Hartree-Fock and MP2 energy calculation

1.0

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Chapter 1

File Index

1.1 File List

Here is a list of all files with brief descriptions:

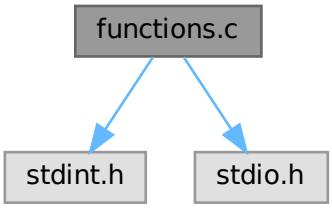
Chapter 2

File Documentation

2.1 functions.c File Reference

```
#include <stdint.h>
#include <stdio.h>
```

Include dependency graph for functions.c:



Functions

- double one_electron_energy (double *data, int32_t n_up, int32_t mo_num)

  Calculates the one-electron energy contribution to the Hartree-Fock energy.
- double two_electron_energy (int32_t *index, double *value, int32_t n_up, int64_t n_integrals)

  Calculates the two-electron energy contribution to the Hartree-Fock energy.
- double hartree_fock_energy (double nuc_repul, double one_el_energy, double two_el_energy)

  Calculates the total Hartree-Fock energy.
- double get_integral (int i, int j, int k, int l, const int32_t *index, const double *value, int64_t n_integrals)
- double MP2_energy_correction (int32_t *index, double *value, double *mo_energy, int32_t n_up, int32_t mo_num, int64_t n_integrals)
- double get_integral_2 (int i, int j, int k, int l, const int32_t *index, const double *value, int64_t n_integrals)

  Retrieves integral value.
- double MP2_alter (int32_t *index, double *value, double *mo_energy, int32_t n_up, int64_t n_integrals)

  MP2 energy correction calculation.

2.1.1 Function Documentation

2.1.1.1 get_integral()

```
double get_integral (
            int i,
            int j,
            int k,
            int l,
            const int32_t * index,
            const double * value,
            int64_t n_integrals )
```

2.1.1.2 get_integral_2()

```
double get_integral_2 (
            int i,
            int j,
            int k,
            int l,
            const int32_t * index,
            const double * value,
            int64_t n_integrals )
```

Retrieves integral value.

Parameters

i	First index
j	Second index
k	Third index
l	Fourth index
index	Array containing four-index combinations
value	Array containing integral values
n_integrals	Total number of integrals

Returns

Value of the requested integral or 0.0 if not found

2.1.1.3 hartree_fock_energy()

```
double hartree_fock_energy (
            double nuc_repul,
            double one_el_energy,
            double two_el_energy )
```

Calculates the total Hartree-Fock energy.

Parameters

nuc_repul	Nuclear repulsion energy
one_el_energy	One-electron energy contribution
two_el_energy	Two-electron energy contribution

Returns

Total Hartree-Fock energy

2.1.1.4 MP2_alter()

```
double MP2_alter (
            int32_t * index,
            double * value,
            double * mo_energy,
            int32_t n_up,
            int64_t n_integrals )
```

MP2 energy correction calculation.

Parameters

index	Array containing four-index combinations
value	Array containing integral values
mo_energy	Array of molecular orbital energies
n_up	Number of occupied orbitals
n_integrals	Total number of integrals

Returns

MP2 energy correction

< Variable used by MP2_alter() to store the alternative MP2 energy

< Variable used by MP2_alter() to store the integral with indices ijab

< Variable used by MP2_alter() to store the integral with indices ijba

< Variable used by MP2_alter() to store the denominator

< Variable used by MP2_alter to account for permutational symmetry op the integrals

Iterate over the stored integrals

< Variable used by MP2_alter() for storing index i

< Variable used by MP2_alter() for storing index j

< Varibale used by MP2_alter() for storing index a

< Variable used by MP2_alter() for storing index b

2.1.1.5 MP2_energy_correction()

```
double MP2_energy_correction (
            int32_t * index,
            double * value,
            double * mo_energy,
            int32_t n_up,
            int32_t mo_num,
            int64_t n_integrals )
```

< Variable used by MP2_energy_correction() while calculating the MP2 energy

< Variable used by MP2_energy_correction() for storing the integral ijab

< Variable used by MP2_energy_correction() for stpring the integral ijba

2.1.1.6 one_electron_energy()

```
double one_electron_energy (
            double * data,
            int32_t n_up,
            int32_t mo_num )
```

Calculates the one-electron energy contribution to the Hartree-Fock energy.

Parameters

data	Array containing one-electron integrals
n_up	Number of occupied orbitals
mo_num	Total number of molecular orbitals

Returns

One-electron energy contribution

< Variable used by one_electron_energy() while calculating the one-electron energy

2.1.1.7 two_electron_energy()

```
double two_electron_energy (
            int32_t * index,
            double * value,
            int32_t n_up,
            int64_t n_integrals )
```

Calculates the two-electron energy contribution to the Hartree-Fock energy.

Parameters

index	Array containing four-index combinations for two-electron integrals
value	Array containing values of two-electron integrals
n_up	Number of occupied orbitals
n_integrals	Total number of two-electron integrals

Returns

Two-electron energy contribution

< Variable used by two_electron_energy() while calculating the two-electron interaction energy

Iterate over the stored integrals

< Variable used by two_electron_energy() for storing the index i

< Variable used by two_electron_energy() for storing the index j

< Variable used by two_electron_energy() for storing the index k

< Variable used by two_electron_energy() for storing the index l

Check if the first two indices belong to occupied orbitals

if all indices are the same, only add once

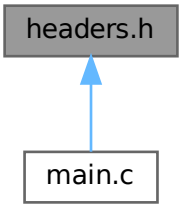
Add x2 the Coulomb integral, ∗2 for permutational symmetry

Substract the exchange integral, ∗2 for permutational symmetry

Break the loop once there are only integrals with virtual orbitals in the list

2.2 headers.h File Reference

This graph shows which files directly or indirectly include this file:



Functions

- double one_electron_energy (double ∗data, int32_t n_up, int32_t mo_num)
  Calculates the one-electron energy contribution to the Hartree-Fock energy.
- double two_electron_energy (int32_t ∗index, double ∗value, int32_t n_up, int64_t n_integrals)
  Calculates the two-electron energy contribution to the Hartree-Fock energy.
- double hartree_fock_energy (double nuc_repul, double one_el_energy, double two_el_energy)
  Calculates the total Hartree-Fock energy.
- double get_integral (int i, int j, int k, int l, const int32_t ∗index, const double ∗value, int64_t n_integrals)
- double get_integral_2 (int i, int j, int k, int l, const int32_t ∗index, const double ∗value, int64_t n_integrals)
  Retrieves integral value.
- double MP2_energy_correction (int32_t ∗index, double ∗value, double ∗mo_energy, int32_t n_up, int32_t mo_num, int64_t n_integrals)
- double MP2_alter (int32_t ∗index, double ∗value, double ∗mo_energy, int32_t n_up, int64_t n_integrals)
  MP2 energy correction calculation.

2.2.1 Function Documentation

2.2.1.1 get_integral()

```
double get_integral (
            int i,
            int j,
            int k,
            int l,
            const int32_t * index,
            const double * value,
            int64_t n_integrals )
```

2.2.1.2 get_integral_2()

```
double get_integral_2 (
            int i,
            int j,
            int k,
            int l,
            const int32_t * index,
            const double * value,
            int64_t n_integrals )
```

Retrieves integral value.

Parameters

i	First index
j	Second index
k	Third index
l	Fourth index
index	Array containing four-index combinations
value	Array containing integral values
n_integrals	Total number of integrals

Returns

Value of the requested integral or 0.0 if not found

2.2.1.3 hartree_fock_energy()

```
double hartree_fock_energy (
            double nuc_repul,
            double one_el_energy,
            double two_el_energy )
```

Calculates the total Hartree-Fock energy.

Parameters

nuc_repul	Nuclear repulsion energy
one_el_energy	One-electron energy contribution
two_el_energy	Two-electron energy contribution

Returns

Total Hartree-Fock energy

2.2.1.4 MP2_alter()

```
double MP2_alter (
            int32_t * index,
            double * value,
            double * mo_energy,
            int32_t n_up,
            int64_t n_integrals )
```

MP2 energy correction calculation.

Parameters

index	Array containing four-index combinations
value	Array containing integral values
mo_energy	Array of molecular orbital energies
n_up	Number of occupied orbitals
n_integrals	Total number of integrals

Returns

MP2 energy correction

< Variable used by MP2_alter() to store the alternative MP2 energy

< Variable used by MP2_alter() to store the integral with indices ijab

< Variable used by MP2_alter() to store the integral with indices ijba

< Variable used by MP2_alter() to store the denominator

< Variable used by MP2_alter to account for permutational symmetry op the integrals

Iterate over the stored integrals

< Variable used by MP2_alter() for storing index i

< Variable used by MP2_alter() for storing index j

< Varibale used by MP2_alter() for storing index a

< Variable used by MP2_alter() for storing index b

2.2.1.5 MP2_energy_correction()

```
double MP2_energy_correction (
            int32_t * index,
            double * value,
            double * mo_energy,
            int32_t n_up,
            int32_t mo_num,
            int64_t n_integrals )
```

< Variable used by MP2_energy_correction() while calculating the MP2 energy

< Variable used by MP2_energy_correction() for storing the integral ijab

< Variable used by MP2_energy_correction() for stpring the integral ijba

2.2.1.6 one_electron_energy()

```
double one_electron_energy (
            double * data,
            int32_t n_up,
            int32_t mo_num )
```

Calculates the one-electron energy contribution to the Hartree-Fock energy.

Parameters

data	Array containing one-electron integrals
n_up	Number of occupied orbitals
mo_num	Total number of molecular orbitals

Returns

One-electron energy contribution

< Variable used by one_electron_energy() while calculating the one-electron energy

2.2.1.7 two_electron_energy()

```
double two_electron_energy (
            int32_t * index,
            double * value,
            int32_t n_up,
            int64_t n_integrals )
```

Calculates the two-electron energy contribution to the Hartree-Fock energy.

Parameters

index	Array containing four-index combinations for two-electron integrals
value	Array containing values of two-electron integrals
n_up	Number of occupied orbitals
n_integrals	Total number of two-electron integrals

Returns

Two-electron energy contribution

< Variable used by two_electron_energy() while calculating the two-electron interaction energy

Iterate over the stored integrals

< Variable used by two_electron_energy() for storing the index i

< Variable used by two_electron_energy() for storing the index j

< Variable used by two_electron_energy() for storing the index k

< Variable used by two_electron_energy() for storing the index l

Check if the first two indices belong to occupied orbitals

if all indices are the same, only add once

Add x2 the Coulomb integral, ∗2 for permutational symmetry

Substract the exchange integral, ∗2 for permutational symmetry

Break the loop once there are only integrals with virtual orbitals in the list

2.3 headers.h

Go to the documentation of this file.

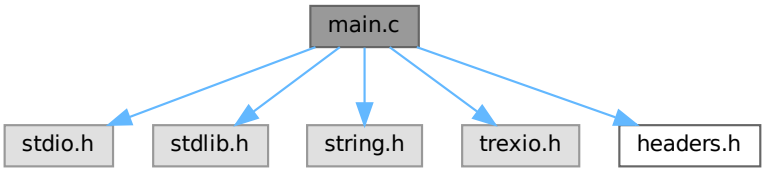
```
00001 // Function headers
00002 #ifndef FUNCTIONS_H
00003 #define FUNCTIONS_H
00004
00005 double one_electron_energy(double* data, int32_t n_up, int32_t mo_num);
00006 double two_electron_energy(int32_t* index, double* value, int32_t n_up, int64_t n_integrals);
00007 double hartree_fock_energy(double nuc_repul, double one_el_energy, double two_el_energy);
00008
00009 double get_integral(int i, int j, int k, int l, const int32_t* index, const double* value, int64_t
      n_integrals);
00010 double get_integral_2(int i, int j, int k, int l, const int32_t* index, const double* value, int64_t
      n_integrals);
00011 double MP2_energy_correction(int32_t* index, double* value, double* mo_energy, int32_t n_up, int32_t
      mo_num, int64_t n_integrals);
00012 double MP2_alter(int32_t* index, double* value, double* mo_energy, int32_t n_up, int64_t n_integrals);
00013
00014 #endif
00015
```

2.4 main.c File Reference

Contains the main program.

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <trexio.h>
#include "headers.h"
```

Include dependency graph for main.c:



Functions

- int main (int argc, char ∗argv[ ])

2.4.1 Detailed Description

Contains the main program.

2.4.2 Function Documentation

2.4.2.1 main()

```
int main (
            int argc,
            char * argv[] )
```

< Variable for the name of the HDF5 file

< Varibale for storing the TREXIO output

< Variable where the nuclear repulsion energy is read

< Variable where the number of spin-up electrons is read

< Variable where the number of molecular orbitals is read

< Array for storing the orbital energies

< Variable for the number of elements to store in data array

< Request mo_num x mo_num doubles for storing the one-electron integrals

< Variable for number of non-zero two-electron integrals

< Array for storing the indices of the two-electron integrals

< Array for storing the values of the two-electron integrals

< Variable buffer size for reading the two-electron integrals, equal to n_integrals

< Variable for the one-electron energy contribution

< Variable for the two-electron energy contribution

< Variable for the overall Hartree-Fock energy

Index