PYQCTools Documentation

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PYQCTools is a collection of python scripts useful to dump quantum chemistry integrals and to perform data post-processing for different quantum chemistry methods.

PYQCTools requires the following prerequisites to work:

- Python 2.6, 2.7, 3.2, 3.3, 3.4
- Numpy 1.6.2 or higher
- Scipy 0.10 or higher (0.12.0 or higher for python 3.3, 3.4)
- PySCF for Integrals Calculation in Integrals Dumpings scripts.

CHAPTER

ONE

CONTENTS

1.1 Tools for Omega Space Green's Functions

`gf_trace.py`: Calculate the Density of States (DOS) value from an ω-dependent Green's Function. It makes the trace of the Green's Function associated with a certain frequency value.

Example :

```
>>> python gf_trace.py /PATH/green.txt omega_value
```

`green.txt`: formatted text file containing the Green's function.

`omega_value`: double frequency value.

1.2 Tools for Real-Time Green's Functions

`rtgf.py`: Calculate the Density of States (DOS) values during a time propagation. It makes the trace of time-dependent Green's Functions calculated along a time propagation and return the DOS values as a function of time both for the real and for the imaginary part of the Green's Function.

Example :

```
>>> python rtgf.py prop_time time_step /PATH/scratch
```

`prop_time`: double value of the full propagation time (period).

`time_step`: double value of the time-step.

`scratch`: directory containing text files of the real (green.$t.$t.txt) and imaginary (green.30000+$t.30000+$t.txt) Green's Functions, where $t indicate the specific time-step.

The script save two output files, `rt_real.txt` and `rt_imag.txt`, containing the real and imaginary part of the time-dependent DOS respectively.

1.3 Tools for Integrals Dumping

You can also download the PDF version of this manual.