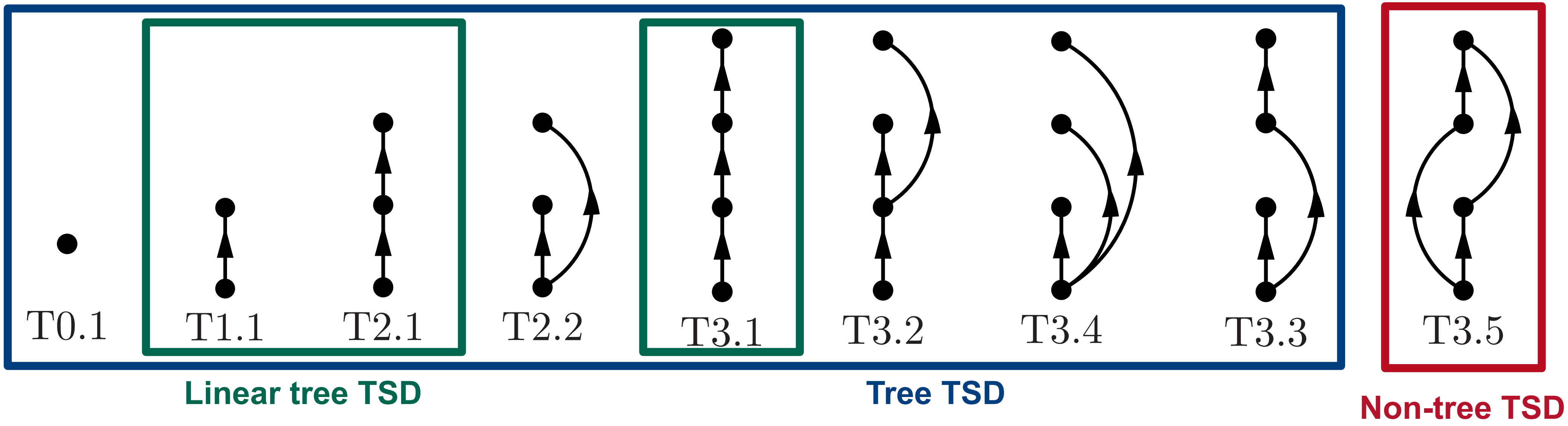


$$TSD = \lim_{\tau \to \infty} \int_0^{\tau} \mathrm{d}\tau_1 \mathrm{d}\tau_2 \mathrm{d}\tau_3 \, \theta(\tau_2 - \tau_1) \theta(\tau_3 - \tau_1) e^{-a_1 \tau_1} e^{-a_2 \tau_2} e^{-a_3 \tau_3}$$

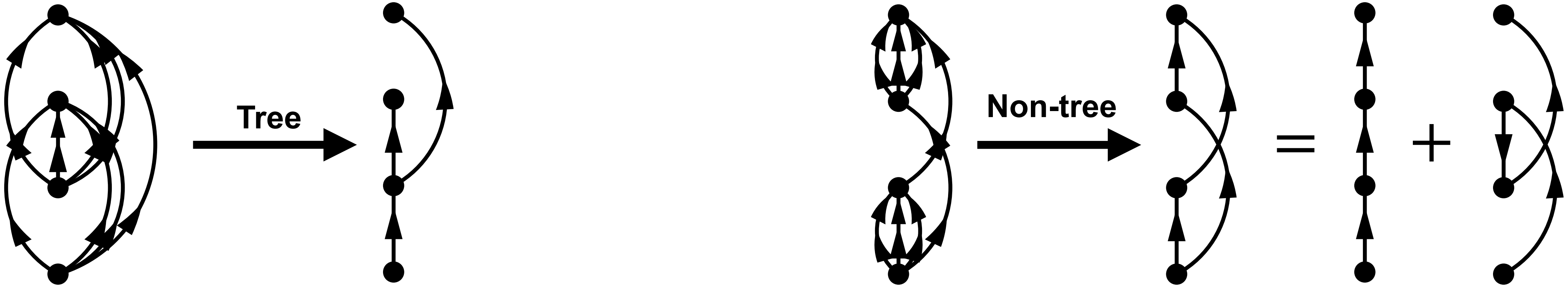
- Several BMBPT diagrams may have same TSD
- Replace a_i with appropriate q.p. energy sum for final expression

TOPOLOGIES OF TIME-STRUCTURE DIAGRAMS

TSD topology crucial for result extraction



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



DENOMINATOR EXTRACTION AND INTEGRAL STRUCTURE

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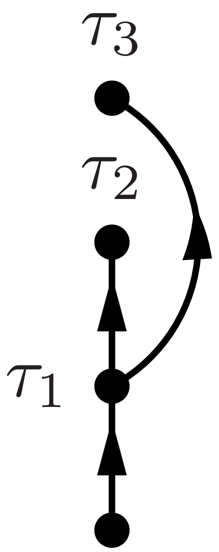
Why a so simple structure for all trees?

Link between tree TSD structure and time integrals structure



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

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

NEW DIAGRAMMATIC RULE

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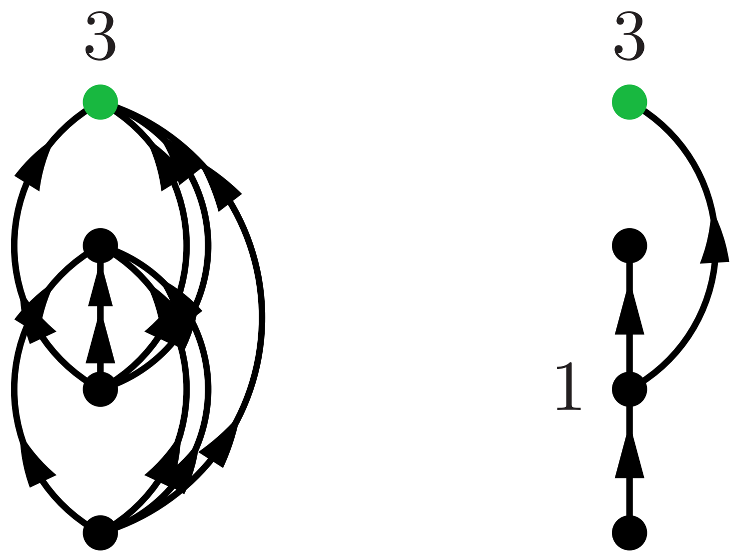
Direct time-integrated expression extraction from time-unordered diagrams

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

- Determine all its descendants using the TSD
- Form a subgraph using the vertex and its descendants
- For all propagators entering the subgraph, add the associated qpe



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

New rule yields double, not quadruple

Physics of whole topology captured at once

NEW DIAGRAMMATIC RULE

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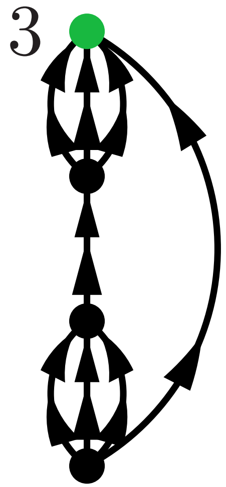
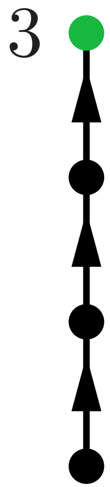
For each perturbation vertex in a diagram associated to a tree TSD:

- Determine all its descendants using the TSD
- Form a subgraph using the vertex and its descendants
- For all propagators entering the subgraph, add the associated qpe





New rule reduces to resolvent rule for time-ordered diagrams

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

DENOMINATOR EXTRACTION: NON-TREE CASE

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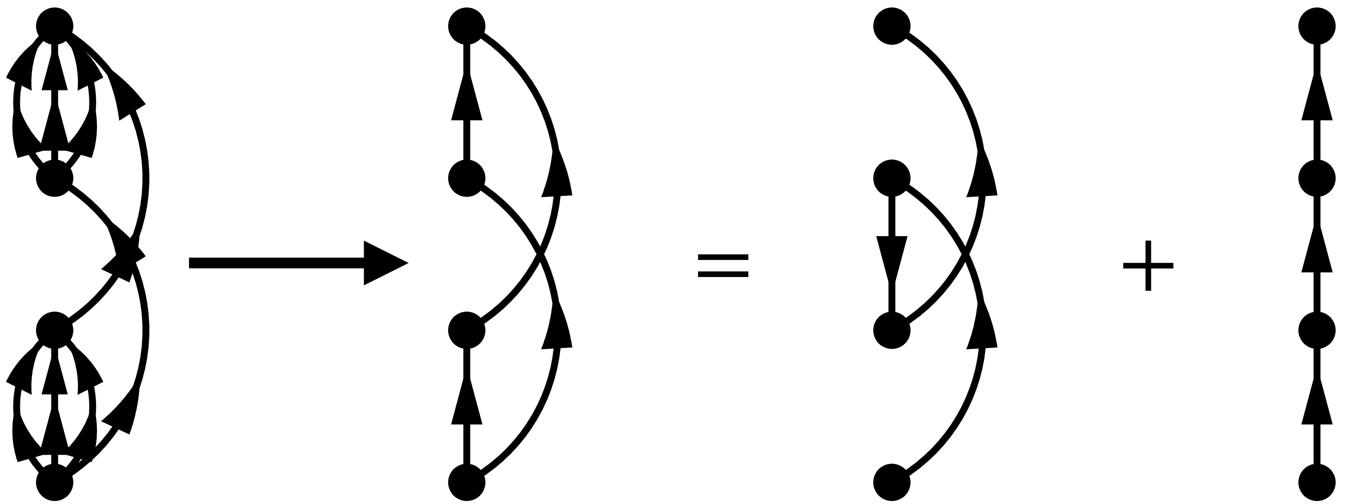
If the associated TSD is not a tree:

- Separate the TSD into a sum of tree TSDs
- Apply the tree denominator algorithm to each of them
- Sum the results



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

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

HOW TO BUILD AN AUTOMATED FRAMEWORK

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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 → Arbitrary order expressions

TIME-UNORDERED VS TIME-ORDERED DIAGRAMMATICS

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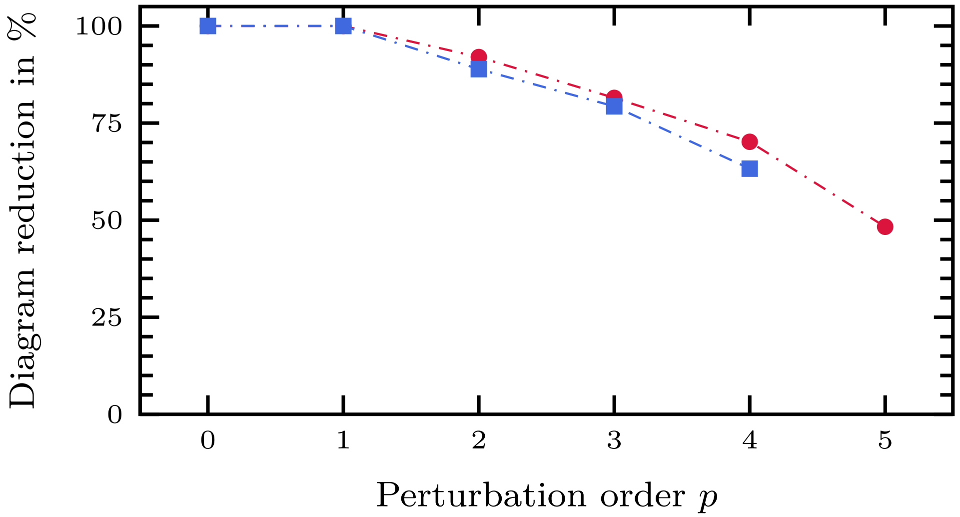
Time-dependent perturbation theory = Time-unordered diagrams

Time-independent perturbation theory = Time-ordered diagrams

- 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



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

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

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?

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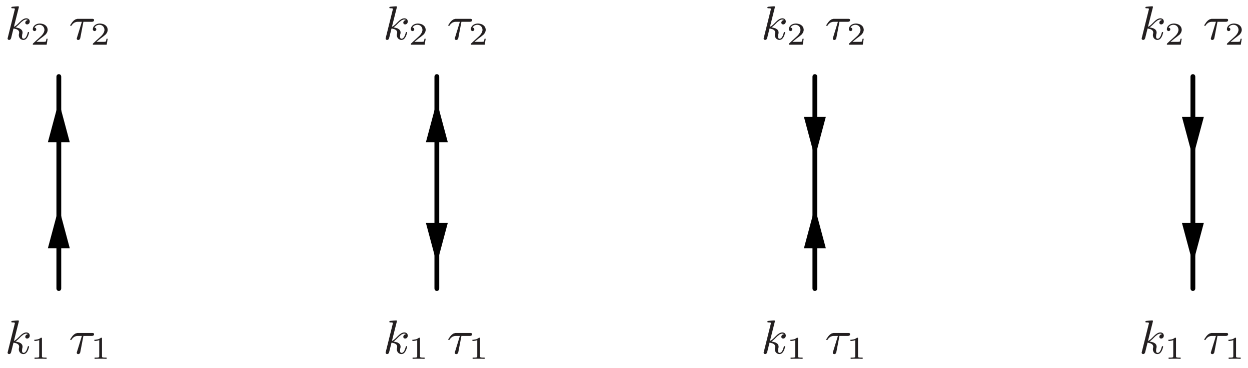

$G^{+-(0)}_{k_1k_2}(\tau_1,\tau_2)$ $G^{--(0)}_{k_1k_2}(\tau_1,\tau_2)$ $G^{++(0)}_{k_1k_2}(\tau_1,\tau_2)$ $G^{-+(0)}_{k_1k_2}(\tau_1,\tau_2)$

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

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

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

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

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

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

Only one more

HOW TO PRODUCE AN OFF-DIAGONAL PBMBPT DIAGRAM?

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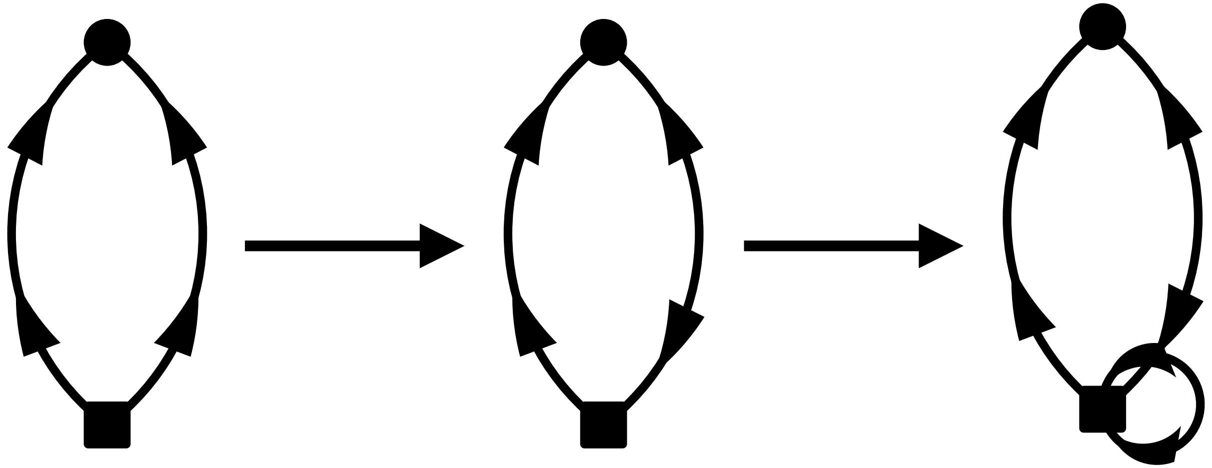
Naive algorithm:

- 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)



The combinatorics is not looking good…

A NAIVE REPRESENTATION OF PBMBPT DIAGRAMS

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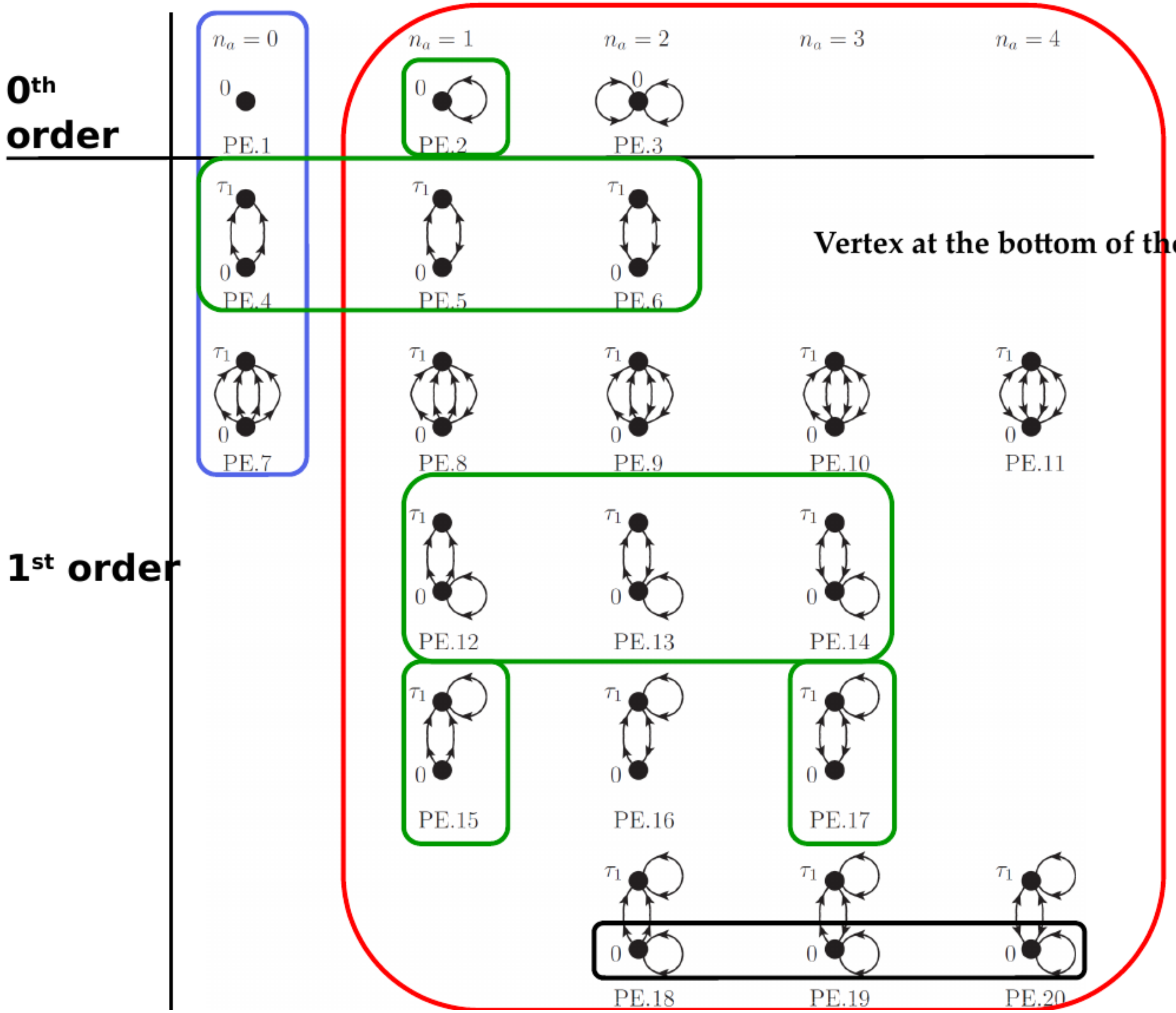

20 diagrams
3 diagrams
17 diagrams
9 diagrams

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

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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

Similarity transformation

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

Reduction in the number of diagrams:

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

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

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	…

WHAT ABOUT EXPRESSIONS?

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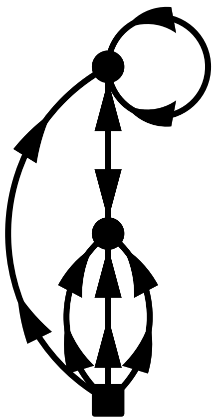
Extend on diagonal BMBPT rules:

- 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



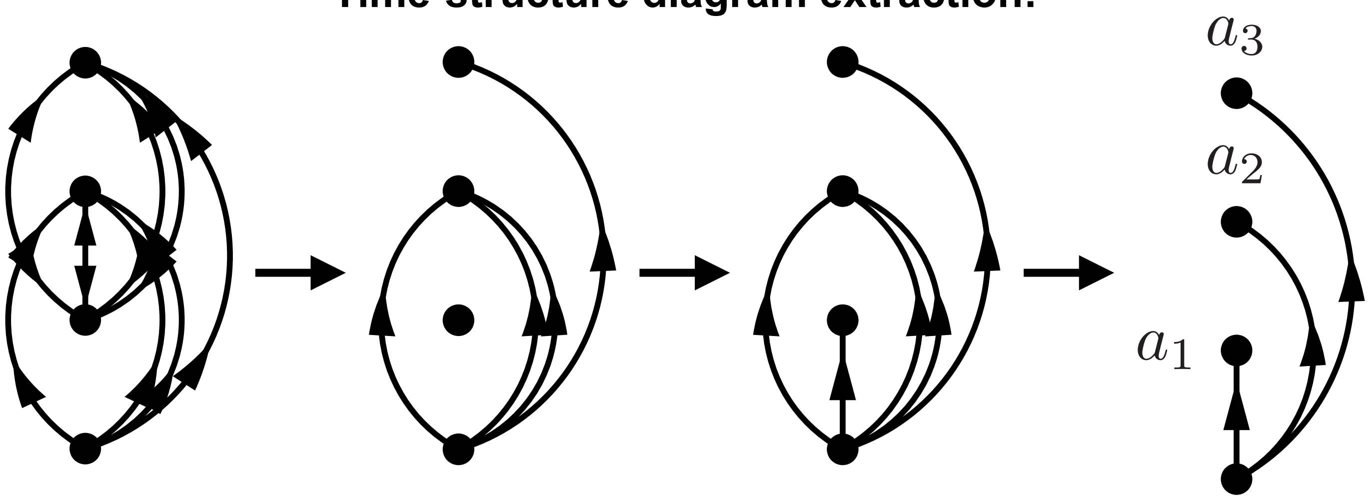
$$\text{PO2.3.3} = \lim_{\tau\to\infty} \frac{(-1)^2}{(3!)} \sum_{k_i} \tilde{O}^{40}_{k_1k_2k_3k_4}(\varphi)\Omega^{04}_{k_1k_2k_3k_5}\Omega^{04}_{k_6k_4k_7k_8}R^{--}_{k_6k_5}(\varphi)R^{--}_{k_8k_7}(\varphi)$$

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

EXTENDING THE TSD RULES BY LEAVING THEM UNCHANGED

Remove all anomalous lines then proceed as before

Time-structure diagram extraction:



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

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

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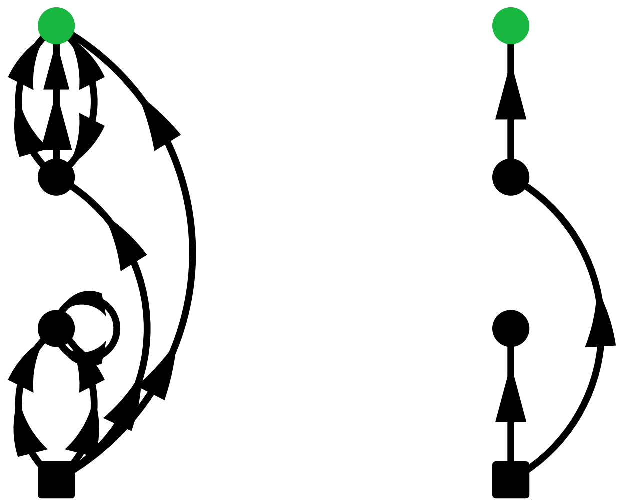
For each perturbation vertex in a diagram associated to a tree TSD:

- Determine all its descendants using the TSD
- Form a subgraph of **normal propagators** using the vertex and its descendants
- Form all **normal** propagators entering the subgraph, add associated q.p.e.
- For all **anomalous propagator halves** entering the subgraph, dd associated q.p.e.



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

Anomalous propagators contribute as separate q.p.e.

AUTOMATED GENERATION AND EVALUATION OF DIAGRAMS

CASE STUDY B: BOGOLIUBOV IN-MEDIUM SRG

[Tichai, Arthuis, Hergert, Duguet, EPJA 58 (2022)]

IN-MEDIUM SIMILARITY RENORMALIZATION GROUP

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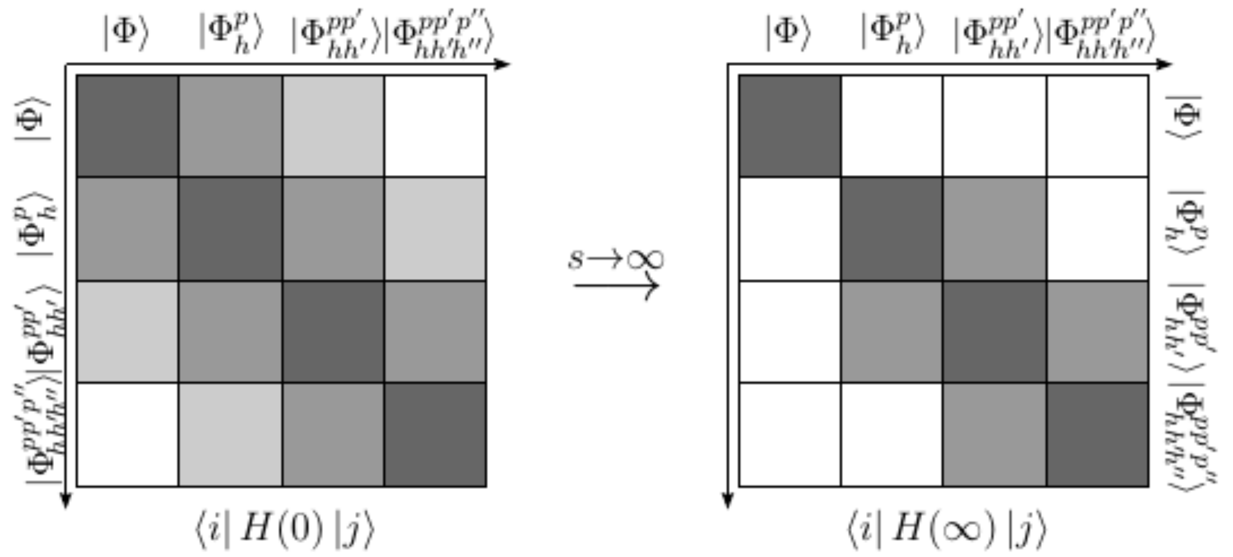
Continuous unitary transformation acting on operators

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

IMSRG flow equation

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

Decouple reference state from excitations



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

See Matthias' talk!

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

BOGOLIUBOV IMSRG

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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):

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

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

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

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

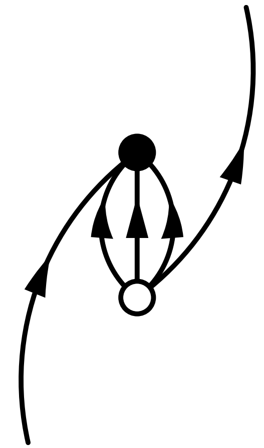
DIAGRAMMATIC BIMSRG

BIMSRG terms have a simple, recurring structure: $C = [A, B]$

$$C^{11}_{k_1 k_2}(04, 40) = \frac{1}{3!} \sum_{pqr} A^{04}_{k_2 pqr} B^{40}_{pqr k_1}$$

Only two operators A and B:

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

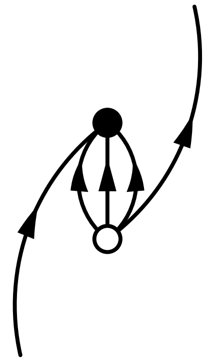


$C^{11}(04, 40)$

That makes for an easy automation!

CONSTRAINING MATRICES FROM THE DIAGRAMS

Open diagrams: top/bottom considered as vertices



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

$\longleftrightarrow$

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

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

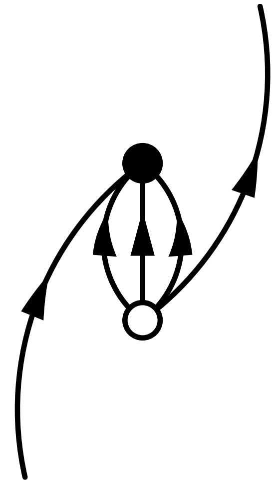
Select A or B as the top operator
Not relevant for the matrix but its treatment

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

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

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

Contract A and B up to a valid vertex degree



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

GENERATING BIMSRG DIAGRAMS

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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

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

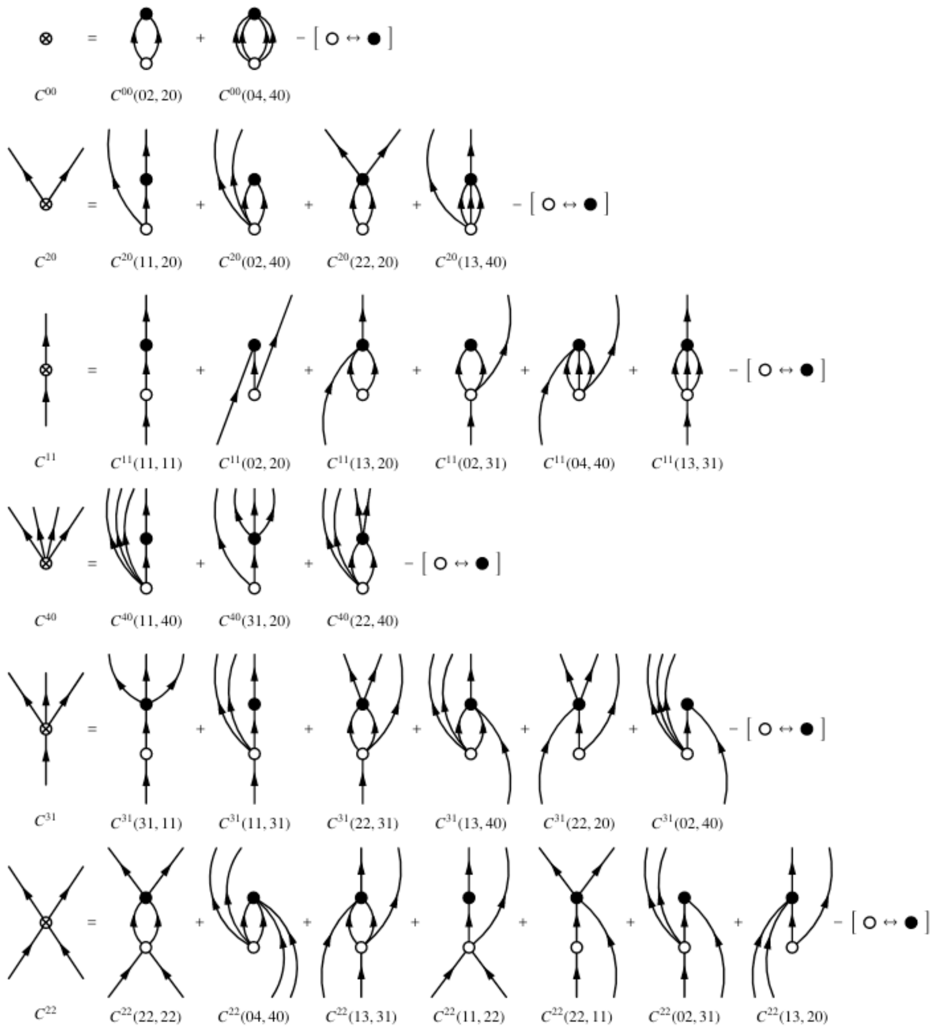

Fig. 6 Diagrams contributing to the (2, 2; 2) commutator under the hypothesis that C is Hermitian or anti-Hermitian, i.e., only the subset $\{C^{ij}, i \geq j\}$ is explicitly computed.

THE FUTURE WITH ADG

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Extension to three-body forces with MBPT

- Putting the MBPT part of ADG on par with other formalisms
- Access to full-three body calculations at high orders for e.g. infinite matter
- Other properties: divergent diagrams, …

→

Already existing code generator

Drischler, Hebeler, Schwenk, *PRL* **122** (2019)

Single- and multi-reference symmetry-conserving IMSRG

- Make future extensions of IMSRG safer (issues raised for IMSRG(3))
  [Heinz, Tichai, Hoppe, Hebeler, Schwenk, *PRC* **103** (2021)]
- Include triples in MR-IMSRG calculations → Connection with IM-GCM
  [Yao, Bally, Engel, Wirth, Rodriguez, Hergert, *PRL* **124** (2020)]

→

Automated code generator

Somewhere in the future….

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CONCLUSION AND OUTLOOK

Tremendous progress of ab initio methods

- Now reaching A ~ 100
- Progress driven by formal and numerical developments
- Higher-order calculations slowly becoming feasible

Automated diagram generator

- Flexible software to generate many-body diagrams and expressions
- Several methods already covered
- Theoretical insights gained from the implementation work
- Results mainly formal for now, waiting for numerical progress for proper leveraging

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Thank your for your attention!

SFB 1245

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