GHF

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RESTRICTED HARTREE FOCK, BY MEANS OF SCF PROCEDURE

This function calculates the RHF energy of a given molecule and the number of occupied orbitals. The molecule has to be created in pySCF: molecule = gto.M(atom = geometry, spin = diff. in alpha and beta electrons, basis = basis set) number of occupied orbitals: number of doubly occupied orbitals (1 for H_2, 2 for H_4,...) The function prints the number of iterations and the converged SCF energy, while also returning the energy value for eventual subsequent calculations

class `ghf.RHF`.**RHF** (*molecule*, *number_of_electrons*)

Input is a molecule and the number of occupied orbitals.

Molecules are made in pySCF and calculations are performed as follows, eg.: The following snippet prints and returns RHF energy of h_2 and the number of iterations needed to get this value.

```
>>> h_2 = gto.M(atom = 'h 0 0 0; h 0 0 1', spin = 0, basis = 'cc-pvdz')
>>> x = RHF(h_2, 2)
>>> x.get_scf_solution()
Number of iterations: 109
Converged SCF energy in Hartree: -1.9403598392831243 (RHF)
```

get_last_dens ()

Prints the last density matrix of the converged solution.

> **Returns** The last density matrix.

get_last_fock ()

Prints the last fock matrix of the converged solution.

> **Returns** The last Fock matrix.

get_mo_coeff ()

Prints the mo coefficients of the converged solution.

> **Returns** The mo coefficients

get_one_e ()

> **Returns** The one electron integral matrix: T + V

get_ovlp ()

> **Returns** The overlap matrix

get_scf_solution ()

Prints the number of iterations and the converged scf energy.

> **Returns** The converged scf energy.

get_two_e ()

> **Returns** The electron repulsion interaction tensor

nuc_rep()

> **Returns** The nuclear repulsion value

scf()

Performs a self consistent field calculation to find the lowest RHF energy.

> **Returns** number of iterations, scf energy, mo coefficients, last density matrix, last fock matrix

UNRESTRICTED HARTREE FOCK, BY MEANS OF SCF PROCEDURE

This function calculates the UHF energy for a given molecule and the number of occupied alpha and beta orbitals. The molecule has to be created in pySCF: molecule = gto.M(atom = geometry, spin = diff. in alpha and beta electrons, basis = basis set)

number of occupied orbitals: first the number of occupied alpha orbitals second the number of occupied beta orbitals

There are two extra options added into the function:

- extra_e_coeff: when true, the program will add two extra alpha electrons to the system and calculate when the new system's energy converges. From the last density matrix in this calculation, new coefficients for the alpha and beta orbitals will be calculated and used as new guess density for the original system.

- internal_stability_analysis: when true, an internal stability analysis will be performed. When the wave finction is deemed unstable, new coefficients will be calculated that are closer in value to the stable condition, which is done by varying the Hessian by means of a trial vector. These will then be used as a guess density for the energy calculation.

The function prints the number of iterations and the converged SCF energy, while also returning the energy value for eventual subsequent calculations

ghf.UHF.**UHF** (*molecule*, *occ_a*, *occ_b*, *extra_e_coeff=False*, *internal_stability_analysis=False*)

```
>>> h3 = gto.M(atom = 'h 0 0 0; h 0 0.86602540378 0.5; h 0 0 1', spin = 1, basis
↪= 'cc-pvdz')
>>> UHF(h3, 2, 1)
```

```
>>> h3 = gto.M(atom = 'h 0 0 0; h 0 0.86602540378 0.5; h 0 0 1', spin = 1, basis
↪= 'cc-pvdz')
>>> UHF(h3, 2, 1, extra_e_coeff=True)
```

```
>>> h3 = gto.M(atom = 'h 0 0 0; h 0 0.86602540378 0.5; h 0 0 1', spin = 1, basis
↪= 'cc-pvdz')
>>> UHF(h3, 2, 1, internal_stability_analysis=True)
```

prints and returns UHF energy of h3

REAL GENERALISED HARTREE FOCK, BY MEANS OF SCF PROCEDURE

This function calculates the real GHF energy for a given molecule and the number of electrons in the system. The molecule has to be created in pySCF: molecule = gto.M(atom = geometry, spin = diff. in alpha and beta electrons, basis = basis set)

The function can do this in two ways.

- Create the general density matrix and work with this as a whole

- create the density matrix in spin-blocked notation

`ghf.real_GHF.`**`real_GHF`** (*molecule*, *number_of_electrons*)

Input is a molecule and the number of electrons.

Molecules are made in pySCF, eg.:

```
>>> h_2 = gto.M(atom = 'h 0 0 0; h 0 0 1', spin = 0, basis = 'cc-pvdz')
>>> GHF(h_2, 2)
```

prints and returns GHF energy of h_2

USEFUL FUNCTIONS FOR SCF PROCEDURE

A number of functions used throughout the UHF and RHF calculations are summarised here.

`ghf.SCF_functions.`**`density_matrix`**(*f_matrix*, *occ*, *trans*)

- density() creates a density matrix from a fock matrix and the number of occupied orbitals.

- Input is a fock matrix, the number of occupied orbitals, which can be separate for alpha and beta in case of UHF. And

a transformation matrix X.

`ghf.SCF_functions.`**`get_integrals`**(*molecule*)
A function to calculate your integrals & nuclear repulsion with pyscf.

`ghf.SCF_functions.`**`spin`**(*occ_a*, *occ_b*, *coeff_a*, *coeff_b*, *overlap*)

> **Parameters**
>
> - **`occ_a`** – number of occupied alpha orbitals
>
> - **`occ_b`** – number of occupied beta orbitals
>
> - **`coeff_a`** – MO coefficients of alpha orbitals
>
> - **`coeff_b`** – MO coefficients of beta orbitals
>
> - **`overlap`** – overlap matrix of the molecule
>
> **Returns** S^2, S_z and spin multiplicity

`ghf.SCF_functions.`**`trans_matrix`**(*overlap*)

- Define a transformation matrix X, used to orthogonalize different matrices throughout the calculation.

- Input should be an overlap matrix.

`ghf.SCF_functions.`**`uhf_fock_matrix`**(*density_matrix_1*, *density_matrix_2*, *one_electron*, *two_electron*)

- calculate a fock matrix from a given alpha and beta density matrix

- fock alpha if 1 = alpha and 2 = beta and vice versa

- input is the density matrix for alpha and beta, a one electron matrix and a two electron tensor.

`ghf.SCF_functions.`**`uhf_scf_energy`**(*density_matrix_a*, *density_matrix_b*, *fock_a*, *fock_b*, *one_electron*)

- calculate the scf energy value from a given density matrix and a given fock matrix for both alpha and beta, so 4 matrices in total

- then calculate the initial electronic energy and put it into an array

- input is the density matrices for alpha and beta, the fock matrices for alpha and beta and lastly a one electron matrix

TESTING THE RHF AND UHF METHODS

Simple tests to check whether or not the functions return the correct value.

ghf.tests.test_auth.**test_RHF**()
> test_RHF will test whether or not the RHF method returns the wanted result. The accuracy is 10^16.

ghf.tests.test_auth.**test_UHF**()
> test_UHF will test the regular UHF method, by checking whether or not it returns the expected result. The accuracy is 10^-6.

ghf.tests.test_auth.**test_extra_e**()
> test_extra_e will test the UHF method, with the added option of first adding 2 electrons to the system and using those coefficients for the actual system, by checking whether or not it returns the expected result. The accuracy is 10^-6.

ghf.tests.test_auth.**test_stability**()
> test_stability will test the UHF method, with stability analysis, by checking whether or not it returns the expected result. The accuracy is 10^-6.

PYTHON MODULE INDEX

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