ADG - Automated Diagram Generator Documentation

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CHAPTER 1

The ADG Project

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 by ADG id needed. Other computer-readable files may be produced as well.

1.2 Status

As for now, the code is capable of handling three different formalisms, i.e. Many-Body Perturbation Theory (MBPT), Bogoliubov Many-Body Perturbation Theory (BMBPT). and Projected Bogoliubov Many-Body Perturbation Theory (PBMBPT).

- 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.

1.3 Future developments

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

CHAPTER 2

Install ADG on your computer

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 >= 2.7.1 and the following Python libraries:

- networkx >= 2.0
- numpy
- scipy
- future

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

Generate diagrams with ADG

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]
-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`.

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'
```

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*, *pdiag*)
Compile the program's LaTeX ouput file.

Parameters

- **directory** (*str*) – Path to the ouput folder.
- **pdiag** (*bool*) – `True` if one wants to draw the diagrams.

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.**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()`
Return run commands from the Command Line Interface.

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

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,
↪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)`
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.

`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,␣
↪3], [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`*) – Fistance 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 ouput 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 subgaph 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 tha appropriate header for the LaTeX file for MBPT diagrams.

Parameters

- **tex_file** (*file*) – The LaTeX ouput 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 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

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 dictionnaries.

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 euivalent 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)

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 obervable 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)
```

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```
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.pbmbpt.**ProjectedBmbptDiagram**(*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 dictionnaries.

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 euivalent 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.

Attibutes: 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-stucture 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 BmbptFeymmanDiagrams.

Returns All the identifiers of associated BmbptFeymmanDiagrams.

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** (*BmbptFeymmanDiagram*) – 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 BmbptFeymmanDiagrams.

4.8 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 attributedto 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

Developers Team

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

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CHAPTER 6

Citing

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

CHAPTER 7

License

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```
Copyright (C) 2018-2020 ADG Dev Team
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```

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