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# **ADG - Automated Diagram Generator Documentation**

***Release 3.0.2***

**ADG Dev Team**

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# CHAPTER 1

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## The ADG Project

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### 1.1 Description

ADG is a tool generating diagrams and producing their expressions for given many-body formalisms. Diagrammatic rules from the formalism are combined with graph theory objects to produce diagrams and expressions in a fast, simple and error-safe way.

The only input consists in the theory and order of interest, and the N-body character of the operators of interest. The main output is a LaTeX file containing the diagrams, their associated expressions and additional informations that can be compiled into PDF by ADG if needed. Other computer-readable files may be produced as well.

### 1.2 Status

As for now, the code is capable of handling four different formalisms, i.e. Many-Body Perturbation Theory (MBPT), Bogoliubov Many-Body Perturbation Theory (BMBPT), Projected Bogoliubov Many-Body Perturbation Theory (PBMBPT), and Bogoliubov In-Medium Similarity Renormalization Group (BIMSRG).

- For MBPT, the code generates all Hartree-Fock energy diagrams at any given order along with their expression and additional information (conjugate diagram, excitation level...).
- For (P)BMBPT, the code generates all diagrams for a generic observable commuting with the Hamiltonian, along with their time-dependent and time-integrated expressions.
- For BIMSRG, the code generates all diagrams and expressions at any given truncation order for the two operators as well as the commutator itself. The traditional BIMSRG(n) truncation order corresponds to truncating both operators as well as the commutator at the same rank.

### 1.3 Future developments

ADG is currently being extended to diagrams and expressions generation for Gorkov Self-Consistent Green's Functions (GSCGF).



# CHAPTER 2

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## Install ADG on your computer

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### 2.1 Install

To install ADG, download the source files and run

```
pip install <project_folder>
```

or alternatively

```
python setup.py install
```

If you want to install ADG in develop mode, then run

```
pip install -e <project_folder>
```

### 2.2 Dependencies

In order to run the code, you will need a Python2 install  $\geq 2.7.1$  and the following Python libraries:

- networkx  $\geq 2.0$
- numpy
- scipy
- future
- more-itertools

If you want ADG to compile the LaTeX output file, you will need a Latex install with the PDFLaTeX compiler and the feynmp and feynmp-auto packages installed, which are standard packages in most recent distributions.



# CHAPTER 3

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## Generate diagrams with ADG

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### 3.1 Run ADG

To run the program and generate BMBPT diagrams at order 4 for example, use

```
adg -o 4 -t BMBPT -d -c
```

where the `-o` flag is for the order, `-t` for the type of theory, `-d` indicates you want the diagrams to be drawn and `-c` that you want ADG to compile the LaTeX output.

You can alternatively run the program in interactive mode by typing

```
adg -i
```

Finally, to obtain more information on all the available flags, use

```
adg -h
```

### 3.2 CLI options

#### 3.2.1 Generic options:

- o, --order**      order of the diagrams [1-9] or N\_A, N\_B, N\_C truncation for BIMSRG
- t, --theory**      theory of interest: MBPT, BMBPT or PBMBPT
- i, --interactive**    execute ADG in interactive mode

#### 3.2.2 (P)BMBPT options:

- can, --canonical**    consider only canonical diagrams
- nobs, --nbody\_observable**    maximal n-body character of the observable [1-3], default = 2
- 3NF, --with\_3NF**    use two and three-body forces for BMBPT diagrams
- dt, --draw\_tsds**    draw Time-Structure Diagrams

### **3.2.3 MBPT option:**

**-cd, --cd\_output** produce computer-readable output for automated frameworks

### **3.2.4 Run management options:**

**-d, --draw\_diags** draw the diagrams using FeynMF

**-c, --compile** compile the LaTeX output file with PDFLaTeX

## **3.3 Output files**

The output of the program is stored in a folder named after the theory, and a subfolder named after the order, e.g. /MBPT/Order-4. In the case of (P)BMBPT, suffixes are added depending on the n-body forces of the observable, and if three-body forces were used or only canonical diagrams computed, i.e. for our previous example, results would be stored under BMBPT/Order-4\_2body\_observable. For BIMSRG, the folder corresponds e.g. to BIMSRG/Order\_1\_2\_3 if N\_A is 1, N\_B is 2 and N\_B is 3.

The main output file of the program, called `result.tex`, is a LaTeX file containing the expressions of the diagrams along other basic infos on their structure, and, if flag `-d` has been used, drawing instructions. The file is automatically compiled and produces a PDF file `result.pdf` when using the `-c` file.

A list of the adjacency matrices associated with the diagrams is printed separately in the `adj_matrices.list` file to allow for an easy use with another many-body diagrams code.

In the case of a MBPT calculations, it is possible to produce output specifically tailored for automated calculations framework by using the `-cd` flag. The associated output files use `CD_` as a prefix.

# CHAPTER 4

## ADG Reference for Developers

### 4.1 Main script

Main routine of the Automated Diagram Generator.

```
adg.main.main()  
Launch the ADG program.
```

### 4.2 Run & CLI management

Routines handling the run of ADG.

```
adg.run.attribute_directory(commands)  
Create missing directories and return the working directory.
```

**Parameters** `commands` (*Namespace*) – Flags for the run management.

**Returns** Path to the result folder.

**Return type** (str)

```
>>> com = argparse.Namespace()  
>>>  
>>> com.theory, com.order = 'BMBPT', 4  
>>> com.with_3NF, com.nbody_observable, com.canonical = False, 2, False  
>>>  
>>> attribute_directory(com)  
'BMBPT/Order-4_2body_observable'  
>>>  
>>> com.theory, com.order = 'BMBPT', 5  
>>> com.with_3NF, com.nbody_observable, com.canonical = True, 3, False  
>>>  
>>> attribute_directory(com)  
'BMBPT/Order-5_3body_observable_with3N'  
>>>  
>>> com.theory, com.order = 'MBPT', 3  
>>> com.with_3NF, com.nbody_observable, com.canonical = False, 2, False  
>>>
```

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```
>>> attribute_directory(com)
'MBPT/Order-3'
>>>
>>> com.theory, com.order = 'BIMSRG', (1, 2, 3)
>>>
>>> attribute_directory(com)
'BIMSRG/Order_1_2_3'
```

adg.run.**clean\_folders**(*directory, commands*)  
Delete temporary files and folders.

**Parameters**

- **directory** (*str*) – Path to the output folder.
- **commands** (*Namespace*) – Flags to manage the program's run.

adg.run.**compile\_manager**(*directory*)  
Compile the program's LaTeX output file.

**Parameters** **directory** (*str*) – Path to the output folder.

adg.run.**create\_feynmanmp\_files**(*diagrams, theory, directory, diag\_type*)  
Create and move the appropriate feynmanmp files to the right place.

**Parameters**

- **diagrams** (*list*) – The studied diagrams.
- **theory** (*str*) – Name of the theory of interest.
- **directory** (*str*) – Path to the result folder.
- **diag\_type** (*str*) – Type of studied diagrams used for drawing.

adg.run.**generate\_diagrams**(*commands, id\_generator*)  
Return a list with diagrams of the appropriate type.

**Parameters**

- **commands** (*Namespace*) – Flags for the run management.
- **id\_generator** (*UniqueID*) – A unique ID number generator.

**Returns** All the diagrams of the appropriate Class and order.

**Return type** (*list*)

adg.run.**get\_bimsrg\_truncation\_order**(*operator*)  
Return the truncation order of a given operator from the user input.

**Parameters** **operator** (*str*) – The letter corresponding to the operator name.py

**Returns** The truncation rank of the operator.

**Return type** order (*int*)

adg.run.**interactive\_interface**(*commands*)  
Run the interactive interface mode, return the appropriate commands.

**Parameters** **commands** (*Namespace*) – Flags for the run management.

**Returns** Flags initialized through keyboard input.

**Return type** (*Namespace*)

adg.run.**order\_diagrams**(*diagrams, commands*)  
Return the ordered unique diagrams with a dict of numbers per type.

**Parameters**

- **diagrams** (*list*) – The diagrams of the appropriate Class.
- **commands** (*Namespace*) – Flags for the run management.

**Returns** First element is the list of ordered and unique diagrams. Second element is a dict with the number of diagrams per type. Third element is a dict with the identifiers of diagrams starting each output file section.

**Return type** (tuple)

`adg.run.parse_command_line(cli_args)`

Return run commands from the Command Line Interface.

**Parameters** `cli_args` – Command-line arguments submitted with the program.

**Returns** Appropriate commands to manage the program's run.

**Return type** (Namespace)

`adg.run.prepare_drawing_instructions(directory, commands, diagrams, diagrams_time)`

Write FeynMP files for the different diagrams.

**Parameters**

- **directory** (*str*) – Path to the output folder.
- **commands** (*Namespace*) – Flags for the run management.
- **diagrams** (*list*) – All the diagrams of interest.
- **diagrams\_time** (*list*) – All the associated TSDs if appropriate.

`adg.run.print_diags_numbers(commands, diags_nbs)`

Print the number of diagrams for each major type.

**Parameters**

- **commands** (*Namespace*) – Flags for the run management.
- **diags\_nbs** (*dict*) – The number of diagrams for each major type.

`adg.run.write_file_header(latex_file, commands, diags_nbs)`

Write the header of the result tex file.

**Parameters**

- **latex\_file** (*file*) – LaTeX output file of the program.
- **commands** (*Namespace*) – Flags to manage the program's run.
- **diags\_nbs** (*dict*) – Number of diagrams per major type.

## 4.3 Generic Diagram

Routines and class for all types of diagrams, inherited by others.

**class** `adg.diag.Diagram(nx_graph)`  
Bases: `object`

Describes a diagram with its related properties.

**graph**  
The actual graph.

**Type** NetworkX MultiDiGraph

**unsorted\_degrees**  
The degrees of the graph vertices

**Type** tuple

**degrees**

The ascendingly sorted degrees of the graph vertices.

**Type** tuple

**unsort\_io\_degrees**

The list of in- and out-degrees for each vertex of the graph, stored in a (in, out) tuple.

**Type** tuple

**io\_degrees**

The sorted version of unsort\_io\_degrees.

**Type** tuple

**max\_degree**

The maximal degree of a vertex in the graph.

**Type** int

**tags**

The tag numbers associated to a diagram.

**Type** list

**degrees**

**graph**

**io\_degrees**

**max\_degree**

**tags**

**unsort\_degrees**

**unsort\_io\_degrees**

**write\_graph** (*latex\_file*, *directory*, *write\_time*)

Write the graph of the diagram to the LaTeX file.

**Parameters**

- **latex\_file** (*file*) – The LaTeX output file of the program.
- **directory** (*str*) – Path to the result folder.
- **write\_time** (*bool*) – (Here to emulate polymorphism).

**adg.diag.bimsrg\_diagram\_internals** (*graph*, *fmf\_file*, *prop\_type*)

Write to file the vertices and propagators of BIMSRG diagrams.

**Parameters**

- **graph** (*NetworkX MultiDiGraph*) – The graph to be drawn.
- **fmf\_file** (*file*) – The FeynmanMF file to be written to.
- **prop\_type** (*str*) – The FeynmanMF type for drawing the propagators.

**adg.diag.check\_vertex\_degree** (*matrices*, *three\_body\_use*, *nbody\_max\_observable*, *canonical\_only*, *vertex\_id*)

Check the degree of a specific vertex in a set of matrices.

**Parameters**

- **matrices** (*list*) – Adjacency matrices.
- **three\_body\_use** (*bool*) – True if one uses three-body forces.
- **nbody\_max\_observable** (*int*) – Maximum body number for the observable.
- **canonical\_only** (*bool*) – True if one draws only canonical diagrams.

- **vertex\_id** (*int*) – The position of the studied vertex.

```
>>> test_matrices = [numpy.array([[0, 1, 2], [1, 0, 1], [0, 2, 0]]),
    ↪numpy.array([[2, 0, 2], [1, 2, 3], [1, 0, 0]]), numpy.array([[0, 1, 0,
    ↪3], [2, 0, 8], [2, 1, 0]])]
>>> check_vertex_degree(test_matrices, True, 3, False, 0)
>>> test_matrices #doctest: +NORMALIZE_WHITESPACE
[array([[0, 1, 2], [1, 0, 1], [0, 2, 0]]),
 array([[2, 0, 2], [1, 2, 3], [1, 0, 0]])]
>>> check_vertex_degree(test_matrices, False, 2, False, 0)
>>> test_matrices #doctest: +NORMALIZE_WHITESPACE
[array([[0, 1, 2], [1, 0, 1], [0, 2, 0]])]
```

`adg.diag.create_checkable_diagram(pbmbpt_graph)`

Return a graph with anomalous props going both ways for topo check.

**Parameters** `pbmbpt_graph` (*NetworkX MultiDiGraph*) – The graph to be copied.

**Returns** Graph with double the anomalous props.

**Return type** (*NetworkX MultiDiGraph*)

`adg.diag.draw_diagram(directory, result_file, diagram_index, diag_type)`

Copy the diagram feynmanmp instructions in the result file.

**Parameters**

- `directory` (*str*) – The path to the output folder.
- `result_file` (*file*) – The LaTeX ouput file of the program.
- `diagram_index` (*str*) – The number associated to the diagram.
- `diag_type` (*str*) – The type of diagram used here.

`adg.diag.extract_denom(start_graph, subgraph)`

Extract the appropriate denominator using the subgraph rule.

**Parameters**

- `start_graph` (*NetworkX MultiDiGraph*) – The studied graph.
- `subgraph` (*NetworkX MultiDiGraph*) – The subgraph used for this particular denominator factor.

**Returns** The denominator factor for this subgraph.

**Return type** (*str*)

`adg.diag.feynmf_generator(graph, theory_type, diagram_name)`

Generate the feynmanmp instructions corresponding to the diagram.

**Parameters**

- `graph` (*NetworkX MultiDiGraph*) – The graph of interest.
- `theory_type` (*str*) – The name of the theory of interest.
- `diagram_name` (*str*) – The name of the studied diagram.

`adg.diag.label_vertices(graphs_list, theory_type, switch_flag)`

Account for different status of vertices in operator diagrams.

**Parameters**

- `graphs_list` (*list*) – The Diagrams of interest.
- `theory_type` (*str*) – The name of the theory of interest.
- `switch_flag` (*int*) – When to switch A and B operators for BIMSRG.

`adg.diag.no_trace(matrices)`

Select matrices with full 0 diagonal.

**Parameters** `matrices` (`list`) – A list of adjacency matrices.

**Returns** The adjacency matrices without non-zero diagonal elements.

**Return type** (`list`)

```
>>> test_matrices = [[[0, 1, 2], [2, 0, 1], [5, 2, 0]],      [[2, 2, 2], [1, 2, 0], [0, 0, 0]],      [[0, 1, 3], [2, 0, 8], [2, 1, 0]]]
>>> no_trace(test_matrices)
[[[0, 1, 2], [2, 0, 1], [5, 2, 0]], [[0, 1, 3], [2, 0, 8], [2, 1, 0]]]
```

`adg.diag.print_adj_matrices(directory, diagrams)`

Print a computer-readable file with the diagrams' adjacency matrices.

**Parameters**

- `directory` (`str`) – The path to the output directory.
- `diagrams` (`list`) – All the diagrams.

`adg.diag.prop_directions(vert_distance, nb_props)`

Return a list of possible propagators directions.

**Parameters**

- `vert_distance` (`int`) – Distance between the two connected vertices.
- `nb_props` (`int`) – Number of propagators to be drawn.

**Returns** Propagators directions stored as strings.

**Return type** (`list`)

`adg.diag.propagator_style(prop_type)`

Return the FeynMF definition for the appropriate propagator type.

**Parameters** `prop_type` (`str`) – The type of propagators used in the diagram.

**Returns** The FeynMF definition for the propagator style used.

**Return type** (`str`)

`adg.diag.self_contractions(graph)`

Return the instructions for drawing the graph's self-contractions.

**Parameters** `graph` (`NetworkX MultiDiGraph`) – The graph being drawn.

**Returns** FeynMF instructions for drawing the self-contractions.

**Return type** (`str`)

`adg.diag.to_skeleton(graph)`

Return the bare skeleton of a graph, i.e. only non-redundant links.

**Parameters** `graph` (`NetworkX MultiDiGraph`) – The graph to be turned into a skeleton.

**Returns** The skeleton of the initial graph.

**Return type** (`NetworkX MultiDiGraph`)

`adg.diag.topologically_distinct_diagrams(diagrams)`

Return a list of diagrams all topologically distinct.

**Parameters** `diagrams` (`list`) – The Diagrams of interest.

**Returns** Topologically unique diagrams.

**Return type** (`list`)

---

```
adg.diag.update_permutations (comp_graph_perms, comp_graph_tag, mapping)
```

Update permutations associated to the BMBPT diags for a shared TSD.

#### Parameters

- **comp\_graph\_perms** (*dict*) – Permutations to be updated.
- **comp\_graph\_tag** (*int*) – The tag associated to the TSD configuration.
- **mapping** (*dict*) – permutations to go from previous ref TSD to new one.

```
adg.diag.vertex_positions (graph, order)
```

Return the positions of the graph's vertices.

#### Parameters

- **graph** (*NetworkX MultiDiGraph*) – The graph of interest.
- **order** (*int*) – The perturbative order of the graph.

**Returns** The FeynMP instructions for positioning the vertices.

**Return type** (str)

## 4.4 MBPT diagram

Routines and class for Many-Body Perturbation Theory diagrams.

```
class adg.mbpt.MbptDiagram (mbpt_graph, tag_num)
```

Bases: *adg.diag.Diagram*

Describes a MBPT diagram with its related properties.

#### incidence

The incidence matrix of the graph.

**Type** NumPy array

#### excitation\_level

The single, double, etc., excitation character.

**Type** int

#### complex\_conjugate

The tag number of the diagram's complex conjugate. -1 is the graph has none.

**Type** int

#### expr

The MBPT expression associated to the diagram.

**Type** str

#### cd\_expr

The expression associated to the diagram in a computer-readable format.

**Type** str

#### adjacency\_mat

The adjacency matrix of the graph.

**Type** NumPy array

#### adjacency\_mat

#### attribute\_expression ()

Initialize the expression associated to the diagram.

#### attribute\_ph\_labels ()

Attribute the appropriate qp labels to the graph's propagators.

```
calc_excitation()
    Return an integer coding for the excitation level of the diag.

    Returns The singles / doubles / etc. character of the graph.

    Return type (int)

cd_denominator()
    Return the computer-readable denominator of the graph.

    Returns The graph denominator tailored for automated frameworks.

    Return type (str)

cd_expr

cd_numerator()
    Return the computer-readable numerator.

    Returns The graph numerator tailored for automated frameworks.

    Return type (str)

complex_conjugate

count_hole_lines()
    Return an integer for the number of hole lines in the graph.

    Returns The number of holes in the diagram.

    Return type (int)

degrees

excitation_level

expr

extract_denominator()
    Return the denominator for a MBPT graph.

    Returns The denominator of the diagram.

    Return type (str)

extract_numerator()
    Return the numerator associated to a MBPT graph.

    Returns The numerator of the diagram.

    Return type (str)

graph

incidence

io_degrees

is_complex_conjug_of (test_diagram)
    Return True if self and test_diagram are complex conjugate.

    Parameters test_diagram (MbptDiagram) – A diagram to compare with.

    Returns The complex conjugate status of the pair of diagrams.

    Return type (bool)

loops_number()
    Return the number of loops in the diagram as an integer.

    Returns The number of loops in the graph.

    Return type (int)

max_degree
```

**tags****unsort\_degrees****unsort\_io\_degrees****write\_graph** (*latex\_file*, *directory*, *write\_time*)

Write the graph of the diagram to the LaTeX file.

**Parameters**

- **latex\_file** (*file*) – The LaTeX output file of the program.
- **directory** (*str*) – Path to the result folder.
- **write\_time** (*bool*) – (Here to emulate polymorphism).

**write\_section** (*result*, *commands*, *flags*)

Write sections for MBPT result file.

**Parameters**

- **result** (*file*) – The LaTeX output file to be written in.
- **commands** (*dict*) – The flags associated with run management.
- **flags** (*dict*) – The identifier of each section-starting graph.

adg.mbpt.**attribute\_conjugate** (*diagrams*)

Attribute to each diagram its complex conjugate.

The diagrams involved in conjugate pairs receive the tag associated to their partner in the `complex_conjugate` attribute.**Parameters** **diagrams** (*list*) – The topologically unique MbptDiagrams.adg.mbpt.**diagrams\_generation** (*order*)

Generate the diagrams for the MBPT case.

**Parameters** **order** (*int*) – The perturbative order of interest.**Returns** A list of NumPy arrays with the diagrams adjacency matrices.**Return type** (*list*)

```
>>> diagrams_generation(2) # doctest: +NORMALIZE_WHITESPACE
[array([[0, 2], [2, 0]])]
>>> diagrams_generation(3) # doctest: +NORMALIZE_WHITESPACE
[array([[0, 2, 0], [0, 0, 2], [2, 0, 0]]),
 array([[0, 1, 1], [1, 0, 1], [1, 1, 0]]),
 array([[0, 0, 2], [2, 0, 0], [0, 2, 0]])]
>>> diagrams_generation(1)
[]
```

adg.mbpt.**extract\_cd\_denom** (*start\_graph*, *subgraph*)

Extract the computer-readable denominator using the subgraph rule.

**Parameters**

- **start\_graph** (*NetworkX MultiDiGraph*) – The studied graph.
- **subgraph** (*NetworkX MultiDiGraph*) – The subgraph for this particular factor.

**Returns** The denominator factor associated to this subgraph.**Return type** (*str*)adg.mbpt.**order\_diagrams** (*diagrams*)

Order the MBPT diagrams and return the number of diags for each type.

**Parameters** **diagrams** (*list*) – The unordered MbptDiagrams.

**Returns** First element are the ordered MbptDiagrams. Second element is the number of diagrams for each excitation level type.

**Return type** (tuple)

```
adg.mbpt.print_cd_output(directory, diagrams)
```

Print a computer-readable file for automated frameworks.

**Parameters**

- **directory** (str) – The path to the output directory.
- **diagrams** (list) – All the MbptDiagrams.

```
adg.mbpt.write_diag_exp(latex_file, mbpt_diag)
```

Write the expression associated to a diagram in the LaTeX file.

**Parameters**

- **latex\_file** (file) – The LaTeX output file to be written in.
- **mbpt\_diag** (MbptDiagram) – The diagram which expression is being written.

```
adg.mbpt.write_header(tex_file, diags_nbs)
```

Write the appropriate header for the LaTeX file for MBPT diagrams.

**Parameters**

- **tex\_file** (file) – The LaTeX output file to be written in.
- **diags\_nbs** (dict) – A dict with the number of diagrams per excitation level type.

## 4.5 BMBPT Diagram

Routines and class for Bogoliubov MBPT diagrams.

```
class adg.bmbpt.BmbptFeynmanDiagram(nx_graph, tag_num)
```

Bases: *adg.diag.Diagram*

Describes a BMBPT Feynman diagram with its related properties.

**two\_or\_three\_body**

The 2 or 3-body character of the vertices.

**Type** int

**time\_tag**

The tag number associated to the diagram's associated TSD.

**Type** int

**tsd\_is\_tree**

The tree or non-tree character of the associated TSD.

**Type** bool

**feynman\_exp**

The Feynman expression associated to the diagram.

**Type** str

**diag\_exp**

The Goldstone expression associated to the diagram.

**Type** str

**vert\_exp**

The expression associated to the vertices.

**Type** list

**hf\_type**

The Hartree-Fock, non-Hartree-Fock or Hartree-Fock for the energy operator only character of the graph.

**Type** str

**unique\_id**

A unique number associated to the diagram.

**Type** int

**vertex\_exchange\_sym\_factor**

Lazy-initialized symmetry factor associated to the vertex exchange, stored to avoid being computed several times.

**Type** int

**attribute\_expressions** (*time\_diag*)

Attribute the correct Feynman and Goldstone expressions.

**Parameters** **time\_diag** (TimeStructureDiagram) – The associated TSD.

**attribute\_qp\_labels** ()

Attribute the appropriate qp labels to the graph's propagators.

**degrees****diag\_exp****equivalent\_permutations** ()

Return the permutations generating equivalent diagrams.

**Returns** Vertices permutations as dictionnaires.

**Return type** (list)

**extract\_integral** ()

Return the integral part of the Feynman expression of the diag.

**Returns** The integral part of its Feynman expression.

**Return type** (str)

**extract\_numerator** ()

Return the numerator associated to a BMBPT graph.

**Returns** The numerator of the graph.

**Return type** (str)

**feynman\_exp****graph****has\_crossing\_sign** ()

Return True for a minus sign associated with crossing propagators.

Use the fact that all lines propagate upwards and the canonical representation of the diagrams and vertices.

**Returns**

**Encode for the sign factor associated with crossing** propagators.

**Return type** (bool)

**has\_sign\_factor** ()

Return True if a sign factor is associated to the diagram.

Wrapper allowing for easy refactoring of expression code.

**Returns** The presence of a sign factor.

**Return type** (boolean)

**hf\_type**

**io\_degrees**

**max\_degree**

**multiplicity\_symmetry\_factor()**  
Return the symmetry factor associated with propagators multiplicity.

**Returns** The symmetry factor associated with equivalent lines.

**Return type** (str)

**symmetry\_factor()**  
Return the overall symmetry factor of the diagram.

**Returns** The combination of all symmetry factors.

**Return type** (str)

**tags**

**time\_tag**

**time\_tree\_denominator(*time\_graph*)**  
Return the denominator for a time-tree graph.

**Parameters** **time\_graph** (*NetworkX MultiDiGraph*) – Its associated time-structure graph.

**Returns** The denominator of the graph.

**Return type** (str)

**tsd\_is\_tree**

**two\_or\_three\_body**

**unique\_id**

**unsort\_degrees**

**unsort\_io\_degrees**

**vert\_exp**

**vertex\_exchange\_sym\_factor**  
Return the symmetry factor associated with vertex exchange.

**Returns** The symmetry factor for vertex exchange.

**Return type** (int)

**vertex\_expression(*vertex*)**  
Return the expression associated to a given vertex.

**Parameters** **vertex** (*int*) – The vertex of interest in the graph.

**Returns** The LaTeX expression associated to the vertex.

**Return type** (str)

**write\_diag\_exps(*latex\_file*, *norder*)**  
Write the expressions associated to a diagram in the LaTeX file.

**Parameters**

- **latex\_file** (*file*) – The LaTeX outputfile of the program.
- **norder** (*int*) – The order in BMBPT formalism.

**write\_graph(*latex\_file*, *directory*, *write\_time*)**  
Write the BMBPT graph and its associated TSD to the LaTeX file.

**Parameters**

- **latex\_file** (*file*) – The LaTeX output file of the program.
- **directory** (*str*) – The path to the result folder.
- **write\_time** (*bool*) – True if we want informations on the associated TSDs.

**write\_section** (*result, commands, section\_flags*)

Write section and subsections for BMBPT result file.

**Parameters**

- **result** (*file*) – The LaTeX output file of the program.
- **commands** (*dict*) – The flags associated with run management.
- **section\_flags** (*dict*) – UniqueIDs of diags starting each section.

**write\_tsd\_info** (*diagrams\_time, latex\_file*)

Write info related to the BMBPT associated TSD to the LaTeX file.

**Parameters**

- **diagrams\_time** (*list*) – The associated TSDs.
- **latex\_file** (*file*) – The LaTeX output file of the program.

**write\_vertices\_values** (*latex\_file, mapping*)

Write the qp energies associated to each vertex of the diag.

**Parameters**

- **latex\_file** (*file*) – The LaTeX output file of the program.
- **mapping** (*dict*) – A mapping between the vertices in the diagram and the vertices in its equivalent TSD, since permutations between vertices are possible.

adg.bmbpt.**check\_topologically\_equivalent** (*matrices, max\_vertex*)

Exclude matrices that would spawn topologically equivalent graphs.

**Parameters**

- **matrices** (*list*) – Adjacency matrices to be checked.
- **max\_vertex** (*int*) – The maximum vertex which have been filled.

**Returns** The topologically unique matrices.**Return type** (*list*)

```
>>> import numpy
>>> mats = [numpy.array([[0, 2, 0, 0], [2, 0, 0, 1], [0, 0, 0, 0], [0, 0, 0, 0]]),
             numpy.array([[0, 0, 2, 0], [0, 0, 0, 0], [2, 0, 0, 1], [0, 0, 0, 0]])]
>>>
>>> mats = check_topologically_equivalent(mats, 2)
>>> mats # doctest: +NORMALIZE_WHITESPACE
[array([[0, 2, 0, 0], [2, 0, 0, 1], [0, 0, 0, 0], [0, 0, 0, 0]])]
>>>
>>> mats = check_topologically_equivalent([], 2)
>>> mats # doctest: +NORMALIZE_WHITESPACE
[]
```

adg.bmbpt.**check\_unconnected\_spawn** (*matrices, max\_filled\_vertex*)

Exclude some matrices that would spawn unconnected diagrams.

Do several permutations among the rows and columns corresponding to already filled vertices, and check if one obtains a block-diagonal organisation, where the off-diagonals blocks connecting the already-filled and yet-unfilled parts of the matrix would be empty. In that case, remove the matrix.

## Parameters

- **matrices** (*list*) – The adjacency matrices to be checked.
- **max\_filled\_vertex** (*int*) – The furthest vertex until which the matrices have been filled.

```
>>> import numpy
>>> mats = [numpy.array([[0, 2, 0], [2, 0, 0], [0, 0, 0]]),
->           numpy.array([[0, 2, 1], [2, 0, 1], [0, 0, 0]])]
>>>
>>> check_unconnected_spawn(mats, 1)
>>> mats # doctest: +NORMALIZE_WHITESPACE
[array([[0, 2, 1], [2, 0, 1], [0, 0, 0]])]
```

`adg.bmbpt.diagrams_generation(p_order, three_body_use, nbody_obs, canonical)`

Generate diagrams for BMBPT from bottom up.

## Parameters

- **p\_order** (*int*) – The BMBPT perturbative order of the studied diagrams.
- **three\_body\_use** (*bool*) – Flag for the use of three-body forces.
- **nbody\_obs** (*int*) – N-body character of the observable of interest.
- **canonical** (*bool*) – True if one draws only canonical diagrams.

**Returns** NumPy arrays encoding the adjacency matrices of the graphs.

**Return type** (*list*)

```
>>> diags = diagrams_generation(1, False, 2, False)
>>> len(diags)
2
>>> any(np.array_equal([[0, 4], [0, 0]], diag) for diag in diags)
True
>>> any(np.array_equal([[0, 2], [0, 0]], diag) for diag in diags)
True
>>> diags = diagrams_generation(1, True, 3, False)
>>> len(diags)
3
>>> any(np.array_equal([[0, 6], [0, 0]], diag) for diag in diags)
True
>>> any(np.array_equal([[0, 4], [0, 0]], diag) for diag in diags)
True
>>> any(np.array_equal([[0, 2], [0, 0]], diag) for diag in diags)
True
>>> diags = diagrams_generation(2, False, 2, True)
>>> len(diags)
2
>>> any(np.array_equal([[0, 2, 2], [0, 0, 2], [0, 0, 0]], d) for d in diags)
True
>>> any(np.array_equal([[0, 1, 1], [0, 0, 3], [0, 0, 0]], d) for d in diags)
True
```

`adg.bmbpt.order_and_remove_topologically_equiv(matrices, max_vertex)`

Order the matrices in sub-list and remove topologically equivalent ones.

## Parameters

- **matrices** (*list*) – The adjacency matrices to be checked.
- **max\_vertex** (*int*) – The maximum vertex which has been filled.

**Returns** The ordered topologically unique matrices.

**Return type** (*list*)

```
adg.bmbpt.order_diagrams(diagrams)
```

Order the BMBPT diagrams and return number of diags for each type.

**Parameters** `diagrams` (`list`) – Possibly redundant BmbptFeynmanDiagrams.

**Returns**

**First element is the list of topologically unique, ordered** diagrams. Second element is a dict with the number of diagrams for each major type. Third element is a dict with the identifiers of diagrams starting each output file section.

**Return type** (`tuple`)

```
adg.bmbpt.produce_expressions(diagrams, diagrams_time)
```

Produce and store the expressions associated to the BMBPT diagrams.

**Parameters**

- `diagrams` (`list`) – The list of all BmbptFeynmanDiagrams.
- `diagrams_time` (`list`) – Their associates TSDs.

```
adg.bmbpt.remove_disconnected_matrices(matrices)
```

Remove matrices corresponding to disconnected diagrams.

**Parameters** `matrices` (`list`) – List of adjacency matrices.

```
adg.bmbpt.write_header(tex_file, commands, diags_nbs)
```

Write overall header for BMBPT result file.

**Parameters**

- `tex_file` (`file`) – The ouput LaTeX file of the program.
- `commands` (`Namespace`) – Flags for the program run.
- `diags_nbs` (`dict`) – The number of diagrams per type.

## 4.6 PBMBPT Diagram

Routines and class for Projected Bogoliubov MBPT diagrams.

```
class adg.pbmpt.ProjectedExceptionDiagram(graph, unique_id, tag, child_tag)
```

Bases: `adg.bmbpt.BmbptFeynmanDiagram`

Describes a PBMBPT diagram with its related properties.

**two\_or\_three\_body**

The 2 or 3-body characted of the vertices.

**Type** int

**time\_tag**

The tag number associated to the diagram's associated TSD.

**Type** int

**tsd\_is\_tree**

The tree or non-tree character of the associated TSD.

**Type** bool

**feynman\_exp**

The Feynman expression associated to the diagram.

**Type** str

**diag\_exp**

The Goldstone expression associated to the diagram.

**Type** str

**vert\_exp**  
The expression associated to the vertices.

**Type** list

**hf\_type**  
The Hartree-Fock, non-Hartree-Fock or Hartree-Fock for the energy operator only character of the graph.

**Type** str

**unique\_id**  
A unique number associated to the diagram.

**Type** int

**vertex\_exchange\_sym\_factor**  
Lazy-initialized symmetry factor associated to the vertex exchange, stored to avoid being computed several times.

**Type** int

**check\_graph**  
A copy of the graph that can be used for topological equivalence checks (lazy-initialized).

**Type** NetworkX MultiDiGraph

**anomalous\_contractions\_factor()**  
Return the factor associated with anomalous self-contractions.

**Returns** The anomalous self-contractions factor.

**Return type** (int)

**attribute\_expressions(time\_diag)**  
Attribute the correct Feynman and Goldstone expressions.

**Parameters** `time_diag` (TimeStructureDiagram) – The associated TSD.

**attribute\_qp\_labels()**  
Attribute the appropriate qp labels to the graph's propagators.

**check\_graph**  
Return a graph that can be used for topological equivalence checks.

Lazy-initialized to reduce memory and CPU costs as this operation requires a deep copy.

**Returns** The graph with doubled anomalous props.

**Return type** (NetworkX MultiDiGraph)

**degrees**

**diag\_exp**

**equivalent\_permutations()**  
Return the permutations generating equivalent diagrams.

**Returns** Vertices permutations as dictionnaires.

**Return type** (list)

**extract\_integral()**  
Return the integral part of the Feynman expression of the diag.

**Returns** The integral part of its Feynman expression.

**Return type** (str)

**extract\_numerator()**  
Return the numerator associated to a PBMBPT graph.

**Returns** The numerator of the graph.

**Return type** (str)

**feynman\_exp**

**graph**

**has\_anom\_non\_selfcontracted\_props()**  
Return True if the diagram has anomalous propagators.

**Returns** The presence of anomalous propagators.

**Return type** (bool)

**has\_anom\_props\_linked\_sign()**  
Return True if there is a minus sign associated to anom props.

Anomalous propagators departing to higher vertices introduce a sign factor if a normal propagator is going to an even higher vertex, as it departs from the canonical representation used for numerator extraction.

**Returns** The presence of the sign factor.

**Return type** (bool)

**has\_crossing\_sign()**  
Return True for a minus sign associated with crossing propagators.

Use the fact that all lines propagate upwards and the canonical representation of the diagrams and vertices.

**Returns**

**Encode for the sign factor associated with crossing** propagators.

**Return type** (bool)

**has\_sign\_factor()**  
Return True if a sign factor is associated to the diagram.

Wrapper allowing for easy refactoring of expression code.

**Returns** The presence of a sign factor.

**Return type** (boolean)

**hf\_type**

**io\_degrees**

**max\_degree**

**multiplicity\_symmetry\_factor()**  
Return the symmetry factor associated with propagators multiplicity.

**Returns** The symmetry factor associated with equivalent lines.

**Return type** (str)

**set\_io\_degrees()**  
Attribute the correct in- and out-degrees to a PBMBPT diagram.

**symmetry\_factor()**  
Return the overall symmetry factor of the diagram.

**Returns** The combination of all symmetry factors.

**Return type** (str)

**tags**

**time\_tag**

**time\_tree\_denominator**(*time\_graph*)

Return the denominator for a time-tree graph.

**Parameters** **time\_graph** (*NetworkX MultiDiGraph*) – Its associated time-structure graph.

**Returns** The denominator of the graph.

**Return type** (str)

**tsd\_is\_tree****two\_or\_three\_body****unique\_id****unsort\_degrees****unsort\_io\_degrees****vert\_exp****vertex\_exchange\_sym\_factor**

Return the symmetry factor associated with vertex exchange.

**Returns** The symmetry factor for vertex exchange.

**Return type** (int)

**vertex\_expression**(*vertex*)

Return the expression associated to a given vertex.

**Parameters** **vertex** (*int*) – The vertex of interest in the graph.

**Returns** The LaTeX expression associated to the vertex.

**Return type** (str)

**write\_diag\_exps**(*latex\_file*, *norder*)

Write the expressions associated to a diagram in the LaTeX file.

**Parameters**

- **latex\_file** (*file*) – The LaTeX outputfile of the program.
- **norder** (*int*) – The order in BMBPT formalism.

**write\_graph**(*latex\_file*, *directory*, *write\_time*)

Write the PBMBPT graph and its associated TSD to the LaTeX file.

**Parameters**

- **latex\_file** (*file*) – The LaTeX output file of the program.
- **directory** (*str*) – The path to the result folder.
- **write\_time** (*bool*) – True if we want informations on the associated TSDs.

**write\_section**(*result*, *commands*, *section\_flags*)

Write section and subsections for BMBPT result file.

**Parameters**

- **result** (*file*) – The LaTeX output file of the program.
- **commands** (*dict*) – The flags associated with run management.
- **section\_flags** (*dict*) – UniqueIDs of diags starting each section.

**write\_tsd\_info**(*diagrams\_time*, *latex\_file*)

Write info related to the BMBPT associated TSD to the LaTeX file.

**Parameters**

- **diagrams\_time** (*list*) – The associated TSDs.

- **latex\_file** (*file*) – The LaTeX output file of the program.

**write\_vertices\_values** (*latex\_file, mapping*)

Write the qp energies associated to each vertex of the diag.

#### Parameters

- **latex\_file** (*file*) – The LaTeX output file of the program.
- **mapping** (*dict*) – A mapping between the vertices in the diagram and the vertices in its equivalent TSD, since permutations between vertices are possible.

adg.pbmbpt.**equiv\_generating\_permutations** (*graph*)

Return the list of permutations generating equivalent PBMBPT diags.

adg.pbmbpt.**graph**

The graph to be checked.

**Type** Networkx MultiDiGraph

**Returns** The mappings giving equivalent graphs, inc. identity.

**Return type** (list)

adg.pbmbpt.**filter\_new\_diagrams** (*new\_diags, old\_diags*)

Eliminate diagrams having a topologically equivalent diag.

**Attributes:** new\_diags (list): The list of newly created PBMBPT diagrams. old\_diags (list): The list of already checked PBMBPT diagrams.

adg.pbmbpt.**generate\_anomalous\_diags** (*diag, nbody\_max*)

Generate PBMBPT graphs with anomalous lines, with some redundancy.

#### Parameters

- **diag** ([BmbptFeynmanDiagram](#)) – The diagram to generate children from.
- **nbody\_max** (*int*) – The maximal n-body character of a graph vertex.

**Returns** The anomalous graphs generated.

**Return type** (list)

adg.pbmbpt.**generate\_combinations** (*iter\_list*)

Generate all possible combinations of length 1 to total.

adg.pbmbpt.**iter\_list**

A list of iterable objects.

**Type** list

**Returns** A list with all the possible combinations of all lengths.

**Return type** (list)

```
>>> print(generate_combinations([1, 2, 3]))
[(1,), (1, 2), (1, 2, 3), (1, 3), (2,), (2, 3), (3,)]
```

adg.pbmbpt.**unique\_edge\_combinations** (*edges, permutations*)

Return all edge combinations not producing equivalent anomalous graphs.

adg.pbmbpt.**edges**

The edges that can be modified.

**Type** list

adg.pbmbpt.**permutations**

The permutation generating equivalent diagrams.

**Type** list

**Returns** The list of edges producing unique anomalous diagrams.

**Return type** (list)

```
>>> edges = [(1, 3), (2, 3)]
>>> permutations = [{1: 1, 2: 2}, {1: 2, 2: 1}]
>>> print(unique_edge_combinations(edges, permutations))
[((1, 3), (2, 3)), ((2, 3),)]
```

`adg.pbmbpt.unique_vertex_combinations(vertices, permutations)`

Return vertex combinations generating unique anomalous diagrams.

Return combinations of vertices on which self-contractions can be added without producing topologically equivalent PBMBPT diagrams.

`adg.pbmbpt.vertices`

Vertices that can be self-contracted.

**Type** list

`adg.pbmbpt.permutations`

The permutations that generate equivalent diags.

**Type** list

**Returns** Vertex combinations that do not produce equivalent diags.

**Return type** (list)

```
>>> vertices = [1, 3]
>>> permutations = [{1: 1, 3: 3}, {1: 3, 3: 1}]
>>> print(unique_vertex_combinations(vertices, permutations))
[(1, 3), (3,)]
```

## 4.7 Time-Structure Diagram

Module with functions relative to time-structure diagrams, called by ADG.

`class adg.tsd.TimeStructureDiagram(bmbpt_diag)`

Bases: `adg.diag.Diagram`

Describes a time-structure diagram with its related properties.

**perms**

The permutations on the vertices for all the BMBPT diagrams associated to this TSD.

**Type** dict

**equivalent\_trees**

The tag numbers of the equivalent tree TSDs associated to a non-tree TSD.

**Type** list

**is\_tree**

The tree or non-tree character of a TSD.

**Type** bool

**expr**

The Goldstone denominator associated to the TSD.

**Type** str

---

```

resum
The resummation power of a tree TSD.

Type int

degrees

draw_equivalent_tree_tsds (latex_file)
Draw the equivalent tree TSDs for a given non-tree TSD.

Parameters latex_file (file) – The output LaTeX file of the program.

equivalent_trees

expr

get_feynman_diags (feyn_diagrams)
Return the list of Feynman diagrams associated to the TSD.

Parameters feyn_diagrams (list) – All produced BmbptFeynmanDiagrams.

Returns All the identifiers of associated BmbptFeynmanDiagrams.

Return type (str)

graph

io_degrees

is_tree

max_degree

perms

resum

resummation_power ()
Calculate the resummation power of the tree TSD.

Returns The resummation power associated to the TSD.abs

Return type (int)

tags

treat_cycles ()
Find and treat cycles in a TSD diagram.

Returns The unique tree TSDs associated to a non-tree TSD.

Return type (list)

unsort_degrees

unsort_io_degrees

write_graph (latex_file, directory, write_time)
Write the graph of the diagram to the LaTeX file.

Parameters

- latex_file (file) – The LaTeX ouput file of the program.
- directory (str) – Path to the result folder.
- write_time (bool) – (Here to emulate polymorphism).

adg.tsd.disentangle_cycle (time_graph, cycle_nodes)
Separate a cycle in a sum of tree diagrams.

Parameters

- time_graph (NetworkXn MultiDiGraph) – A time-structure diagram.

```

- **cycle\_nodes** (*tuple*) – Integers encoding the positions of the end nodes of the cycle.

**Returns** New graphs produced from treating the cycles in the TSD.

**Return type** (list)

`adg.tsd.equivalent_labelled_tsds (equivalent_trees, labelled_tsds)`

Return the list of labelled TSDs corresponding to equivalent TSDs.

**Parameters**

- **equivalent\_trees** (*list*) – The equivalent tree TSDs of a non-tree TSD.
- **labelled\_tsds** (*list*) – The labelled TSDs obtained from BMBPT diagrams.

**Returns** The list of tag numbers of the equivalent TSDs.

**Return type** (str)

`adg.tsd.find_cycle (graph)`

Return start and end nodes for an elementary cycle.

**Parameters** **graph** (*NetworkX MultiDiGraph*) – A TSD with cycle(s) to be treated.

**Returns** Positions of the two end nodes of a cycle in the graph.

**Return type** (tuple)

`adg.tsd.time_structure_graph (diag)`

Return the time-structure graph associated to the graph.

**Parameters** **diag** (*BmbptFeynmanDiagram*) – The BMBPT graph of interest.

**Returns** The time-structure diagram.

**Return type** (NetworkX MultiDiGraph)

`adg.tsd.treat_tsds (diagrams_time)`

Order TSDs, produce their expressions, return also number of trees.

**Parameters** **diagrams\_time** (*list*) – All the associated TSDs.

**Returns** List of TSDs, number of tree TSDs

**Return type** (tuple)

`adg.tsd.tree_time_structure_den (time_graph)`

Return the denominator associated to a tree time-structure graph.

**Parameters** **time\_graph** (*NetworkX MultiDiGraph*) – The TSD of interest.

**Returns** The denominator associated to the TSD.

**Return type** (str)

`adg.tsd.write_section (latex_file, directory, pdiag, time_diagrams, nb_tree_tsds, diagrams)`

Write the appropriate section for tsd diagrams in the LaTeX file.

**Parameters**

- **latex\_file** (*file*) – The LaTeX output file of the program.
- **directory** (*str*) – Path to the output folder.
- **pdiag** (*bool*) – True if diagrams are to be drawn.
- **time\_diagrams** (*list*) – The ensemble of TSDs.
- **nb\_tree\_tsds** (*int*) – Number of tree TSDs.
- **diagrams** (*list*) – All produced BmbptFeynmanDiagrams.

## 4.8 BIMSRG Diagram

Routines and class for Bogoliubov IMSRG diagrams.

```
class adg.bimsrg.BimsrgDiagram(nx_graph, tag_num)
Bases: adg.diag.Diagram
```

Describes a B-IMSRG Feynman diagram with its related properties.

**adjacency\_mat**

The adjacency matrix of the diagram.

**Type** Numpy array

**unique\_id**

A unique number associated to the diagram.

**Type** int

**expr**

The B-IMSRG expression associated to the diagram.

**Type** str

**ext\_io\_degree**

The degree of the operator component the diagram corresponds to.

**Type** tuple

**is\_AB**

True if the diagram contributes to +AB, false if to -BA.

**Type** bool

**adjacency\_mat**

**attribute\_expression()**

Returns the LaTeX expression of the diagram.

The expression is extracted in a way that assumes the canonical representation of the vertices as well as a labeling of the external lines that would correspond to a canonical representation of the C operator vertex. As such, there is no sign factor associated to departing from the canonical representation of the diagram. This additionally prevents any line crossing from appearing.

**Returns** The LaTeX expression for the diagram.

**Return type** (str)

**degrees**

**expr**

**ext\_io\_degree**

**graph**

**io\_degrees**

**is\_AB**

**max\_degree**

**permulator()**

Return the permulator associated to the diagram.

The labelling of the external lines correspond to the canonical representation of the C operator vertex.

**Returns** The permulator associated to the diagram in LaTeX format.

**Return type** (str)

**sign()**

Return the sign of the diagram.

As the diagrams are made with vertices in canonical representation and avoiding crossings, the only sign left is associated with the commutator.

**Returns** The sign of the diagram.

**Return type** (str)

**symmetry\_factor()**

Returns the symmetry factor of the diagram in LaTeX format.

**Returns** The LaTeX-formatted symmetry factor.

**Return type** (str)

**tags****unique\_id****unsort\_degrees****unsort\_io\_degrees****vertices\_expression()**

Return the expression associated to the vertices in LaTeX format.

The expressions are extracted in a way that assumes the canonical representation of the vertices as well as a labeling of the external lines that would correspond to a canonical representation of the C operator vertex. This prevents any crossing as well as additional sign tied to departing from the canonical representation.

**Returns** The LaTeX-formatted expression for the vertices.

**Return type** (str)

**write\_graph(latex\_file, directory, write\_time)**

Write the graph of the diagram to the LaTeX file.

**Parameters**

- **latex\_file** (file) – The LaTeX ouput file of the program.
- **directory** (str) – Path to the result folder.
- **write\_time** (bool) – (Here to emulate polymorphism).

**write\_section(result, commands, section\_flags)**

Write section and subsections for BMBPT result file.

**Parameters**

- **result** (file) – The LaTeX output file of the program.
- **commands** (dict) – The flags associated with run management.
- **section\_flags** (dict) – UniqueIDs of diags starting each section.

**adg.bimsrg.diagrams\_generation(orders)**

Generate diagrams for B-IMSRG.

**Parameters** **orders** (tuple) – The B-IMSRG (N\_A, N\_B, N\_C) order of the diagrams.

**Returns**

**NumPy arrays encoding the adjacency matrices of the graphs**, and number of diagrams with the A vertex on top.

**Return type** (tuple)

**adg.bimsrg.diagrams\_subset(deg\_max\_top, deg\_max\_bot, deg\_max\_ext)**

Generate diagrams for B-IMSRG.

**Parameters** `orders` (*tuple*) – The max ranks ( $2*N_A, 2*N_B, 2*N_C$ ) of the vertices.

**Returns** NumPy arrays encoding the adjacency matrices of the graphs.

**Return type** (*list*)

```
>>> diagrams_subset(2, 2, 0) # doctest: +NORMALIZE_WHITESPACE
[array([[0, 0, 0, 0],
       [0, 0, 2, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0]])]
>>> len(diagrams_subset(2, 2, 2))
5
>>> len(diagrams_subset(4, 4, 4))
41
>>> len(diagrams_subset(0, 0, 0))
0
```

`adg.bimsrg.order_diagrams(diagrams, order)`

Order the BIMSRG diagrams and return the number of diags for each type.

**Parameters**

- `diagrams` (*list*) – The unordered BimsrgDiagrams.
- `order` (*int*) – The order of the B-IMSRG truncation.

**Returns** First element are the ordered BimsrgDiagrams. Second element is the number of diagrams for each type. Third element is flags for the output processing.

**Return type** (*tuple*)

`adg.bimsrg.permutator(set_1, set_2)`

Write the definition of the permutation operator given by the two sets.

**Parameters**

- `set_1` (*list*) – The list of the left-hand-side qp labels.
- `set_2` (*list*) – The list of the right-hand-side qp labels.

**Returns** The LaTeX expression for the permutation operator.

**Return type** (*str*)

```
>>> print(permutator([1, 2], [3])) # doctest: +NORMALIZE_WHITESPACE
P(k_{1}k_{2}/k_{3}) \&= 1 - P_{k_{1}} k_{3} - P_{k_{2}} k_{3} \\
```

`adg.bimsrg.two_partitions(number)`

Return 2-partitions of the given integer.

**Parameters** `numbr` (*int*) – The integer to partition.

**Returns** All the 2-partitions as tuples.

**Return type** (*list*)

```
>>> two_partitions(3)
[(0, 3), (1, 2), (2, 1), (3, 0)]
```

```
>>> two_partitions(0)
[(0, 0)]
```

```
>>> two_partitions(-1)
[]
```

`adg.bimsrg.write_header(tex_file, commands, diags_nbs)`

Write overall header for BIMSRG result file.

**Parameters**

- **tex\_file** (*file*) – The output LaTeX file of the program.
- **commands** (*Namespace*) – Flags for the program run.
- **diags\_nbs** (*dict*) – The number of diagrams per type.

```
adg.bimsrg.write_permutator_section(tex_file, commands)
```

Write the section defining permutation operators.

**Parameters**

- **tex\_file** (*file*) – The output LaTeX file of the program.
- **commands** (*Namespace*) – Flags for the program run.

## 4.9 Tools and utilities

Miscellaneous diagram-unrelated tools for ADG.

```
class adg.tools.UniqueID
```

Bases: object

Counter making sure of generating a unique ID number for diagrams.

**current**

The unique identifier to be attributed to a diagram.

**Type** int

**current**

**get()**

Iterate on counter value and return current value.

**Returns** A unique identifier for the diagram.

**Return type** (int)

```
adg.tools.reversed_enumerate(data)
```

Return the index and item of the data in reversed order.

**Parameters** **data** (*iterable data structure*) – The data to be used..

**Returns** Index and item.

**Return type** (tuple)

```
>>> list(reversed_enumerate(['A', 'B', 'C']))
[(2, 'C'), (1, 'B'), (0, 'A')]
```

# CHAPTER 5

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## Developers Team

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They have been involved in the making of ADG over the past years:

- Pierre Arthuis - TU Darmstadt & ExtreMe Matter Institute EMMI, GSI, Darmstadt (previously University of Surrey & Irfu, CEA, Université Paris-Saclay & CEA, DAM, DIF)
- Thomas Duguet - Irfu, CEA, Université Paris-Saclay & KU Leuven, IKS
- Jean-Paul Ebran - CEA, DAM, DIF
- Heiko Hergert - NSCL/FRIB Laboratory & Department of Physics and Astronomy, Michigan State University
- Raphaël-David Lasseri - ESNT, Irfu, CEA, Université Paris-Saclay (previously IPN, CNRS/IN2P3, Université Paris-Sud, Université Paris-Saclay)
- Julien Ripoche - CEA, DAM, DIF
- Alexander Tichai - MPI fuer Kernphysik, Heidelberg & TU Darmstadt & ExtreMe Matter Institute EMMI, GSI, Darmstadt (previously ESNT, Irfu, CEA, Université Paris-Saclay)



# CHAPTER 6

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## Citing

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If you use ADG in your research work, we kindly ask you to cite the following papers:

- P. Arthuis, T. Duguet, A. Tichai, R.-D. Lasseri and J.-P. Ebran, Comput. Phys. Commun. **240**, 202-227 (2019). It is available under the following [DOI](#).
- P. Arthuis, A. Tichai, J. Ripoche and T. Duguet, Comput. Phys. Commun. **261**, 107677 (2021). It is available [here](#).
- A. Tichai, P. Arthuis, H. Hergert and T. Duguet, Eur. Phys. J. A **58**, 2 (2022). It is available under this [URL](#).



# CHAPTER 7

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## License

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Pierre Arthuis  
Thomas Duguet  
Jean-Paul Ebran  
Heiko Hergert  
Raphaël-David Lasseri  
Julien Ripoche  
Alexander Tichai



# CHAPTER 8

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## Python Module Index

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