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# Class uni10::Qnum

#### **Quantum number of states**

A Qnum is comprised of one or more eigenvalues of following three symmetry operators:

- U1: If the system has some U1 symmetry, for example, conservation of total Sz or total particle number, we can write down the state with the U1 symmetry eigenstates. U1 eigenvalues here is the U1 in Qnum of the state.
- Z2(parity of Bosonic system): it corresponds to the conservation of the parity of the total particle number, or the parity of total spin up(or down) sites in spin system.
- Z2(parity of Fermionic system): This symmetry is reserved for the parity of the total particle number in fermionic system. In fermionic system, this symmetry is used to take care of the fermionic signs in operations.

# relavant datatype

# uni10::parityType

enum parityType{ PRT\_EVEN = 0, PRT\_ODD = 1};

Type of quantum number parity, belong to Z<sub>2</sub> symmetry group.

# uni10::parityFType

enum parityType{ PRT\_EVEN = 0, PRT\_ODD = 1};

Type of quantum number parity for **fermionic system**, belong to Z<sub>2</sub> symmetry group.

# member functions:

# uni10::Qnum::Qnum

- (1) Qnum(int U1 = 0, parityType prt = PRT\_EVEN);
- (2) Qnum(parityFType prtF, int U1=0, parityType prt=PRT\_EVEN);
- (3) Qnum(const Qnum& qnum);

#### **Construct Qnum**

- (1) Constructs a quantum number for bosonic system.
- (2) Constructs a quantum number for fermionic system.
- (3) Copy constructor.

see example: egQ1

### **Parameters**

U1: int, optional(0)

Initial U1 value for quantum number. the value must bounded by (uni10::Qnum::U1\_UPB, uni10::Qnum::U1\_LOB).

prt: parityType, optional(PRT\_EVEN)

Initial parity value for quantum number.

prtF: parityFType

Initial fermionic parity value for quantum number.

# uni10::Qnum::~Qnum

~Qnum();

#### **Destruct Qnum**

Destroys Qnum.

# uni10::Qnum::assign

- (1) void assign(int U1 = 0, parityType prt = PRT\_EVEN);
- (2) void assign(parityFType prtF, int U1 = 0, parityType prt = PRT\_EVEN);

### **Assign Qnum content**

Assigns new content to Qnum, replacing its current content.

(2) assigns a fermionic quantum number.

see example: egQ1

### **Parameters**

U1: int, optional(0)

Initial U1 value for quantum number. the value must bounded by (uni10::Qnum::U1\_UPB, uni10::Qnum::U1\_LOB).

prt: parityType, optional(PRT\_EVEN)

Initial parity value for quantum number.

prtF: parityFType

Initial fermionic parity value for quantum number.

# uni10::Qnum::**U1**

int U1()const;

#### Return U1

Returns the value of U1 quantum number.

### **Return Value**

The value of U1 quantum number, bounded by (uni10::Qnum::U1\_UPB, uni10::Qnum::U1\_LOB).

# uni10::Qnum::prt

parityType prt()const;

## **Return parity**

Returns the value of parity quantum number.

### **Return Value**

The value of parity quantum number.

# uni10::Qnum::prtF

parityFType prtF()const;

### **Return parity**

Returns the value of fermionic parity quantum number.

### **Return Value**

The value of fermionic parity quantum number.

# static member functions:

## uni10::Qnum::isFermionic

static bool isFermionic();

## Test whether the system is fermionic

Tests whether fermionic parity *PRTF\_ODD* exists in the system,

#### **Return Value**

true if the fermionic odd parity exists, false otherwise.

# Example: egQ1

```
source: http://uni10.org/examples/egQ1.cpp
```

```
1) #include <iostream>
2) #include <uni10.hpp>
3)
4) int main(){
5)  // U1 = 1, parity even.
6)  uni10::Qnum q10(1, uni10::PRT_EVEN);
7)  // U1 = -1, parity odd.
8)  uni10::Qnum q_11(-1, uni10::PRT_ODD);
9)
10) std::cout<<"q10: "<<q10<<std::endl;</pre>
```

```
11) std::cout<<"q_11: "<<q_11<<std::endl;</pre>
12) std::cout<<"q_11: U1 = "<<q_11.U1()<<", parity = "<<q_11.prt()<<std::endl;
13) q_11.assign(-2, uni10::PRT_EVEN);
14) std::cout<<"q_11(after assign): "<<q_11<<std::endl;
15) // check the for fermionic
16) std::cout<<"isFermioinc: "<<uni10::0num::isFermionic()<<std::endl :
17)
18) // Fermionic system
19) std::cout<<"---- Fermionic ----\n";</pre>
20) // fermionic parity even, U1 = 1, parity even.
21) uni10::Qnum f0_q10(uni10::PRTF_EVEN, 1, uni10::PRT_EVEN);
22) // fermionic parity odd, U1 = 1, parity even.
23) uni10::Qnum f1_q10(uni10::PRTF_ODD, 1, uni10::PRT_EVEN);
24)
25) std::cout<<"f0 q10: "<<f0 q10<<std::endl;</pre>
26) std::cout<<"f1_q10: "<<f1_q10<<std::endl;</pre>
27) std::cout<<"f1_q10: fermionic parity = " <<f1_q10.prtF()<<std::endl;</pre>
28) std::cout<<"isFermioinc: "<<uni10::Qnum::isFermionic()<<std::endl;</pre>
29)
30) return 0;
31)}
```

### Output:

```
q10: (U1 = 1, P = 0, 0)

q_11: (U1 = -1, P = 1, 0)

q_11: U1 = -1, parity = 1

q_11(after assign): (U1 = -2, P = 0, 0)

isFermioinc: 0

---- Fermionic -----

f0_q10: (U1 = 1, P = 0, 0)

f1_q10: (U1 = 1, P = 0, 1)

f1_q10: fermionic parity = 1

isFermioinc: 1
```

### non-member overloads:

# operator<

friend bool operator< (const Qnum& q1, const Qnum& q2); friend bool operator<= (const Qnum& q1, const Qnum& q2);

### **Define less than operator**

Defines q1 < q2

### **Parameters**

```
q1, q2: Qnum
```

Two *Qnums* being compared.

#### **Return Value**

true if q1 < q2, false otherwise.

# operator==

friend bool operator== (const Qnum& q1, const Qnum& q2);

## **Define equal operator**

Defines q1 == q2

### **Parameters**

q1, q2: Qnum

Two Qnums being compared.

### **Return Value**

true if q1 == q2, false otherwise.

# operator-

friend Qnum operator- (const Qnum& q1);

### **Define minus operator**

Defines the minus sign behavior. Minus sign is defined by the change be when quantum number on in-coming bond *permute* to out-coming bond, or vice versa.

For U1 symmetry in Qnum, minus sign corresponds to minus U1 value. As for parity, minus sign have no effect.

### **Parameters**

q1: Qnum

Original Qnum

### **Return Value**

Returns the resulting Qnum q = -q1.

# operator\*

friend Qnum operator\* (const Qnum& q1, const Qnum& q2);

### **Define multiplication operator**

Defines the fusion rules for quantum numbers. For U1 symmetry in Qnum, q1 \* q2 corresponds to q1.U1() + q2.U1(). For parity, q1 \* q2 corresponds to  $q1.prt() ^q2.prt()$ .  $(q1.prtF() ^q2.prtF()$  in fermionic case)

### **Parameters**

q1, q2: Qnum

Two Qnums being multiplied, q1 multiplied by q2.

### **Return Value**

Returns the resulting Qnum q = q1 \* q2.

# operator<<

friend std::ostream& operator<< (std::ostream& os, const Qnum& g);

#### **Print out Qnum**

Prints out a quantum number Qnum *q* as: (for example)

```
std::cout << q;
```

```
(U1 = 1, P = 0, 1)
```

Which means q.U1() is 1, q.prt() is 0(PRT\_EVEN) and q.prtF() is 1(PRTF\_ODD)

### **Parameters**

os: std::ostream

ostream in standard library, see http://www.cplusplus.com/reference/ostream/ostream/? kw=ostream

q: Qnum

Qnum to be printed out.

### **Return Value**

Returns std::ostream&

# Example: egQ2

```
source: http://uni10.org/examples/egQ2.cpp
1) int main(){
    // U1 = 1, parity even.
    uni10::Qnum q10(1, uni10::PRT_EVEN);
    // U1 = -1, parity odd.
5)
    uni10::Qnum q_11(-1, uni10::PRT_ODD);
7)
    std::cout<<"q10: "<< q10 << std::endl;
    std::cout<<"q_11: "<< q_11 << std::endl;
9)
10) std::cout<<"---- Operations ----\n";</pre>
11) std::cout<<"-q_11 = " << -q_11 << std::endl;
12) std::cout<<"q10 * q_11 = " << q10 * q_11 <<std::endl;
13) std::cout << "q10 * (-q 11) = " << q10 * (-q 11) << std::endl;
15) return 0;
16)}
```

# Output:

```
q10: (U1 = 1, P = 0, 0)

q_11: (U1 = -1, P = 1, 0)

---- Operations ----

-q_11 = (U1 = 1, P = 1, 0)

q10 * q_11 = (U1 = 0, P = 1, 0)

q10 * q_11 = (U1 = 2, P = 1, 0)
```

# Class uni10::Bond

#### Bond of a tensor

A tensor is comprised of bonds. The number of bonds corresponds to the rank of a tensor. A bond usually represents states of a particular basis of a physical system. For example, a bond could represents the states of a spin 1 particle, which has three possible states in the basis of Sz, -1, 0, 1. In this case, the dimension of bond is three. If there are some symmetries in the system, each state of bond can has a *Qnum*, which is the eigenvalue of the symmetry operators. For example, the conservation of total Sz in spin system(U1 symmetry), if we choose Sz as our basis, we can have a bond of three *Qnum* of *U1* values corresponding to the Sz eigenvalues.

# relavant datatype

# uni10::bondType

enum bondType{ BD\_IN = 1, BD\_OUT = -1 };

Two types of bond, in-coming bond, out-going bond.

# member functions

## uni10::Bond::Bond

- (1) Bond(bondType, int dim);
- (2) Bond(bondType, const std::vector<Qnum>& gnums);
- (3) Bond(const Bond& bd);

### **Construct Bond**

Constructs a Bond, initializing depending on the constructor version used:

- (1) Constructs a Bond with dimension *dim* and without symmetry quantum number
- (2) Constructs a Bond by the given *Qnum* vector *qnums*. *qnums* is the quantum numbers of the states on the bond.
- (3) Copy constructor.

#### **Parameters**

gnums: std::vector<Qnum>

Quantum number array to fill the bond with.

bd: Bond

Bond to be copied.

# uni10::Bond::~Bond

~Bond();

#### **Destruct Bond**

Destroys a Bond.

# uni10::Bond::assign

- void assign(bondType, int dim);
- (2) void assign(bondType, const std::vector<Qnum>& qnums);

### **Assign bond content**

Assigns new quantum numbers, bondType and dimension dim to Bond, replacing its current content.

#### **Parameters**

gnums: std::vector<Qnum>

Quantum number array to fill the bond with.

# uni10::Bond::type

bondType type()const;

### Return type

Returns the type of a bond, either BD\_IN or BD\_OUT.

### **Return Value**

The type of the bond.

## uni10::Bond::dim

int dim()const;

#### **Return dimension**

Returns the dimension of a bond, that is, the number of quantum states.

### **Return Value**

The dimension of the bond.

# uni10::Bond::degeneracy

std::map<Qnum, int> degeneracy()const;

### Return the numbers of degeneracy of various Qnum

Returns a map, which shows the degeneracy of various *Qnum*.

### **Return Value**

The mapping of *Qnum* to its degeneracy value.

# uni10::Bond::Qlist

std::vector<Qnum> Qlist()const;

### Return its quantum number array

Returns an array of *Qnum* of states in the bond. the size of the vector is the same as the dimension of the bond.

# **Return Value**

The vector of its Qnum array.

# uni10::Bond::change

void change(bondType type);

## Change type of a bond

Changes the type of the bond, together with the *Qnums* of the bond. If bond is changed from incoming(BD\_IN) to out-going(BD\_OUT) type or vice versa, the change of its *Qnums* is defined by the minus sign "-" of *Qnum* itself.

### **Parameters**

type: bondType

Type to change to.

# uni10::Bond::combine

Bond& combine(const Bond bd);

### Combine a bond

Combines another bond *db*, expand the bond dimension by direct product of it *Qnums* and the *Qnums* of the given bond *bd*. The resulting bondType is unchanged.

### **Parameters**

bd: Bond

The bond to be combined.

### **Return Value**

The resulting Bond.

# static member functions:

## uni10::Bond::combine

- (1) static Bond combine(const std::vector<Bond>& bds);
- (2) static Bond combine(bondType type, const std::vector<Bond>& bds);

#### **Combine bonds**

Combines an array of bonds by successively combining the bonds in the order of bonds in the given array *bds*.

- (1) The resulting Bond is of type of the first bond in bds.
- (2) The resulting Bond is of type of the given *bondType*.

### **Parameters**

bds: std::vector<Bond>

An array of *Bond* to be combined.

type: bondType

The type for the resulting bond to be.

### **Return Value**

The resulting Bond.

## non-member overloads:

## operator==

friend bool operator== (const Bond& b1, const Bond& b2);

### Compare two bonds

The equality condition is that:

b1.type() == b2.type() && b1.Qlist() == b2.Qlist()

#### **Parameters**

b1, b2: Bond

The bonds to be compared.

### **Return Value**

true if b1 == b2, false otherwise.

# operator<<

friend std::ostream& operator<< (std::ostream& os, const Bond& b);

#### **Print out Qnum**

Prints out a bond as(for example):

std::cout << b;

IN: (U1 = 1, P = 0, 0)|1, (U1 = 0, P = 0, 0)|2, (U1 = -1, P = 0, 0)|1, Dim = 4

In above example, it is in-coming bond with three Qnums: one U1=1, two U1=0 and one U1=-1. The dimension of the bond is 4.

### **Parameters**

os: std::ostream&

ostream in standard library, see http://www.cplusplus.com/reference/ostream/ostream/? kw=ostream

b: Bond

Bond to be printed out.

### **Return Value**

Returns std::ostream&

# Example: egB1

```
source: http://uni10.org/examples/egB1.cpp
```

```
1) #include <iostream>
2) #include <uni10.hpp>
3)
4) int main(){
    uni10::Qnum q1(1);
    uni10::Qnum q0(0);
6)
7)
    uni10::Qnum q_1(-1);
    // Create an array of Qnums for the states of a bond.
9)
    std::vector<uni10::Onum> anums:
10) qnums.push_back(q1);
11) qnums.push_back(q1);
12) gnums.push back(q0);
13) qnums.push_back(q0);
14) gnums.push_back(q0);
15) gnums.push back(q 1);
16)
17) // Constrcut Bond with Qnum array
18) uni10::Bond bd(uni10::BD IN, gnums);
19) // Print out a Bond
20) std::cout<<"Bond bd: \n"<<bd<<std::endl;</pre>
21) std::cout<<"Bond type: "<<bd.type()<<"(IN)"<<", Bond dimension:</pre>
    "<<bd.dim()<<std::endl<<std::endl;
23) // List the degeneracy of states
24) std::cout<<"Degeneracies: "<<std::endl;</pre>
25) std::map<uni10::Qnum, int> degs = bd.degeneracy();
26) for(std::map<uni10::Qnum,int>::const_iterator it=degs.begin(); it!
    =degs.end(); ++it)
         std::cout<<it->first<<": "<<it->second<<std::endl;
28) std::cout<<std::endl:</pre>
30) std::vector<uni10::Qnum> qlist = bd.Qlist();
31) std::cout<<"Qnum list: "<<std::endl;</pre>
32) for(int i = 0; i < qlist.size(); i++)</pre>
         std::cout<<qlist[i]<<", ";</pre>
```

```
34) std::cout<<std::endl<<std::endl;</pre>
36) // Change bond type
         bd.change(uni10::BD OUT);
         std::cout<<"bd changes to BD_OUT:\n"<<bd<<std::endl;</pre>
40) bd.change(uni10::BD IN);
41)
42) // Combine bond
43) qnums.clear();
44) qnums.push_back(q1);
45) gnums.push back(q0);
46) gnums.push back(q0);
47) qnums.push_back(q_1);
48) uni10::Bond bd2(uni10::BD IN, gnums);
49) std::cout<<"Bond bd2: \n"<<bd2<<std::endl;</pre>
50)
51) // bd.combine(bd2);
52) std::cout<<"bd2.combine(bd): \n"<<bd2.combine(bd)<<std::endl;</pre>
53)
54) std::cout<<"Degeneracies of bd2 after combining bd: "<<std::endl;
55) degs = bd2.degeneracy();
56) for(std::map<uni10::Qnum,int>::const_iterator it=degs.begin(); it!
          =degs.end(); ++it)
                    std::cout<<it->first<<": "<<it->second<<std::endl;</pre>
57)
58) std::cout<<std::endl;</pre>
59)
60) return 0;
61)}
Output:
Bond bd:
IN: (U1 = 1, P = 0, 0)|2, (U1 = 0, P = 0, 0)|3, (U1 = -1, P = 0, 0)|1, Dim = 6
Bond type: 1(IN), Bond dimension: 6
Degeneracies:
(U1 = -1, P = 0, 0): 1
(U1 = 0, P = 0, 0): 3
(U1 = 1, P = 0, 0): 2
Onum list:
(U1 = 1, P = 0, 0), (U1 = 1, P = 0, 0), (U1 = 0, P = 0, 0), (U1 = 0, P = 0, 0),
(U1 = 0, P = 0, 0), (U1 = -1, P = 0, 0),
bd changes to BD OUT:
OUT: (U1 = -1, P = 0, 0)|2, (U1 = 0, P = 0, 0)|3, (U1 = 1, P = 0, 0)|1, Dim = 6
Bond bd2:
IN: (U1 = 1, P = 0, 0)|1, (U1 = 0, P = 0, 0)|2, (U1 = -1, P = 0, 0)|1, Dim = 4
bd2.combine(bd):
IN: (U1 = 2, P = 0, 0)|2, (U1 = 1, P = 0, 0)|3, (U1 = 0, P = 0, 0)|1, (U1 = 1, P)|
= 0, 0)|2, (U1 = 0, P = 0, 0)|3, (U1 = -1, P = 0, 0)|1, (U1 = 1, P = 0, 0)|2, (U1 = 0, 0)|2, (
```

```
= 0, P = 0, 0) |3, (U1 = -1, P = 0, 0) |1, (U1 = 0, P = 0, 0) |2, (U1 = -1, P = 0, 0) |3, (U1 = -2, P = 0, 0) |1, Dim = 24

Degeneracies of bd2 after combining bd:
(U1 = -2, P = 0, 0) : 1
(U1 = -1, P = 0, 0) : 5
(U1 = 0, P = 0, 0) : 9
(U1 = 1, P = 0, 0) : 7
(U1 = 2, P = 0, 0) : 2
```

# Class uni10::Matrix

#### A common matrix

Class *Matrix* is made for some linear algebra operations on matrix. In addition, *Matrix* is perfectly cooperate with the class *UniTensor*. A tensor with symmetries contains blocks of various *Qnums*. Each block is a matrix with tensor elements. We can take a block out of a tensor as a *Matrix*, do whatever operations you want on the matrix elements and put *Matrix* back to the tensor. The *Matrix* follows C convention that it is row-major and indices start from 0. For now, *Matrix* only supports datatype *double*.

# member functions:

# uni10::Matrix::Matrix

- (1) Matrix(int Rnum, int Cnum, bool diag=false);
- (2) Matrix(int Rnum, int Cnum, double\* elem, bool diag=false);
- (3) Matrix(const Matrix& m);

#### **Construct Matrix**

Constructs a *Matrix*, initializing depending on the constructor version used:

- (1) Allocate memory of size Rnum \* Cnum( or min(*Rnum, Cnum*) if *diag* is *true*) for matrix elements and set the elements to zero
- (2) Allocate memory of size Rnum \* Cnum( or min(*Rnum, Cnum*) if *diag* is *true*) for matrix elements and copy the elements from the given *elem*.
- (3) copy constructor. The properties of the *Matrix* are copied. It allocates new memory for elements and copied the content from the given *Matrix* m.

### **Parameters**

Rnum: int

The number of rows of the matrix.

Cnum: int

The number of columns of the matrix.

diag: bool, optional(false)

If it's true, only the memory of the diagonal elements are allocated.

m: Matrix

Another *Matrix* being copied from.

# uni10::Matrix::~Matrix

~Matrix();

#### **Destruct Matrix**

Destroys the *Matrix* and freeing all the allocated memory for matrix elements.

# uni10::Matrix::row

int row()const;

### **Return number of rows**

Returns the number of rows of the *Matrix*.

### **Return Value**

Number of rows

# uni10::Matrix::col

int col()const;

### **Return number of columns**

Returns the number of columns of the Matrix.

### **Return Value**

Number of columns.

# uni10::Matrix::isDiag

bool isDiag()const;

## Test whether *Matrix* is diagonal

Returns whether the *Matrix* is diagonal

### **Return Value**

true if diagonal, false otherwise.

# uni10::Matrix::elemNum

size\_t elemNum()const;

#### Return size

Returns the number of allocated elements. If diagonal, the return value is equal to the number of diagonal elements.

## **Return Value**

The number of elements in *Matrix* 

# uni10::Matrix::operator[]

double& operator[](size\_t idx);

#### **Access element**

Returns a reference to the element at position idx in the Matrix. The value idx is serial index counted in row-major from the first element (idx = 0) of the Matrix.

This function works similar to member function *Matrix::at()*.

### **Parameters**

idx: int

Position of an element in the *Matrix* 

### **Return Value**

The element at the specified position in the *Matrix*.

## uni10::Matrix::at

double& at(int i, int j);

### **Access element**

Returns a reference to the element in *i*-th row and *j*-th column of the *Matrix*. The values *i* and *j* are counted from 0.

### **Parameters**

i, j: int

Index of the Matrix

### **Return Value**

The element at the index (i, j) in the *Matrix*.

## uni10::Matrix::elem

double\* elem()const;

#### **Access element**

Returns a pointer of type *double* to the *Matrix* elements.

### **Return Value**

double pointer of the Matrix elements

# uni10::Matrix::operator=

Matrix& operator=(const Matrix& mat);

### **Assign Matrix**

Assigns new content to the *Matrix* from the given matrix *mat*, replacing the original memory of elements by reallocating new memory fit for *mat*.

### **Parameters**

mat: Matrix

The Matrix to be copied from.

# uni10::Matrix::addElem

void addElem(double\* elem);

# Copy elements

Copies the first *elemNum()* elements from the given double pointer elem, replacing the original ones.

### **Parameters**

elem: double pointer

The *Matrix* elements to be copied from.

# uni10::Matrix::save

void save(const std::string& fname);

## **Output to file**

Writes the elements of the *Matrix* out to a binary file of file name *fname*. The output file size is elemNum()\*sizeof(double).

### **Parameters**

fname: std::string

File name to write elements out.

# uni10::Matrix::load

void load(const std::string& fname);

### Input from file

Reads the elements of the *Matrix* from the binary file of file name *fname*. Reads in *double* array of size *elemNum*()\*sizeof(*double*) from file stream and replacing the origin elements.

### **Parameters**

fname: std::string

File name to read elements in.

# uni10::Matrix::set zero

void set\_zero();

#### **Assign elements**

Sets all the double elements of the *Matrix* to zero.

# uni10::Matrix::randomize

void randomize();

### **Assign elements**

Randomly assigns double values ranged (0, 1) to the elements of the *Matrix*.

# uni10::Matrix::orthoRand

void orthoRand();

## **Assign elements**

Randomly generates orthogonal bases. Assigns to the elements of the *Matrix*.

Let Nr = row() and Nc = col().

If the Nr < Nc, randomly generates Nr's orthogonal bases with each basis having dimension Nc, generating Nr's row-vectors of size Nc.

If the Nr > Nc, randomly generates Nc's orthogonal bases with each basis having dimension Nr, generating Nc's column-vectors of size Nr.

# uni10::Matrix::transpose

void transpose();

### **Transpose Matrix**

Exchanges the number of rows and the number of columns and transposes the elements of the *Matrix*.

# uni10::Matrix::diagonalize

std::vector<Matrix> diagonalize();

### **Perform diagonalization on the Matrix**

Diagonalizes the *Matrix* and returns the a vector of two matrices of diagonalization. Notice that, the matrix being diagonalized must be symmetry.

For a *n* by *n* matrix *A*:

A = UT \* D \* U

The operation is a wrapper of Lapack function *dsyev()*.

### **Return Value**

A vector of Matrices [D, U] of the diagonalization results.

For *n* by *n Matrix*:

*D* is *n* by *n* diagonal *Matrix* of eigenvalues.

*U* is *n* by *n* row-vectors of eigenvectors.

# uni10::Matrix::svd

std::vector<Matrix> svd();

### **Perform SVD on the Matrix**

Performs singular value decomposition(SVD) on the Matrix and returns a vector of three resulting matrices of SVD.

For *m* by *n* matrix *A*, it is decomposed as:

 $A = U * \Sigma * VT$ 

The operation is a wrapper of Lapack function *dgesvd*().

### **Return Value**

A vector of Matrices  $[U, \Sigma, VT]$  of the diagonalization results.

For *m* by *n Matrix*:

*U* is m by n row-major matrix.

 $\Sigma$  is n by n diagonal matrix.

VT is n by m row-major matrix.

# uni10::Matrix::trace

double trace();

#### **Trace of the Matrix**

Performs trace of the Matrix.

#### **Return Value**

Trace value of the Matrix.

# uni10::Matrix::operator\*=

- (1) Matrix& operator\*= (const Matrix& Mb);
- (2) Matrix& operator\*= (double a);

### **Perform multiplication**

- (1) Performs matrix multiplication with another Matrix Mb.
- (2) Performs element-wise multiplication with a scalar a of type double.

### **Parameters**

Mb: Matrix

The given matrix to multiplied with.

a: double

The scalar of type double to multiplied with.

### **Return Value**

The resulting Matrix.

# uni10::Matrix::operator+=

Matrix& operator+= (const Matrix& Mb);

#### Perform additions of elements

Performs element by element addition.

### **Parameters**

Mb: Matrix

The given matrix to add.

### **Return Value**

The resulting Matrix.

# non-member overloads:

# operator\*

- (1) friend Matrix operator\* (const Matrix& Ma, const Matrix& Mb);
- (2) friend Matrix operator\*(const Matrix& Ma, double a);
- (3) friend Matrix operator\*(double a, const Matrix& Ma)

### **Perform multiplication**

- (1) Performs matrix multiplication, Ma \* Mb;
- (2) Performs element-wise multiplication with a scalar a of type double, Ma \* a
- (3) The same as (2), a \* Ma

#### **Parameters**

Ma, Mb: Matrix

Matrices for matrix multiplication Ma \* Mb

a: double

The scalar of type *double* to multiplied with *Matrix*.

### **Return Value**

The resulting *Matrix*.

# operator+

friend Matrix operator+(const Matrix& Ma, const Matrix& Mb);

#### Matrix addition

Performs element-wise additions on matrix *Ma* and *Mb*, *Ma* + *Mb*.

### **Parameters**

Ma, Mb: Matrix

Matrices for matrix addition Ma + Mb

#### **Return Value**

The resulting Matrix.

# operator==

friend bool operator== (const Matrix& Ma, const Matrix& Mb);

## **Compare Matrices**

Compare all the elements in *Ma* and *Mb*, returning *true* if all the elements are the same, false otherwise.

### **Parameters**

Ma, Mb: Matrix

Matrices for comparison.

### **Return Value**

true if all the elements in Ma and Mb are the same, false otherwise.

# operator<<

std::ostream& operator<< (std::ostream& os, const Matrix& M);

#### **Print out Matrix**

Prints out a *Matrix* as(for example):

std::cout << M:

$$2 \times 3 = 6$$

$$-0.254 - 0.858 - 0.447$$

In the above example, M is a 2 by 3 matrix with number of elements 6 and the following 2 by 3 matrix are its elements.

### **Parameters**

os: std::ostream

ostream in standard library, see http://www.cplusplus.com/reference/ostream/ostream/?kw=ostream

M: Matrix

Matrix to be printed out.

#### **Return Value**

Returns std::ostream&

# Example: egM1

source: http://uni10.org/examples/egM1.cpp

```
1) #include <iostream>
2) #include <uni10.hpp>
3)
4) int main(){
5)
    // Spin 1/2 Heisenberg hamiltonian
6)
    double elem[] = \{1.0/4,
7)
                           0, -1.0/4, 1.0/2,
8)
                           0, 1.0/2, -1.0/4,
9)
                                   0,
                                          0, 1.0/4};
10) uni10::Matrix H(4, 4, elem);
11) std::cout<<H;</pre>
12) // Diagonlize H
13) std::vector<uni10::Matrix> results = H.diagonalize();
14) std::cout<<"The eigen values: \n\n"<<results[0];
15) std::cout<<"The eigen vectors: \n\n"<<results[1];
16)
17) // Access element in a diagonal matrix
18) uni10::Matrix D = results[0];
19) std::cout<<"D.at(1, 1) = "<<D.at(1, 1)<<std::endl;;</pre>
20) std::cout<<"D[2] = " << D[2]<<std::endl;
21) // Assign element
22) std::cout<<"\nAssign D.at(3, 3) = 7.0\n\n";</pre>
23) D.at(3, 3) = 7.0;
24) std::cout<<D;
25)
26) // Access element
27) std::cout<<"H.at(1, 2) = "<<H.at(1, 2)<<std::endl;;</pre>
28) std::cout<<"H[5] = " << H[5]<<std::endl;</pre>
29)
30) // Make a pure density matrix from ground state
31) uni10::Matrix U = results[1];
32) // Generate ground state by taking the first H.rol() elements from U.
33) uni10::Matrix GS(1, H.col(), U.elem());
34) // Transposed GS
35) uni10::Matrix GST = GS;
36) GST.transpose();
38) std::cout<<"\nThe ground state: \n\n";
39) std::cout<< GS;</pre>
40) std::cout<< GST;
41)
42) // Compose a pure density matrix from ground state
43) uni10::Matrix Rho = GST * GS;
44) std::cout<<"\nPure density matrix of ground state: \n\n";
45) std::cout<< Rho;
46)
47) // Measure ground state energy
48) std::cout<<"\nThe ground state energy: " << (Rho * H).trace() << std::endl;
49)}
```

Output:

```
4 \times 4 = 16
```

### The eigen values:

$$4 \times 4 = 4$$
, Diagonal

### The eigen vectors:

$$4 \times 4 = 16$$

$$D.at(1, 1) = 0.250$$

$$D[2] = 0.250$$

Assign D.at(3, 3) = 
$$7.0$$

$$4 \times 4 = 4$$
, Diagonal

$$H.at(1, 2) = 0.500$$

$$H[5] = -0.250$$

### The ground state:

$$1 \times 4 = 4$$

```
0.000 0.707 -0.707 0.000
4 \times 1 = 4
  0.000
  0.707
-0.707
  0.000
Pure density matrix of ground state:
4 \times 4 = 16
  0.000
       0.000 0.000
                       0.000
  0.000 0.500 -0.500
                       0.000
  0.000 -0.500 0.500
                       0.000
  0.000 0.000 0.000
                      0.000
The ground state energy: -0.750
```

# Example: egM2

```
source: http://uni10.org/examples/egM2.cpp
1) #include <iostream>
2) #include <uni10.hpp>
3)
4) int main(){
    uni10::Matrix M(4, 5);
    M.randomize();
6)
7)
    std::cout<<M;</pre>
    // carry out SVD
9)
    std::vector<uni10::Matrix> rets = M.svd();
10)
11) // write matrice out to file
12) rets[0].save("mat U");
13) rets[1].save("mat_Sigma");
14) rets[2].save("mat_VT");
15)
16) uni10::Matrix U(rets[0].row(), rets[0].col(), rets[0].isDiag());
17) uni10::Matrix S(rets[1].row(), rets[1].col(), rets[1].isDiag());
18) uni10::Matrix VT(rets[2].row(), rets[2].col(), rets[2].isDiag());
19)
```

```
20) // read in the matrice we just write out
21) U.load("mat_U");
22) S.load("mat_Sigma");
23) VT.load("mat_VT");
24) std::cout<< S;
25) std::cout<< U * S * VT;
26)}</pre>
```

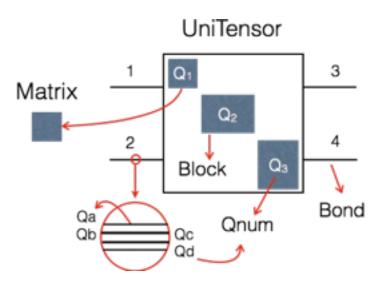
# Output:

```
4 \times 5 = 20
 0.840 0.394 0.783 0.798 0.912
 0.198 0.335 0.768 0.278 0.554
 0.477 0.629 0.365 0.513 0.952
 0.916 0.636 0.717
                      0.142 0.607
4 \times 4 = 4, Diagonal
 2.736 0.000 0.000
                      0.000
 0.000 0.555
               0.000
                      0.000
 0.000 0.000
               0.449
                      0.000
 0.000 0.000
               0.000
                      0.382
4 \times 5 = 20
 0.840 0.394
               0.783 0.798
                           0.912
 0.198 0.335 0.768 0.278
                            0.554
 0.477 0.629 0.365 0.513 0.952
 0.916 0.636 0.717 0.142 0.607
```

## Class uni10::UniTensor

#### **Universal Tensor**

Class *UniTensor* is made for tensor contractions and permutes of tensor *Bonds*(Indices) with symmetry block diagonal elements. A tensor is comprised of *Bonds* and blocked elements with various quantum number *Qnum(Q1, Q2, Q3* in the figure). The *Qnums* on the *Bonds* decide the sizes of those *Qnum* blocks and the rank of tensor is decided by the number of Bonds. Each Bond has a label(1, 2, 3, 4 in the figure). Labels are used to manipulate tensors, such as in operations *permute*, *partialTrace* and tensor contraction. For manipulation of ten



elements, one can use *getBlock* function to take out block elements out as a *Matrix*, performs whatever operations on it and puts it back with function *putBlock*. For the operations about *Matrix*, see class *Matrix*.

## member functions

# uni10::UniTensor::UniTensor

- (1) UniTensor(double val = 1.0);
- (2) UniTensor(const std::vector<Bond>& bonds, const std::string& name = "");
- (3) UniTensor(const std::vector<Bond>& bonds, int\* labels, const std::string& name = "");
- (4) UniTensor(const std::vector<Bond>& bonds, std::vector<int>& labels, const std::string& name = "");
- (5) UniTensor(const std::string& fname);
- (6) UniTensor(const UniTensor& uT);

### **Construct UniTensor**

Constructs a *UniTensor*, initializing depending on the constructor version used:

- (1) Constructs without *Bonds* to create a rank 0 tensor, a scalar. The default value for the scalar is 1.0.
- (2) Constructs a tensor with the given *Bond* array *bonds*, allocating memories for blocks of sizes decided by the input *bonds* and naming the tensor *name* if given.
- (3) Constructs a tensor with the given *Bond* array *bonds* and int array *labels*. It initializes the same way as (2) above, then assigns *labels* to the *Bonds* of the *UniTensor*.
- (4) It is similar to (3). Instead of taking int\* *labels*, it takes std::vector type *labels*.
- (5) Loads a tensor from the binary file of file name *fname*. Note that, the file *fname* is a binary file of specific format which is generated by the function *UniTensor*::save(fname).
- (6) Copy constructor. The properties of the *UniTensor* are copied. It allocates new memory for elements and copied the content from the given *UniTensor uT*.

### **Parameters**

val: double, optional(1.0)

The value for the rank 0 *UniTensor*(1).

bonds: std::vector<Bond>

An array of bonds of the *UniTensor*. For initializing the structure of tensor.

name: std::string, optional("")

Given name of the *UniTensor*.

fname: std::string

The file name of the *UniTensor* being read in

uT: UniTensor

Another *UniTensor* being copied from.

# uni10::UniTensor::~UniTensor

~UniTensor();

#### **Destruct UniTensor**

Destroys the *UniTensor* and freeing all the allocated memory for tensor content.

# uni10::UniTensor::addLabel

- (1) void addLabel(int\* newLabels);
- (2) void addLabel(const std::vector<int>& newLabels);

### **Assign labels**

Assign the labels *newLabels* to each bond of the *UniTensor*, replacing the origin labels on the bonds.

#### **Parameters**

newLabels: int\*

int pointer to the array of labels.

newLabels: std::vector<int> vector of the array of labels.

# uni10::UniTensor::label

- (1) std::vector<int> label()const;
- (2) int label(int idx)const;

#### Access labels

Returns the label of the bond at the position *idx*, the order of bonds are decided at initialization. If no input given, return the array of labels of type std::<int>vector.

#### **Parameters**

idx: int

The position of the bond from which the label is retrieved.

### **Return Value**

The value of label (2) or the array of labels (1).

# uni10::UniTensor::bondNum

size t bondNum()const;

### Access the number of bonds

Returns the number of bonds.

### **Return Value**

The value of the number of bonds of the *UniTensor*.

# uni10::UniTensor::inBondNum

int inBondNum()const;

## Access the number of in-coming bonds

Returns the number of in-coming bonds.

## **Return Value**

The value of the number of in-coming bonds of the *UniTensor*.

# uni10::UniTensor::bond

- (1) std::vector<Bond> bond()const;
- (2) Bond bond(int idx)const;

#### **Access bonds**

Returns the bond of type *Bond* at the position *idx*, the order of bonds is decided at initialization. If no input given, return the array of bonds of type std::<*Bond*>vector.

### **Parameters**

idx: int

The position of the *bond* being retrieved.

#### **Return Value**

The bond in type *Bond* (2) or the array of bonds (1).

# uni10::UniTensor::addRawElem

void addRawElem(double\* rawElem);

### **Assign elements**

Assigns elements to the UniTensor from the given "raw elements" rawElem. Raw elements mean non-block-diagonal elements which are written down with a chosen basis. This function will reorganize the raw elements into block-diagonal elements.

### **Parameters**

rawElem: double\*

double pointer pointing to the array of input non-block-diagonal elements.

# uni10::UniTensor::blockNum

size\_t blockNum()const;

### Access the number of blocks

Returns the number of blocks of elements

#### **Return Value**

The value of the number of blocks.

# uni10::UniTensor::blockQnum

- (1) std::vector<Qnum> blockQnum()const;
- (2) Qnum blockQnum(int idx)const;

#### **Access Qnums of blocks**

Returns the quantum number of type *Qnum* of the block at the position *idx*, the order of blocks is in ascending order of *Qnum*. If no input given, returns an array of *Qnum* of all blocks. The returned array of *Qnums* is in ascending order of *Qnum*.

#### **Parameters**

idx: int

The position of the block from which the *Qnum* is retrieved.

#### **Return Value**

The quantum number in type *Qnum* (2) or the array of *Qnums* in type std::vector<*Qnum*>(1).

# uni10::UniTensor::getBlocks

std::map<Qnum, Matrix> getBlocks()const;

#### **Access block elements**

Returns the element blocks of various *Qnums* as std::map<*Qnum*, *Matrix*>. The returned std::map is a mapping from Qnum to a corresponding elements as a *Matrix* of the *UniTensor*. The order for iterating through all the *Qnum*'s blocks is defined by the smaller than sign "<" of *Qnum*.

## **Return Value**

A std::map of *Qnum* and *Matrix*, they are the quantum number and the block elements of the *UniTensor*.

# uni10::UniTensor::getBlock

Matrix getBlock(const Qnum& qnum, bool diag = false)const;

## Get specific block elements

Returns the block elements of specific quantum number *qnum* as a *Matrix*. If the *diag* flag is set, only the diagonal elements of the block will be picked out to a diagonal *Matrix*.

### **Parameters**

gnum: Qnum

The quantum number of the block to be retrieved.

diag: bool, optional(false)

A flag to specify whether the block elements are diagonal.

### **Return Value**

*Matrix* of the block elements of the quantum number *qnum*.

# uni10::UniTensor::putBlock

void putBlock(const Qnum& qnum, const Matrix& mat);

### Assign elements to specific block

Assigns elements of the given matrix *mat* to the specific block of quantum number *qnum*, replacing the origin elements. If the given matrix *mat* is diagonal, it sets all the elements to zero and assigns elements of *mat* to the diagonal elements of the block.

## **Parameters**

gnum: Qnum

The quantum number of the block which is being assigned elements to.

mat: Matrix

The matrix elements to be assigned to.

# uni10::UniTensor::elemNum

size t elemNum()const;

#### Access the number of elements.

Returns the number of total elements of the blocks.

### **Return Value**

The value of the number of elements.

# uni10::UniTensor::at

double at(std::vector<int>idxs)const;

### Access element.

Returns the element at position specified by the indices *idxs*. The given vector *idxs* is of size equal to the number of bonds, specifying the indices at each bond.

#### **Parameters**

idxs: std::vector<int>

An array of indices of the element in the *UniTensor*.

### **Return Value**

The element at indices idxs.

# uni10::UniTensor::operator[]

double& operator[](size\_t idx);

#### **Access element**

Returns the element at position *idx*. The position *idx* is counted by lining up all the elements in a sequence. The first bond's dimension is the most significant dimension.

### **Parameters**

idx: int

The position of the element in the *UniTensor*.

#### **Return Value**

The element at indices idx.

# uni10::UniTensor::rawElem

Matrix rawElem()const;

# Access non-block-diagonal elements

Returns the non-block-diagonal elements(raw elements) as a *Matrix*. The row(or column) bases of the elements are defined by the in-coming bonds(or out-going) bonds.

#### **Return Value**

The Matrix of the raw elements.

# uni10::UniTensor::printRawElem

void printRawElem()const;

## Print out raw elements

Prints out raw elements as(for example):

	2,0	1,0	0,0	1,0	0,0	-1,0	0,0	-1,0	-2 <b>,</b> 0
2 01	0 142	0 000	0 000	0 000	0 000	0 000	0 000	0 000	0.000
2,0  									
1,0	0.000	0.952	0.000	0.916	0.000	0.000	0.000	0.000	0.000
0,0	0.000	0.000	0.198	0.000	0.335	0.000	0.768	0.000	0.000
1,0	0.000	0.636	0.000	0.717	0.000	0.000	0.000	0.000	0.000
0,0	0.000	0.000	0.278	0.000	0.554	0.000	0.477	0.000	0.000
-1,0	0.000	0.000	0.000	0.000	0.000	0.394	0.000	0.783	0.000
0,0	0.000	0.000	0.629	0.000	0.365	0.000	0.513	0.000	0.000
-1,0	0.000	0.000	0.000	0.000	0.000	0.798	0.000	0.912	0.000
-2,0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.840

In the above example, the UniTensor has two in-coming bonds and two out-going bonds (see example egU1.cpp), with each bond having states with Qnums [q(1), q(0), q(-1)]. The resulting raw elements form a 9 by 9 Matrix. The first row shows the Qnums, U1 and parity, of the columns below and the first column shows the Qnums of the rows on the right.

# uni10::UniTensor::setName

void setName(const std::string& name);

## Assign name to the UniTensor

Assigns *name* to the UniTensor.

## **Parameters**

name: std::string

The string of the *name*.

# uni10::UniTensor::getName

std::string getName();

## Access name of the UniTensor

Return the name of the UniTensor.

# uni10::UniTensor::save

void save(const std::string& fname);

## Write the UniTensor out to file

Writes the UniTensor out to a file of path *fname*. To load in a tensor, use the constructor of *UniTensor*.

#### **Parameters**

fname: std::string

The path of the file.

# uni10::UniTensor::similar

bool similar(const UniTensor& Tb)const;

## Test whether the UniTensor is similar to input tensor Tb

Two tensors are said to be similar if the bonds of the two tensors are exactly the same.

#### **Parameters**

Tb: UniTensor

The *UniTensor* to be compared with.

#### **Return Value**

true if the UniTensor is similar to Tb, false otherwise.

# uni10::UniTensor::elemCmp

bool elemCmp(const UniTensor& Tb)const;

## Test whether the elements of the UniTensor are the same as in Tb

Compares the elements of the two tensors one by one. Returns true the all elements are the same.

## **Parameters**

uT: UniTensor

#### **Return Value**

true if the elements of the UniTensor is the same as in Tb, false otherwise.

# uni10::UniTensor::check

void check();

## Print out the memory usage of the existing UniTensor

Prints out the memory usage as(for example):

Existing Tensors: 30
Allocated Elem: 2240
Max Allocated Elem: 4295

Max Allocated Elem for a Tensor: 924

In the above example, currently there are 30 tensors and total number of existing elements is 2240. The maximum element number for now is 4295 and the maximum element number of a tensor is 924.

# uni10::UniTensor::permute

- (1) UniTensor& permute(int\* newLabels, int inBondNum);
- (2) UniTensor& permute(const std::vector<int>& newLabels, int inBondNum);

## Permute the order of bonds

Permutes the order of bonds to the order according to *newLabels*. *inBondNum* specifies the number of in-coming bonds after permuted. By doing so, all the elements are rearranged and the quantum numbers, shapes and even the number of the symmetry blocks may change. For example, default labels for a 4-bond *UniTensor* are [0, 1, 2, 3]. If we want to permute the order of the first two bonds, the *newLabels* are [1, 0, 2, 3].

#### **Parameters**

newLabels: int\*

int pointer pointing to the array of newLabels.

newLabels: std::vector<int>

std::vector of the array newLabels

inBondNum: int

The number of in-coming bonds to be for the permuted *UniTensor*.

#### **Return Value**

The reference of the permuted *UniTensor*.

# uni10::UniTensor::transpose()

UniTensor& transpose();

## **Transpose the block elements**

Transpose each block of various quantum numbers. The bonds are changed from in-coming to outcoming or vice versa without changing the quantum numbers on the bonds. That is, the bases of incoming and out-going are exchanged without any change on the basis itself.

## **Return Value**

The reference of the transposed *UniTensor*.

# uni10::UniTensor::combineBond

UniTensor& combineBond(const std::vector<int>& combined\_labels);

## Combine bonds together

Combines bonds of label in the array *combined\_labels*. The resulting bond has the same label and *bondType* as the bond of the first label in array *combined\_labels*.

## **Parameters**

combined labels: std::vector<int>

std::vector of the array labels of those bonds to be combined together.

#### **Return Value**

The reference of the *UniTensor* after combining bonds.

# uni10::UniTensor::partialTrace

UniTensor& partialTrace(int la, int lb);

#### Trace out two bonds

Traces out the two bond of label la and lb.

## **Parameters**

la, lb: int

The labels of the bonds to be traced out.

#### **Return Value**

The reference of the *UniTensor* after partial tracing two bonds.

## uni10::UniTensor::trace

double trace()const;

## Trace out in-coming bonds and out-going bonds

Traces out in-coming bonds and out-going bonds and returns the trace value.

#### **Return Value**

The trace value.

# uni10::UniTensor::set\_zero

- (1) void set\_zero();
- (2) void set\_zero(const Qnum& qnum);

## **Assign elements**

Set all the elements to zero(1). If *qnum* is given, set all the elements of the block with quantum number equal to *qnum* to zero.

## **Parameters**

qnum: Qnum

The quantum of the block to be set.

# uni10::UniTensor::eye

- (1) void eye();
- (2) void eye(const Qnum& qnum);

## **Assign elements**

Set all the block elements to identity(1). If *qnum* is given, set the block with quantum number equal to *qnum* to identity.

## **Parameters**

qnum: Qnum

The quantum of the block to be set.

## uni10::UniTensor::randomize

void randomize();

## **Assign elements**

Randomly assigns values to the elements.

# uni10::UniTensor::orthoRand

- (1) void orthoRand();
- (2) void orthoRand(const Qnum& gnum);

## **Assign elements**

Randomly generates orthogonal bases. Assigns to the elements of every block or the block with quantum number equal to *qnum*.

Let Nr = row() and Nc = col().

If the Nr < Nc, randomly generates Nr's orthogonal bases with each basis having dimension Nc, generating Nr's row-vectors of size Nc.

If the Nr > Nc, randomly generates Nc's orthogonal bases with each basis having dimension Nr, generating Nc's column-vectors of size Nr.

## **Parameters**

qnum: Qnum

The quantum of the block to be set.

# uni10::UniTensor::exSwap

std::vector<\_Swap> exSwap(const UniTensor& Tb)const;

## **Record swaps**

In fermionic system, the operation of Ta \* Tb != Tb \* Ta. It's not because of compatibility of *Ta* and *Tb*, but it is come from the swap signs of fermionic operators in *Ta* and *Tb*. This function is to record the swaps of the bonds in the *UniTensor* when exchanging the operation order with the *UniTensor Tb*. Returns the array for swaps of the bonds. For adding fermionic swap signs, see function *addGate*().

#### **Parameters**

Tb: UniTensor

The tensor to exchange with.

## **Return Value**

The array of the swaps of the bonds.

# uni10::UniTensor::addGate

void addGate(std::vector<\_Swap> swaps);

## Add swap gate

Adds swap gate when the order of two bonds are swapped in fermionic system. The meaning of adding swap gate is to multiply the corresponding elements by -1.

## **Parameters**

swaps: std::vector<\_Swap>

The swaps of the bonds.

# uni10::UniTensor::operator\*=

- (1) UniTensor& operator\*= (UniTensor& Tb);
- (2) UniTensor& operator\*= (double a)

## **Perform multiplication**

- (1) Performs tensor contraction with another *UniTensor Tb*. It contracts out the bonds of the same labels in the *UniTensor* and *Tb*
- (2) Performs element-wise multiplication with a scalar a of type double.

## **Parameters**

Tb: UniTensor

The given tensor to multiplied with.

a: double

The scalar of type *double* to multiplied with.

## **Return Value**

The reference of the resulting *UniTensor*.

# uni10::UniTensor::operator+=

UniTensor& operator+= (const UniTensor& Tb);

## Perform additions of elements

Performs element by element addition. The tensor *Tb* to be added must be similar to the *UniTensor*. See *UniTensor::similar()* 

## **Parameters**

Tb: UniTensor

The given tensor to add.

## **Return Value**

The reference of the resulting *UniTensor*.

## non-member overloads:

## contract

friend UniTensor contract(UniTensor & Ta, UniTensor & Tb, bool fast = false);

# Perform multiplication

Performs tensor contraction of Ta and Tb. It contracts out the bonds of the same labels in *Ta* and *Tb*. Note that compared with *operator\** (*Ta\* Tb*), It performs contraction without copying *Ta* and *Tb*. Thus it uses less memory. When the flag *fast* is set true, the two tensors *Ta* and *Tb* are contracted without being permuted back to origin labels.

## **Parameters**

Ta, Tb: UniTensor

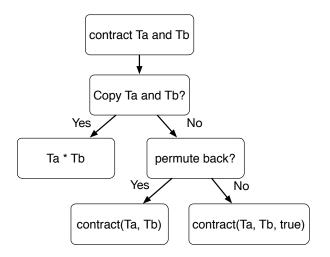
The tensors to carry out contractions.

fast: bool, optional(false)

A flag to decide whether two tensors are permuted back to origin labels. If true, two tensor are not permuted back.

## **Return Value**

Resulting UniTensor.



## outer

friend UniTensor outer(const UniTensor& Ta, const UniTensor& Tb);

# **Perform multiplication**

Performs outer product of Ta and Tb.

Ta, Tb: UniTensor

The tensors to carry out contractions.

# Ta : Tb

## **Return Value**

Resulting UniTensor.

# operator\*

- (1) friend UniTensor operator\* (UniTensor& Ta, UniTensor& Tb);
- (2) friend UniTensor operator\* (const UniTensor& Ta, double a);
- (3) friend UniTensor operator\* (double a, const UniTensor& Ta)

## **Perform multiplication**

- (1) Performs tensor contraction, Ta \* Tb. It contracts out the bonds of the same labels in *Ta* and *Tb*. It copies *Ta* and *Tb* and then call function *contract* to perform the contraction.
- (2)&(3) Performs element-wise multiplication with a scalar a of type double, a \* Ta or Ta \* a.

#### **Parameters**

Ta, Tb: UniTensor

The tensors to carry out contractions.

a: double

The scalar of type double to multiplied with.

## **Return Value**

Resulting UniTensor.

# operator+

friend UniTensor operator+ (const UniTensor& Ta, const UniTensor& Tb);

## Perform additions of elements

Performs element by element addition.

## **Parameters**

Ta, Tb: UniTensor

The tensors to carry out contractions

## **Return Value**

Resulting UniTensor.

# operator<<

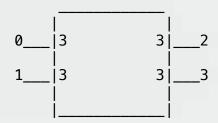
friend std::ostream& operator<< (std::ostream& os, const UniTensor& uT);

#### **Print out UniTensor**

Prints out a *UniTensor* as(for example):

std::cout << uT;

\*\*\*\*\*\*\*\*\*\* Demo \*\*\*\*\*\*\*\*\*\*



=========BONDS===========

IN: 
$$(U1 = 1, P = 0, 0) | 1$$
,  $(U1 = 0, P = 0, 0) | 1$ ,  $(U1 = -1, P = 0, 0) | 1$ ,  $Dim = 3$  IN:  $(U1 = 1, P = 0, 0) | 1$ ,  $(U1 = 0, P = 0, 0) | 1$ ,  $(U1 = -1, P = 0, 0) | 1$ ,  $Dim = 3$  OUT:  $(U1 = 1, P = 0, 0) | 1$ ,  $(U1 = 0, P = 0, 0) | 1$ ,  $(U1 = -1, P = 0, 0) | 1$ ,  $Dim = 3$  OUT:  $(U1 = 1, P = 0, 0) | 1$ ,  $(U1 = 0, P = 0, 0) | 1$ ,  $(U1 = -1, P = 0, 0) | 1$ ,  $Dim = 3$ 

0.840

--- (U1 = -1, 
$$P = 0$$
,  $0$ ):  $2 \times 2 = 4$ 

0.394 0.783

--- (U1 = 0, 
$$P = 0$$
, 0):  $3 \times 3 = 9$ 

0.198 0.335 0.768

0.629 0.365 0.513

--- (U1 = 1, 
$$P = 0$$
,  $0$ ):  $2 \times 2 = 4$ 

0.952 0.916

0.636 0.717

--- (U1 = 2, 
$$P = 0$$
, 0): 1 x 1 = 1

0.142

Total elemNum: 19

In the above example, uT has four bonds with default labels [0, 1, 2, 3]. The bonds 0 and 1 are incoming bonds. and the 2, 3 are out-going bonds. Each bond has dimension three and the three states corresponding to three U1 quantum number [-1, 0, 1]. The following are the block elements of the tensor. There are five blocks of various U1 [-2, -1, 0, 1, 2] and various sizes. The total element number is 19.

## **Parameters**

os: std::ostream

ostream in standard library, see http://www.cplusplus.com/reference/ostream/ostream/?

kw=ostream
uT: UniTensor

The *UniTensor* to be printed out.

double heisenberg s1[] = \

{1, 0, 0, 0, 0, 0, 0, 0, 0, \ 0, 0, 0, 1, 0, 0, 0, 0, \

#### **Return Value**

Returns std::ostream&

# Example: egU1

7)

9)

```
source: http://uni10.org/examples/egU1.cpp
1) #include <iostream>
2) #include <uni10.hpp>
3)
4) int main(){
5)  // Construct spin 1 Heisenberg model
6)  // Raw element
```

```
qnums.push_back(q0);
qnums.push_back(q0);
qnums.push_back(q0);
// Create in-coming and out-going bonds, without any symmetry.
```

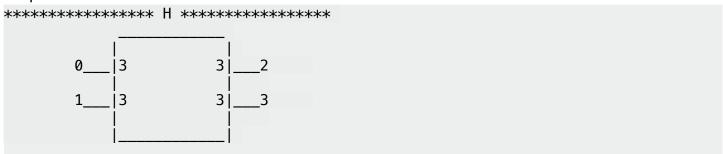
```
uni10::Bond bd_in(uni10::BD_IN, qnums);
uni10::Bond bd_out(uni10::BD_OUT, qnums);
std::vector<uni10::Bond> bonds;
```

29) bonds.push\_back(bd\_in);
30) bonds.push\_back(bd\_in);

bonds.push\_back(bd\_out);

```
32) bonds.push back(bd out);
33) // Create tensor from the bonds and name it "H".
34) uni10::UniTensor H(bonds, "H");
35) H.addRawElem(heisenberg s1);
36) std::cout<< H;</pre>
37)
39) // Since it has U1 symmetry(total Sz conserved)
40) // add U1 quantum number to the states of bonds.
41) uni10::Qnum q1(1);
42) uni10::Qnum q_1(-1);
43) gnums.clear():
44) gnums.push back(q1);
45) qnums.push_back(q0);
46) gnums.push back(q 1);
47)
48) // Create in-coming and out-going bonds
49) bd in.assign(uni10::BD IN, gnums);
50) bd_out.assign(uni10::BD_OUT, qnums);
51) bonds.clear();
52) bonds.push_back(bd_in);
53) bonds.push back(bd in);
54) bonds push_back(bd_out);
55) bonds.push back(bd out);
56)
57) // Create tensor from the bonds and name it "H_U1".
58) uni10::UniTensor H U1(bonds, "H U1");
59) // Add raw elements to tensor
60) H U1.addRawElem(heisenberg s1);
61) std::cout<< H_U1;</pre>
62)
63) // Check the quantum number of the blocks
64) std::cout<<"The number of the blocks = "<< H_U1.blockNum()<<std::endl;
65) std::vector<uni10::Qnum> block gnums = H U1.blockQnum();
66) for(int q = 0; q < block qnums.size(); q++)
        std::cout<< block_qnums[q]<<", ";</pre>
67)
68) std::cout<<std::endl<<std::endl;</pre>
69) // print out non-block diagonal elements, raw elements
70) H U1.printRawElem();
71)
72) // Write out tensor
73) H_U1.save("egU1_H_U1");
74) return 0;
75)}
```

#### Output:



```
========B0NDS=========
IN: (U1 = 0, P = 0, 0)|3, Dim = 3
IN: (U1 = 0, P = 0, 0) | 3, Dim = 3
OUT: (U1 = 0, P = 0, 0)|3, Dim = 3
OUT: (U1 = 0, P = 0, 0) | 3, Dim = 3
=========BL0CKS==========
--- (U1 = 0, P = 0, 0): 9 \times 9 = 81
  1.000 0.000 0.000 0.000 0.000
                                  0.000 0.000 0.000 0.000
  0.000
       0.000
             0.000
                     1.000
                           0.000
                                  0.000
                                         0.000
                                                0.000
                                                      0.000
 0.000
        0.000 - 1.000
                    0.000
                           1.000
                                  0.000
                                         0.000
                                                0.000
                                                      0.000
  0.000
       1.000 0.000
                     0.000
                           0.000
                                  0.000
                                         0.000
                                               0.000
                                                      0.000
  0.000
        0.000
              1.000
                    0.000
                           0.000
                                  0.000
                                         1.000
                                                0.000
                                                      0.000
  0.000
        0.000
              0.000
                    0.000
                           0.000
                                  0.000 0.000
                                               1.000
                                                      0.000
 0.000
       0.000 0.000 0.000
                           1.000
                                  0.000 - 1.000
                                               0.000
                                                      0.000
  0.000 0.000 0.000
                    0.000
                           0.000
                                  1.000 0.000
                                                0.000
                                                      0.000
        0.000 0.000 0.000 0.000 0.000 0.000
  0.000
                                                0.000
                                                     1.000
Total elemNum: 81
************ END **********
*********** H U1 *********
           |3
                           2
                      3|
=======B0NDS=========
IN: (U1 = 1, P = 0, 0)|1, (U1 = 0, P = 0, 0)|1, (U1 = -1, P = 0, 0)|1, Dim = 3
IN: (U1 = 1, P = 0, 0)|1, (U1 = 0, P = 0, 0)|1, (U1 = -1, P = 0, 0)|1, Dim = 3
OUT: (U1 = 1, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = -1, P = 0, 0) | 1, Dim = 3
OUT: (U1 = 1, P = 0, 0)|1, (U1 = 0, P = 0, 0)|1, (U1 = -1, P = 0, 0)|1, Dim = 3
=========BL0CKS==========
--- (U1 = -2, P = 0, 0): 1 \times 1 = 1
 1.000
--- (U1 = -1, P = 0, 0): 2 x 2 = 4
  0.000 1.000
```

# Example: egU2

```
source: http://uni10.org/examples/egU2.cpp
```

```
1) #include <iostream>
2) #include <uni10.hpp>
3)
4) int main(){
   // Construct spin 1 Heisenberg model by reading in the tensor which is
    written out in example egU1
6)
    uni10::UniTensor H U1("eqU1 H U1");
7)
    // Get the block of quantum number q0 as a matrix "block0"
9)
    uni10::Qnum q0(0);
10) uni10::Matrix block0 = H_U1.getBlock(q0);
11) std::cout<<block0;</pre>
12) // Randomly assign "block0" and put it back to H U1
13) block0.randomize();
14) H_U1.putBlock(q0, block0);
15) //std::cout<<H_U1;</pre>
16)
17) // Permute bonds by its label, the default label of it is [0 1 2 3]
18) int permuted_label[] = {1, 2, 3, 0};
19) // Permute bonds to which with label [1, 2, 3, 0] and leaving 1 bond as in-
    coming bonds.
```

```
20) H U1.permute(permuted label, 1);
21) //std::cout<<H_U1;</pre>
22)
23) // Permute bonds by its label.
24) std::vector<int> combined_label;
25) combined label.push back(2);
26) combined_label.push_back(3); // combined_label = [2, 3]
27) // combine the two bonds with label 2 and 3
28) H U1.combineBond(combined label);
29) std::cout<< H_U1;</pre>
31) return 0;
32)}
Output:
3 \times 3 = 9
    -1.000 1.000 0.000
        1.000 0.000 1.000
        0.000 1.000 -1.000
******* eqU1 H U1 ********
                                                                                                                              2
========B0NDS==========
IN: (U1 = 1, P = 0, 0)|1, (U1 = 0, P = 0, 0)|1, (U1 = -1, P = 0, 0)|1, Dim = 3
OUT: (U1 = 2, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1,
= 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = -1, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 0, P = 0
= -1, P = 0, 0) | 1, (U1 = -2, P = 0, 0) | 1, Dim = 9
OUT: (U1 = -1, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, Dim = 3
=======BL0CKS=========
--- (U1 = -1, P = 0, 0): 1 x 6 = 6
        0.840 0.394 0.000 0.783 1.000 1.000
--- (U1 = 0, P = 0, 0): 1 x 7 = 7
         0.000 0.798 1.000 0.912 1.000 0.198 0.000
--- (U1 = 1, P = 0, 0): 1 x 6 = 6
         1.000 1.000 0.335 0.000 0.768 0.278
Total elemNum: 19
```

# Example: egU3

```
source: http://uni10.org/examples/egU3.cpp
```

```
1) #include <iostream>
2) #include <uni10.hpp>
3)
4) int main(){
5)
    // Construct spin 1 Heisenberg model by reading in the tensor which is
    written out in example eqU1
6)
    uni10::UniTensor H_U1("egU1_H_U1");
7)
    // Randomly create an isometry tensor
8)
9)
    uni10::0num q0(0);
10) uni10::Qnum q1(1);
11) uni10::Qnum q_1(-1);
12) uni10::Qnum q2(2);
13) uni10::Qnum q_2(-2);
14) std::vector<uni10::Qnum> in gnums;
15) in_qnums.push_back(q2);
16) in_qnums.push_back(q1);
17) in_qnums.push_back(q0);
18) in_qnums.push_back(q0);
19) in gnums.push back(q 1);
20) in gnums.push back(q 2);
21) std::vector<uni10::Qnum> out_qnums;
22) out_qnums.push_back(q1);
23) out_qnums.push_back(q0);
24) out_qnums.push_back(q_1);
25) uni10::Bond bd_in(uni10::BD_IN, in_qnums);
26) uni10::Bond bd_out(uni10::BD_OUT, out_gnums);
27) std::vector<uni10::Bond> bonds;
28) bonds.push_back(bd_in);
29) bonds.push_back(bd_out);
30) bonds.push_back(bd_out);
31) // Create isometry tensor W and transposed WT
```

```
32) uni10::UniTensor W(bonds, "W");
33) W.orthoRand();
34) uni10::UniTensor WT = W;
35) WT.transpose();
37) // Operate W and WT on H_U1, see the contraction labels in the documentation.
38) int label_H[] = {1, 2, 3, 4};
39) int label_W[] = \{-1, 1, 2\};
40) int label_WT[] = \{3, 4, -2\};
41) H_U1.addLabel(label_H);
42) W.addLabel(label_W);
                                                                         2
43) WT.addLabel(label WT);
44) //std::cout<<W;
45) std::cout<<W * H_U1 * WT;</pre>
                                                                  H U1
46)
47) // Write the tensors W and WT out to file
48) W.save("egU3_W");
49) WT.save("egU3 WT");
50)
51) // Check the memory usage.
52) uni10::UniTensor::check();
53)
54) return 0;
55)}
```

## Output:

```
***********
                                                                                                                                                                                                        6 | _____ – 2
 ========B0NDS==========
IN: (U1 = 2, P = 0, 0)|1, (U1 = 1, P = 0, 0)|1, (U1 = 0, P = 0, 0)|2, (U1 = -1, P = 0, 0)|1, (U1 = 0, P = 0,
 P = 0, 0) | 1, (U1 = -2, P = 0, 0) | 1, Dim = 6
OUT: (U1 = 2, P = 0, 0) | 1, (U1 = 1, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 2, (U1 = -1, P = 0, 0) | 1, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2, (U1 = 0, P = 0, 0) | 2
P = 0, 0) | 1, (U1 = -2, P = 0, 0) | 1, Dim = 6
========BL0CKS=========
--- (U1 = -2, P = 0, 0): 1 \times 1 = 1
                 1.000
 --- (U1 = -1, P = 0, 0): 1 \times 1 = 1
               0.803
--- (U1 = 0, P = 0, 0): 2 x 2 = 4
        -0.264 - 0.427
        -0.427 - 1.164
 --- (U1 = 1, P = 0, 0): 1 \times 1 = 1
```

0.989

--- (U1 = 2, P = 0, 0): 1 x 1 = 1

1.000

Total elemNum: 8

Existing Tensors: 3
Allocated Elem: 43
Max Allocated Elem: 98

Max Allocated Elem for a Tensor: 19

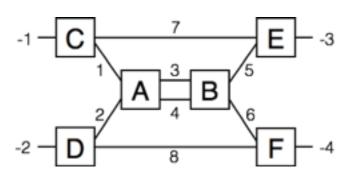
# Class uni10::Network

#### **Tensor Network**

Class *Network* is made for contractions of a whole tensor network. Left figure is an example of tensor network. Each blocks are tensors(in this library *UniTensor*) and tensors are connect together by the bonds(lines) of the same labels. Network is comprised by the connections which is specified by the labels. To construct a network, you have to prepare a file on the left, specifying the labels of the tensors and the out-coming labels of the tensor "TOUT:". Note that

"TOUT" line is necessary in the file. Even if the out-coming tensor having no bond, that is a scalar, you still need to keep the line as "TOUT: ", without any label. Labels are separated by blank or comma and in-coming and out-going labels are divided by semi-colon. The last line, starting from "ORDER: " is optional. It suggests the order to construct the pair-wise contraction order and furthermore you can force the contraction order by the parentheses as(for example):

ORDER: ((((A B) C) E) (D F))



A: 1 2; 3 4
B: 3 4; 5 6
C: -1; 7 1
D: -2; 2 8
E: 7 5; -3
F: 6 8 -4
TOUT: -1 -2; -3 -4
ORDER: A B C E D F

To use a network, one can use the method putTensor() to put tensor to the specific place in the network. After placing all the tensors to the right places. Call the function launch() to contract out all the bonds in between. When the function launch() will generate a contraction order or follow the contraction order if given, carry out the pair-wise contraction. Note that, in fermionic system, even though the labels of contractions are specified, A \* B != B \* A. It is because the swap signs that come from the swapping of the fermionic operators in A and B. The function launch guarantees that no matter what contraction order of the tensors, the resulting tensor is the same as the tensors are contracted by the order when the labels are given in the first few lines. In our example, launch() guarantees the result A \* B \* C \* D \* E \* F.

# member functions

# uni10::Network::Network

- (1) Network(const std::string& fname);
- (2) Network(const std::string& fname, const std::vector<UniTensor\*>& uTptrs);

#### **Construct UniTensor**

Constructs a Network, initializing depending on the constructor version used:

(1) Constructs with the file *fname*. The file specifies the connections between tensors in the network. See more in the introduction of *Network* above.

(2) Constructs with the file *fname* as (1) and also put those *UniTensor* into the right position in the network. The given array of tensor pointers is in the same order of those tensors specified in the network file *fname*.

#### **Parameters**

fname: std::string

Path of the network file.

uTptrs: std::vector<UniTensor\*>

Array of *UniTensor* pointers to put into the network.

# uni10::Network::~Network

~Network();

#### **Destruct Network**

Destroys the Network and freeing all the intermediate tensors.

# uni10::Network::putTensor

- (1) void putTensor(int idx, const UniTensor\* uTptr, bool force=false);
- (2) void putTensor(std::string tname, const UniTensor\* uTptr, bool force=false);

## **Assign tensor to the Network**

- (1) Assigns the tensor uT to the position idx in the network. The order of the position is given in the network file. For the example on the right side, to put tensor uT to the network at position "C", use putTensor(2, uTptr).
- (2) Assigns the tensor uT to the position of the tensor *tname* in the network file. To put tensor uT to the network at position "C", use *putTensor*("C", *uTptr*).

If the force flag is set, the tensor will be put in the network without reconstructing the pair-wise contraction sequence.

A: 1 2; 3 4
B: 3 4; 5 6
C: -1; 7 1
D: -2; 2 8
E: 7 5; -3
F: 6 8 -4
TOUT: -1 -2; -3 -4
ORDER: A B C E D F

## **Parameters**

idx: int

The position in the network at which the tensor uT is placed.

tname: std::string

The name of the tensor in the network file fname. It specifies the position where the tensor uT is put to the network.

uTptr: UniTensor\*

The pointer of the tensor to be added in the network.

force: bool, optional(false)

If false, the contraction sequence will be reconstructed after putting the tensor. If true, contraction sequence remains the same, only the tensor at position idx is replaced with uT.

# uni10::Network::launch

UniTensor launch(const std::string& name="");

## **Contract the tensors in the Network**

Performs contractions of the tensors in the network, returns the out-coming *UniTensor* and naming it as *name*.

## **Parameters**

name: std::string, optional("")

The name for the out-coming *UniTensor*.

## non-member overloads

# operator<<

friend std::ostream& operator<< (std::ostream& os, Network& net);

## **Print out Network**

Before the calling the function *net.launch*()

Prints out the *Network* coming from the example network

file on the right:

```
std::cout << net;
```

```
W1: i[-1] o[0, 1, 3]
W2: i[-2] o[7, 10, 11]
U: i[3, 7] o[4, 8]
Ob: i[1, 4] o[2, 5]
UT: i[5, 8] o[6, 9]
W1T: i[0, 2, 6] o[-3]
W2T: i[9, 10, 11] o[-4]
Rho: i[-3, -4] o[-1, -2]
TOUT:
```

```
W1: -1; 0 1 3

W2: -2; 7 10 11

U: 3 7; 4 8

Ob: 1 4; 2 5

UT: 5 8; 6 9

W1T: 0 2 6; -3

W2T: 9 10 11; -4

Rho: -3 -4; -1 -2

TOUT:

ORDER: W1 W1T W2 W2T U Ob UT Rho
```

The above is the connections of every tensors from the

network file. "i" means labels for in-coming bonds and "o" for out-going.

After we call the function *net.launch*(), besides printing out the connections between tensors above, the contraction sequence, or binary tree of the pair-wise contractions is also printed as:

The output shows clearly how the whole network is contracted. For example, *U* and *Ob* are contracted as the intermediate tensor with labels [3, 7, 8, 1, 2, 5] and element number 20. And the resulting tensor then contracts with *UT* and so on.

## **Parameters**

os: std::ostream

ostream in standard library, see http://www.cplusplus.com/reference/ostream/ostream/?

kw=ostream

net: Network

The Network to be printed out.

## **Return Value**

Returns std::ostream&

# Example: egN1

```
network file: <a href="http://uni10.org/examples/eqN1">http://uni10.org/examples/eqN1</a> network
H: 1 2; 3 4
W: -1; 1 2
WT: 3 4; -2
TOUT: -1; -2
ORDER: ((W H) WT)
                                                                                   H U1
source: http://uni10.org/examples/egN1.cpp
56)#include <iostream>
                                                                                 3
57)#include <uni10.hpp>
58)
59)int main(){
60) // Read in the tensor H_U1 which is written out in example egU1
     and W, WT in example eqU3
61) uni10::UniTensor H_U1("egU1_H_U1");
62) uni10::UniTensor W("eqU3 W");
63) uni10::UniTensor WT("egU3_WT");
64)
```

```
// Create network by reading in network file "egN1_network"
in uni10::Network net("egN1_network");
// Put tensors to the Network net
net.putTensor("H", &H_U1);
net.putTensor("W", &W);
net.putTensor("WT", &WT);
// Perform contractions inside the tensor network
std::cout<<net.launch();
// Print out the network
std::cout<<net;
// return 0;
// return 0;</pre>
```

#### Output:

\*\*\*\*\*\*\*\*\*\*\*



--- (U1 = -2, P = 0, 0):  $1 \times 1 = 1$ 

1.000

--- (U1 = -1, 
$$P = 0$$
,  $0$ ):  $1 \times 1 = 1$ 

0.803

$$---$$
 (U1 = 0, P = 0, 0): 2 x 2 = 4

-0.264 - 0.427

-0.427 -1.164

--- (U1 = 1, 
$$P = 0$$
,  $0$ ):  $1 \times 1 = 1$ 

0.989

--- (U1 = 2, 
$$P = 0$$
, 0): 1 x 1 = 1

1.000

Total elemNum: 8

```
H: i[1, 2] o[3, 4]
W: i[-1] o[1, 2]
WT: i[3, 4] o[-2]
TOUT: i[-1] o[-2]

*(8): -1, -2,

| *(12): -1, 3, 4,

| | W(12): -1, 1, 2,

| | H(19): 1, 2, 3, 4,

| WT(12): 3, 4, -2,
```