Automated generation and evaluation of many-body diagrams

Pierre Arthuis
University of Surrey

Progress in Ab Initio Techniques in Nuclear Physics
TRIUMF, Vancouver - February 28th 2019

Outline

- Why automated tools for many-body diagrams?
- Application to Bogoliubov Many-Body Perturbation Theory
    - Basics of diagrammatic BMBPT formalism
    - Automated generation and evaluation for BMBPT diagrams
- Conclusion and perspectives

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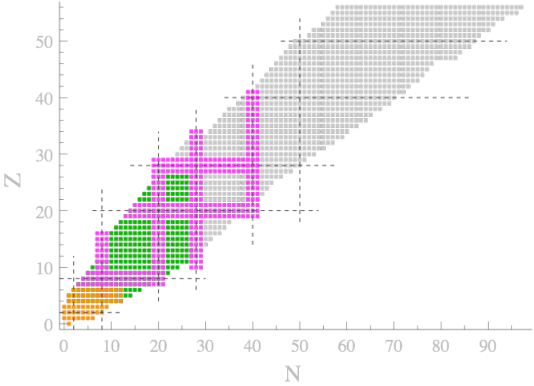
Progress in *ab initio* methods



Courtesy of V. Soma, T. Duguet

"Exact" methods (80's)
- GFMC, NCSM, FY

Closed-shell methods (00's)
- DSCGF, CC, IMSRG

Open-shell methods (10's)
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Ab initio shell model (2014)
- EI via CC, IMSRG, NCSM...

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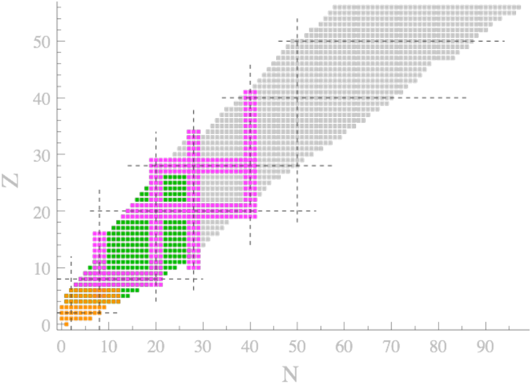

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Two-fold force leading progress

◇ New formal developments

◇ Progress in numerical methods, computing power

Progress in diagrammatic *ab initio* methods

The coming extensions

Keep incorporating more physics

- To higher truncation orders
- To higher-rank forces

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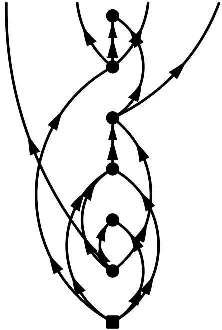
The coming difficulties

More complex topologies appearing

- Time-consuming
- Error-prone



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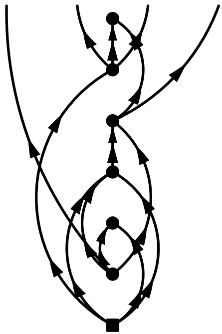

The coming needs

Develop tools to avoid human work

- Automated diagram generation and evaluation
- Automated code-generation

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  - Basics of diagrammatic BMBPT formalism
    [Duguet and Signoracci, *J. Phys. G* **44** (2017)]
    [Tichai, Arthuis, Duguet, Hergert, Somà, Roth, *PLB* **786** (2018)]
    See A. Tichai's talk for numerical implementation
  - Automated generation and evaluation for BMBPT diagrams
- Conclusion and perspectives

Bogoliubov reference state

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

$$\beta_k = \sum_p U^*_{pk} \, c_p + V^*_{pk} \, c^\dagger_p$$

$$\beta^\dagger_k = \sum_p U_{pk} \, c^\dagger_p + V_{pk} \, c_p$$

Particle-number breaking

$$A|\Phi\rangle \neq \mathrm{A}|\Phi\rangle$$

Breaks $U(1)$ symmetry

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

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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

Grand potential partitioning

$$\Omega_0 = \Omega^{00} + \bar{\Omega}^{11} = \Omega^{00} + \sum_k \mathrm{E}_k \beta_k^\dagger \beta_k$$

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

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Time-evolved state

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

Time-dependent BMBPT

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Ground state energy of an open-shell nucleus

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

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Propagators

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

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

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

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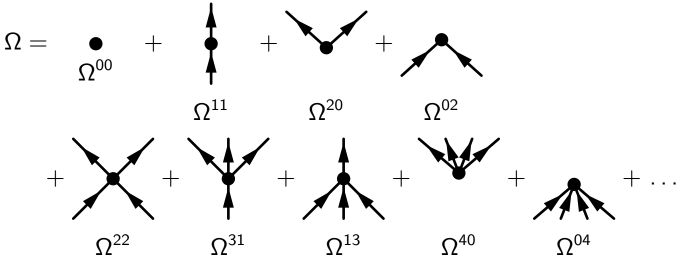
Perturbative expansion of g.s. energy

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

Building blocks of the diagrammatic

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



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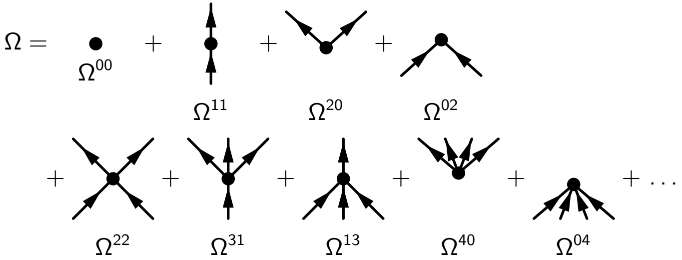
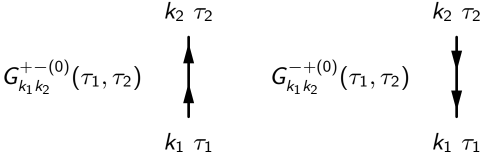


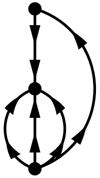
Quasiparticle propagators



Diagrams of observables from building blocks

I. Topological rules

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



Diagrammatic rules for observable $E_0^A - \lambda A$

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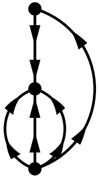
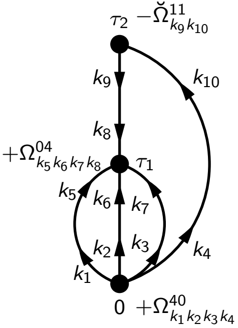


II. Algebraic rules

- 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

$\Updownarrow$

Order $p+1$ in standard counting

Time-dependent and time-integrated expressions:

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

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

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    [Arthuis, Duguet, Tichai, Lasseri, Ebran, *CPC* in print, arXiv:1809.01187]
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How to build an automated framework

Technical goal

p-order diagram production

p-order diagram evaluation

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Challenges

Handling complexity of diagrams	Perform p-tuple time integral

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Tools

Adjacency matrices

Time-structure diagrams

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End product

Open-source computer code

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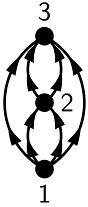
Oriented adjacency matrix from graph theory

a_{ij}: number of edges going from node i to node j

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



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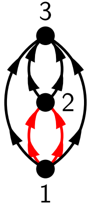

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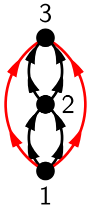

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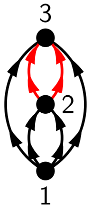

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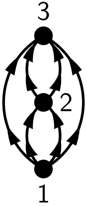

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Generation of BMBPT diagrams of order p

Algorithm

1. Generate all $(p+1) \times (p+1)$ matrices
   - ◇ Fill the matrices "vertex-wise" with all allowed integers
   - ◇ Check the degree of each vertex before moving on

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

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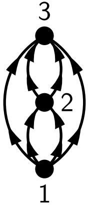

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$$\begin{pmatrix} 0 & \color{red}{2} & \color{red}{2} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Automatic generation of diagrams

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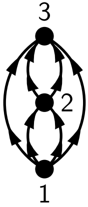

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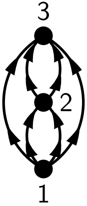

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2. Discard matrices leading to topologically identical diagrams

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

Automatic generation of diagrams

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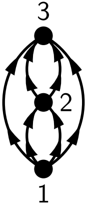

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3. Translate the matrix into drawing instructions

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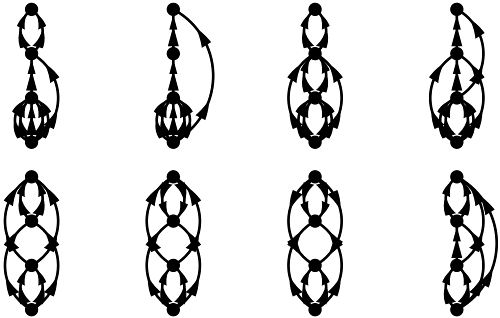
Automatic generation of diagrams

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



+ 388 others...

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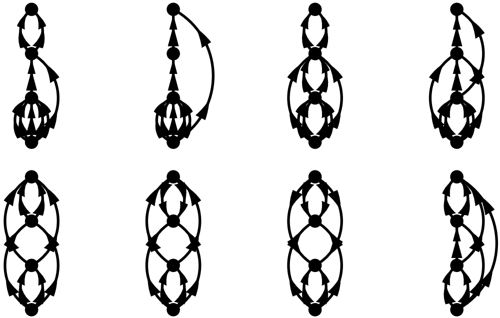

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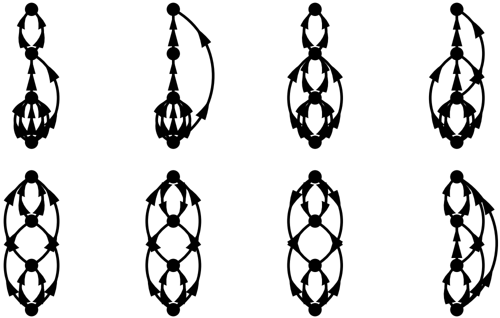
Systematic combinatoric

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

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



+ 388 others...

Systematic combinatoric

Generated by computer code in 2'30

Order		0	1	2	3	4	5
deg_max = 4	General	1	2	8	59	568	6 805
	HFB vacuum	1	1	1	10	82	938
deg_max = 6	General	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

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Time-structure diagrams

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

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

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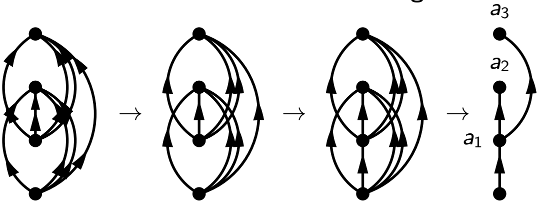
Time-structure diagram extraction



- a_i enter time exponentials
- Links carry time ordering

Time-structure diagrams

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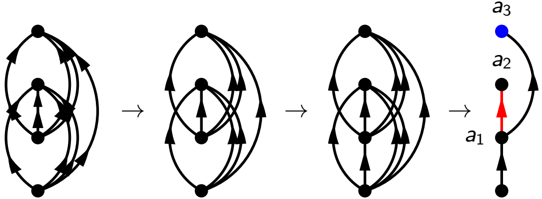

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$$TSD = \lim_{\tau \to \infty} \int_0^{\tau} \mathrm{d}\tau_1 \mathrm{d}\tau_2 \mathrm{d}\tau_3 \, \theta(\tau_2 - \tau_1) \theta(\tau_3 - \tau_1) e^{-a_1 \tau_1} e^{-a_2 \tau_2} e^{-a_3 \tau_3}$$

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

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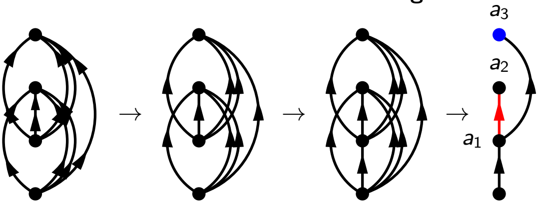

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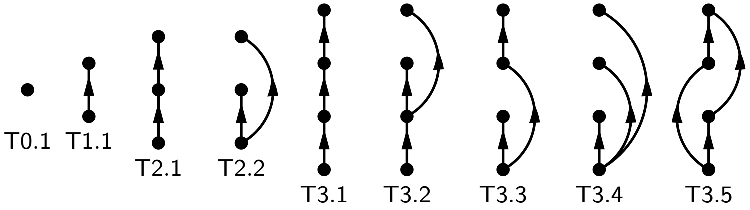
- Several BMBPT diagrams may have same TSD
- Replace a_i with appropriate q.p.e. sum for BMBPT final expression

Topologies of time-structure diagrams

- **TSD topology crucial for result extraction**



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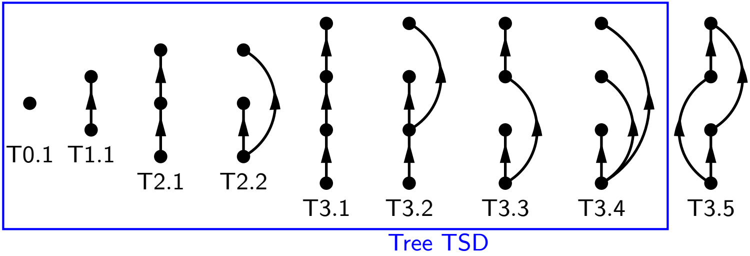

Topologies of time-structure diagrams

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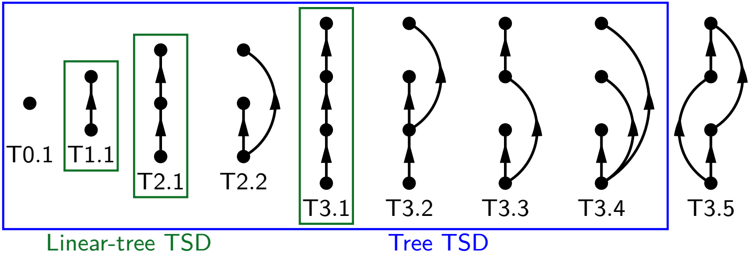

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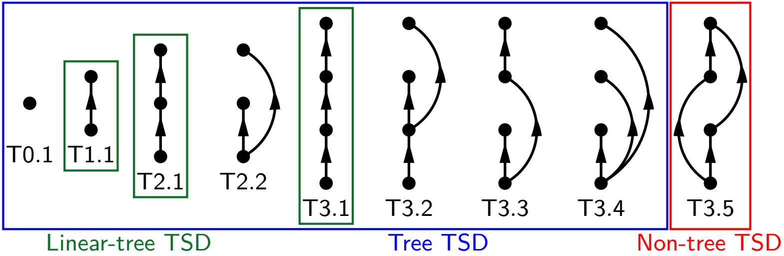

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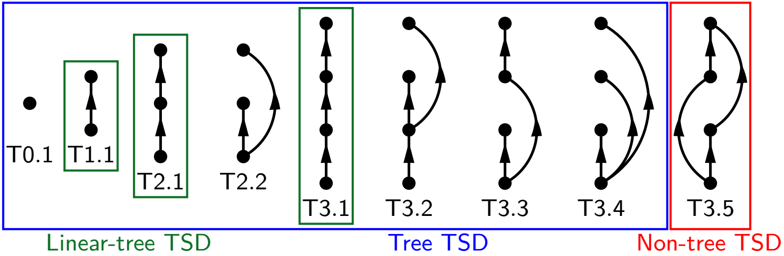
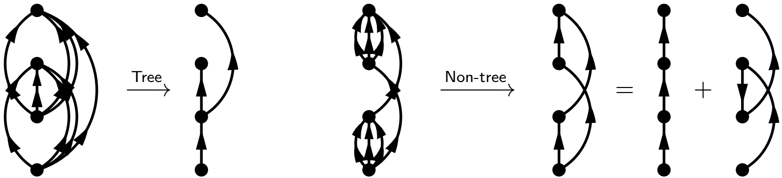


- Extraction of time-integrated expression depends on tree / non-tree



Topologies of time-structure diagrams

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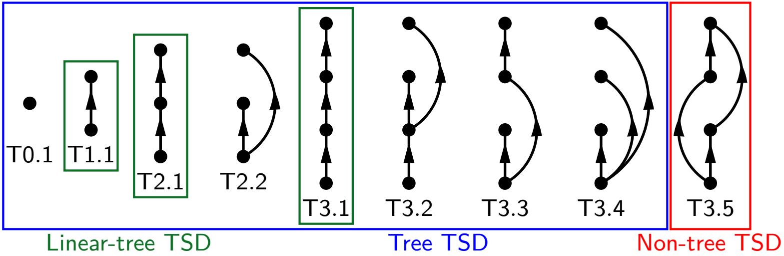

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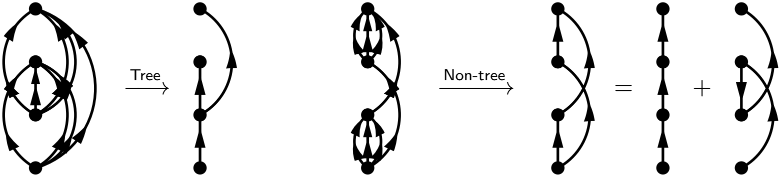
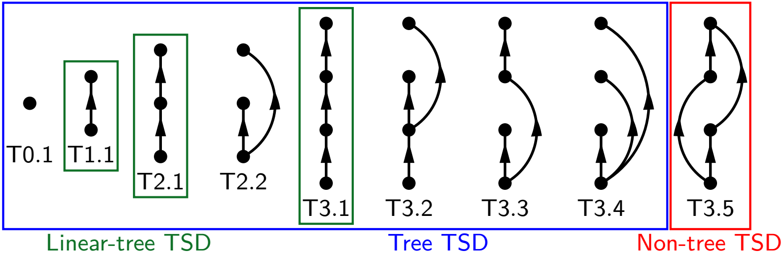


Direct diagrammatic rule

Topologies of time-structure diagrams

- **TSD topology crucial for result extraction**



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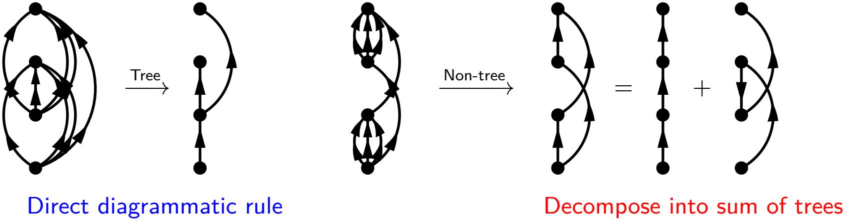

How to build an automated framework

Technical goal

p-order diagram production

p-order diagram evaluation

Challenges

Handling complexity of diagrams

Perform p-tuple time integral

Tools

Adjacency matrices

Time-structure diagrams

End product

Open-source computer code

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Open-source code ADG

UNIVERSITY OF SURREY

Technical aspects

- Python 2
- Use of *NetworkX* and *NumPy* libraries
- OS-independent
- BMBPT, HF-MBPT (NN only)

Diffusion

- Accepted in CPC
- Available on GitHub, PyPI
- GPLv3 license

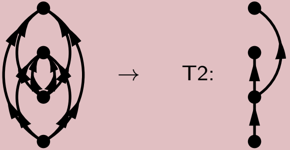
Output example

Diagram 5:

$$\mathrm{P}\Omega 3.5 = \lim_{\tau \to \infty} \frac{(-1)^3}{2(2!)^4} \sum_{k_i} \Omega^{40}_{k_1 k_2 k_3 k_4} \Omega^{40}_{k_5 k_6 k_7 k_8} \Omega^{04}_{k_5 k_6 k_1 k_2} \Omega^{04}_{k_7 k_8 k_3 k_4}$$

$$\times \int_0^{\tau} \mathrm{d}\tau_1 \mathrm{d}\tau_2 \mathrm{d}\tau_3 \theta(\tau_2 - \tau_1)\theta(\tau_3 - \tau_1) e^{-\tau_1 \epsilon^{k_5 k_6 k_7 k_8}} e^{-\tau_2 \epsilon_{k_1 k_2 k_5 k_6}} e^{-\tau_3 \epsilon_{k_3 k_4 k_7 k_8}}$$

$$= \frac{(-1)^3}{2(2!)^4} \sum_{k_i} \frac{\Omega^{40}_{k_1 k_2 k_3 k_4} \Omega^{40}_{k_5 k_6 k_7 k_8} \Omega^{04}_{k_5 k_6 k_1 k_2} \Omega^{04}_{k_7 k_8 k_3 k_4}}{\epsilon_{k_1 k_2 k_3 k_4} \epsilon_{k_1 k_2 k_5 k_6} \epsilon_{k_3 k_4 k_7 k_8}}$$

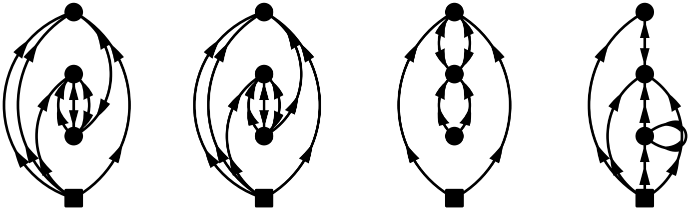


$$\mathrm{T2} = \frac{1}{(a_1 + a_2 + a_3) a_2 a_3}$$

Coming extensions of ADG: v2

Projected BMBPT diagrams now generated as well

[Ripoche, Arthuis, Tichai, Duguet, *in prep.*]



- Co-developped with the method from the start
- Symmetry breaking and restoration at arbitrary order

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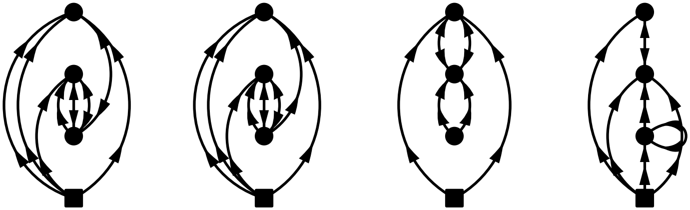
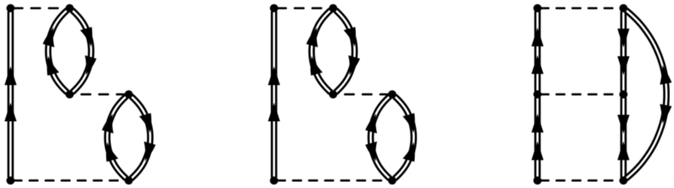


- Co-developped with the method from the start
- Symmetry breaking and restoration at arbitrary order
- Critical need for automatized tools from diagram number

Order	0	1	2	3	4
BMBPT (`deg_max` = 4)	1	2	8	59	568
PBMBPT (`deg_max` = 4)	1	3	37	951	33 985

Extension to Gorkov Self-Consistent Green's Function in progress

[Raimondi, Arthuis, Barbieri, Somà, Duguet, *in prep.*]



$\Sigma_{ab}^{11(C)^{30}_{30}}$ $\Sigma_{ab}^{11(C)^{30}_{12}}$ $\Sigma_{ab}^{11(C)^{21}_{12}}$

- Extend Gorkov SCGF to ADC(3)
  - ◇ Capture more correlations
  - ◇ Put Gorkov SCGF on equal footing with Dyson SCGF
- Incorporate 3NFs from the start

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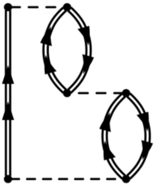
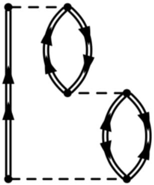
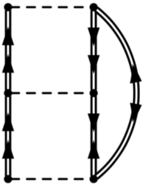


$\Sigma_{ab}^{11(C)^{30}_{30}}$



$\Sigma_{ab}^{11(C)^{30}_{12}}$



$\Sigma_{ab}^{11(C)^{21}_{12}}$

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  - ◇ Capture more correlations
  - ◇ Put Gorkov SCGF on equal footing with Dyson SCGF
- Incorporate 3NFs from the start

See C. Barbieri's colloquium for more SCGF!

Outline

- Why an automated tool for many-body diagrams?
- Application to Bogoliubov Many-Body Perturbation Theory
  - Basics of diagrammatic BMBPT formalism
  - Automated generation and evaluation for BMBPT diagrams
- Conclusion and perspectives

Conclusion and perspectives

(P)BMBPT diagrams generated and evaluated automatically

- ✔ Fast and error-safe
- ✔ Easier numerical implementation

ADG open-source code available

- ✔ HF-MBPT and BMBPT diagrams and expressions
- ✔ PBMBPT to come soon
- ◇ On-going work on GSCGF for ADC(n)

Interface with other codes

- ✔ Text-format output available for interface with numerical codes (e.g. [Drischler, Hebeler and Schwenk, *PRL* **122** (2019)])
- ◇ To be interfaced with *J*-coupling tools (see J. Ripoche's poster)

Behind the ADG project

C. Barbieri

R.-D. Lasseri

T. Duguet
J.-P. Ebran
F. Raimondi
J. Ripoche
V. Somà
A. Tichai

Thank you for your attention!