VQEDriver Documentation

v0.0.0

Python3 driver for the Variational Quantum Eigensolver (VQE) algorithm implemented in IBM's Qiskit for the calculation of the ground-state energy of a molecule. The driver reads a structured input file (commonly named `[molecule].inp`) and runs a complete VQE calculation using IBM's Qiskit and PySCF libraries.

Usage of the program from terminal:

```
$ vqedriver [INPUTFILE]
```

1. Input File

The input file follows a line by line structure, using keywords for each block and their options. In general, keywords are added in the format:

```
%keyword option_keyword1=option option_keyword2=option [...]
```

The input file accepts blank lines and comments beginning with the `#` character. The keywords can be added in any order.

1.1. Geometry

Added using the `%geometry` keyword. Currently, the geometry of the molecule has to be specified using an external XYZ file using the `xyzfile` option keyword.

Optional keywords:

- `charge` (int) – charge of the molecule.
  Default: `charge=0`
- `spin` (int) – $2S$, where S is the total spin angular momentum. Same as the number of unpaired electrons in the molecule.
  Default: `spin=0`

- `units` (str) – length units of the coordinate file.

  Available options: `angstrom`, `bohr`

  Default: `units=angstrom`

Example:

```
%geometry xyzfile=h2.xyz charge=1 spin=1 units=bohr
```

1.2. Basis set

Contains the basis set information for the molecule, added using the keyword `%basis`. Currently, only a single basis set can be added for all the atoms in the molecule using the option keyword `all=[BASIS SET]`.

Example:

```
%basis all=def2-TZVP
```

1.3. Self-Consistent Field (SCF)

Specifies the options for the SCF calculations, added by the `%scf` keyword. By default, the program sets a Restricted Hartree-Fock (RHF) calculation for closed-shell molecules and a Restricted-Open Hartree-Fock (ROHF) for open-shell molecule. Unrestricted Hartree-Fock (UHF) method is also available for open- and close-shell molecules.

Optional keywords:

- `method` (str) – Hartree-Fock method for SCF calculations.

  Available options: `rhf`, `rohf`, `uhf`

  Default: `method=rhf` if `spin==0` (closed-shell), `method=rohf` if `spin!=0` (open-shell)

- `conv` (int) – convergence criteria for the SCF calculations to $10^{-\text{conv}}$ Hartree.

  Default: `conv=9`

- `maxcycles` (int) – maximum number of SCF cycles.

  Default: `maxcycles=50`

- `maxcore` (int) – maximum memory in MB that PySCF should use.

  Default: `maxcore=1000`

Example:

```
%scf method=uhf conv=6 maxcycles=100 maxcore=7500
```

1.4. VQE Settings

Contains general settings for the VQE run, added by the `%vqesets` keyword.

Optional keywords:

- `mapping` (str) – mapping to convert the fermionic operator to a qubit operator.

  Available options: `jordan_wigner`, `parity`, `bravyi_kitaev`, `bksf` (which corresponds to the Braviy-Kitaev Super Fast mapping)

  Default: `mapping=jordan_wigner`

- `threshold` (int) – threshold for Pauli simplification, eliminate the real and imaginary parts of the weight in each Pauli Operator mapped by $10^{-\text{threshold}}$. If a weight is less than $10^{-\text{threshold}}$, the Pauli is removed from the `WeightedPauliOperator` object.

  Default: `threshold=8`

- `z2red` (bool) – whether or not to use Z2 symmetries to taper two qubits from the Qubit Operator.

  Default: `z2red=false`

Example:

```
%vqesets mapping=bksf threshold=9
```