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:

```
from PYQCTools.Omega_GF import gf_trace

gf_trace.run(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:

```
from PYQCTools.RT_GF import rtgf

rtgf.run(prop_time, time_step, 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.

`fft.py`: Perform the fourier transform of the time-dependent Density of States (DOS). It reads the `rt_real.txt` and `rt_imag.txt` generated by the `rtgf.py` script and produces the `ldos.out` and `real_part.txt` files containing the imaginary and real parts of the *omega*-dependent DOS respectively.

Example:

```
from PYQCTools.RT_GF import fft

fft.run(broad, rem_add)
```

broad: double value of the imaginary broadening, rem_add: string specifying if we are working with the addition or removal part of the Green's Function. It can assume only the values 'add' or 'rem'.

extrapolation.py: Perform linear prediction to extend the total propagation time of a time propagation.

It reads N points of time-dependent DOS inside the files rt_real.txt and rt_imag.txt and use the last N/2 data to predict the following N points.

Example:

```
from PYQCTools.RT_GF import extrapolation

extrapolation.run(full_range)
```

full_range: boolean variable. If it is true is return the full range of calculated and predicted values, if it is false it returns only the predicted values.

The script produces new_full_data.out files if full_range = true otherwise it produces predicted.out output files.

iter_extrapolation.py: Perform an interative linear prediction to extend the total propagation time of a time propagatio

It reads 4 points of the time-dependent DOS inside the files rt_real.txt and rt_imag.txt and use the last 2 of them to predict the following N points.

Example:

```
from PYQCTools.RT_GF import iter_extrapolation

iter_extrapolation.run(N)
```

N: integer variable specifying the total number of points that need to be predicted.

The script produces new_full_real.out and new_full_imag.out output files with the real and imaginary parts of the exteded time-dependent DOS respectively.

1.3 Tools for Integrals Dumping

Integrals_dump.py: It dumps 1 and 2-elctron integrals in the MO basis inside a CASCI space in FCIDUMP format.
The PySCF input to calculate integrals is already included in the script.

DipoleIntegrals_dump.py: It dumps dipole integrals in the MO basis in a CASCI space in FCIDUMP format.
The PySCF input to calculate integrals is already included in the script.

LowdinOrtho_Integrals.py: It dumps 1 and 2-electron integrals in the Localized basis obtained by Lowdin Orthogonaliz
The PySCF input to calculate integrals is already included in the script.

hubbard_1d: It dumps 1 and 2-electron integrals got the 1D Hubbard model.

Example:

```
from PYQCTools.Integrals_dump import hubbard_1d

hubbard_1d.run(nsites, t, U, output)
```

nsites: Number of sites, t: Hopping constant, U: Coupling constant, output: Output file name.

You can also download the PDF version of this manual.