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

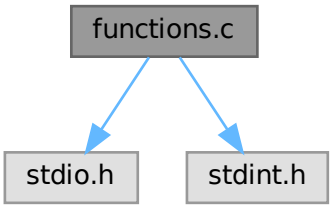
File Documentation

2.1 functions.c File Reference

Contains the functions associated with the HF and MP2 energy calculation.

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

  Retrieves integral value.
- double MP2_energy_correction (int32_t *index, double *value, double *mo_energy, int32_t n_up, int64_t n_integrals)

  MP2 energy correction calculation.

2.1.1 Detailed Description

Contains the functions associated with the HF and MP2 energy calculation.

2.1.2 Function Documentation

2.1.2.1 get_integral()

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

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

2.1.2.2 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

2.1.2.3 MP2_energy_correction()

```
double MP2_energy_correction (
            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

2.1.2.4 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

2.1.2.5 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

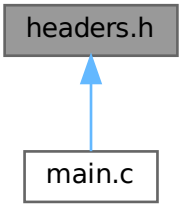
Iterate over the stored integrals

Substract the exchange integral, ∗2 for permutational symmetry

2.2 headers.h File Reference

Contains the function headers.

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)
  Retrieves integral value.
- double MP2_energy_correction (int32_t ∗index, double ∗value, double ∗mo_energy, int32_t n_up, int64_t n_integrals)
  MP2 energy correction calculation.

2.2.1 Detailed Description

Contains the function headers.

2.2.2 Function Documentation

2.2.2.1 get_integral()

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

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

2.2.2.2 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

2.2.2.3 MP2_energy_correction()

```
double MP2_energy_correction (
            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

2.2.2.4 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

2.2.2.5 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

Iterate over the stored integrals

Substract the exchange integral, ∗2 for permutational symmetry

2.3 headers.h

Go to the documentation of this file.

```
00001
00006 #ifndef FUNCTIONS_H
00007 #define FUNCTIONS_H
00008
00009 double one_electron_energy(double* data, int32_t n_up, int32_t mo_num);
00010 double two_electron_energy(int32_t* index, double* value, int32_t n_up, int64_t n_integrals);
00011 double hartree_fock_energy(double nuc_repul, double one_el_energy, double two_el_energy);
00012
00013 double get_integral(int i, int j, int k, int l, const int32_t* index, const double* value, int64_t
      n_integrals);
00014 double MP2_energy_correction(int32_t* index, double* value, double* mo_energy, int32_t n_up, int64_t
      n_integrals);
00015
00016 #endif
00017
```

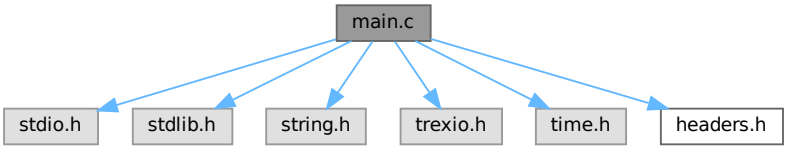
2.4 main.c File Reference

Contains the main program.

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <trexio.h>
#include <time.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[] )
```

2.4.3 Variables

- `char* filename`: Name of the HDF5 file.
- `trexio_exit_code rc`: TREXIO output.
- `trexio_t* trexio_file`: TREXIO file handler.
- `double nuc_repul`: Nuclear repulsion energy.
- `int32_t n_up`: Number of spin-up electrons.
- `int32_t mo_num`: Number of molecular orbitals.
- `double* mo_energy`: Array of molecular orbital energies.
- `int64_t elements`: Number of elements in the data array.
- `double* data`: Array of one-electron integrals.
- `int64_t n_integrals`: Number of non-zero two-electron integrals.
- `int32_t* index`: Array of indices of the two-electron integrals.
- `double* value`: Array of values of the two-electron integrals.
- `int64_t buffer_size`: Buffer size for reading, initially equal to number of two-electron integrals.
- `double one_el_energy`: One-electron energy contribution.
- `double two_el_energy`: Two-electron energy contribution.
- `double HF_energy`: Hartree-Fock energy.
- `double MP2_energy`: MP2 energy correction.

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