# 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:

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2 File Index

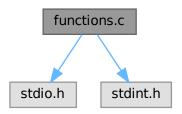
# **Chapter 2**

# **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 1,
    const int32_t * index,
    const double * value,
    int64_t n_integrals )
```

Retrieves integral value.

#### **Parameters**

i	First index
j	Second index
k	Third index
1	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()

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()

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 * 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

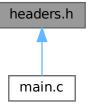
Iterate over the stored integrals

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 1,
    const int32_t * index,
    const double * value,
    int64_t n_integrals )
```

Retrieves integral value.

#### **Parameters**

i	First index
j	Second index
k	Third index
1	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()

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()

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()

2.3 headers.h

```
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.

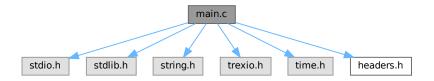
```
00001
00006 #ifndef FUNCTIONS_H
00007 #define FUNCTIONS_H
00008
00009 double one_electron_energy(double* data, int32_t n_up, int32_t mo_num);
00010 double two_electron_energy(int32_t* index, double* value, int32_t n_up, int64_t n_integrals);
00011 double hartree_fock_energy(double nuc_repul, double 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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```