The openMMF library: open source software for multimode driven quantum systems

User manual

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Contents

1	Introduction	1
2	How to build the library and compile the examples	1
3	What does the library calculate and how?	2
4	Use of the library 4.1 Declaration of the Hamiltonian	3 3 4 4 5 5 5
5	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	6 6 6 7
6	C++ wrappers	7
7	Python wrappers	7
8	Bugs and known limitations	8
9	Acknowledgements	8
10	MODULES 10.1 Physical Constants	9 9 9 9
11	DERIVED TYPES (src/modes.f90)	11
12	COMPUTATIONAL SUBROUTINES	11
13	DRIVER SUBROUTINES 13.1 Utility subroutines	17 20
	Python Wrappers prototypes 14.1 Initialisation	23

1 Introduction

2 How to build the library and compile the examples

The openMMF source code includes a Makefilefile for compiling and building the library. The user must ensure that the system's path to the LAPACK and (optionally) the MKL-intel libraries can be found by the Makefile script.

When the paths are set correctly, compiling the library requires invoking a single make command with the following options:

- make lib: compiles the library including support for sparse matrices. This option requires the LAPACK and MKL-intel libraries.
- make lib_lapack: compiles the library without support for sparse matrices. This option requires LAPACK.
- make all_examples: complies all examples under the folders examples/CPP and examples/FORTRAN.
- make: run the options lib and all_examples.

All options of the make command produces the static library libopenmmf saving it in the folder ~/lib. A number of .mod files produced with the building process are moved to the folder ~/include and they are required for running the application.

The Fortran examples that only require the support of the LAPACK library are compiled with:

gfortran -o out SourceCode.f90 -I\$(INCLUDE_OPENMMF) -L\$(LIB_OPENMMF) -lopenmmf \$(GFFLAGS) while code that requires support from the MKL library is compiled by:

```
gfortran -o out SourceCode.f90 -I$(INCLUDE_OPENMMF) -L$(LIB_OPENMMF) -lopenmmf -L$(MKLLIBS) -I$(MKLINC) $(GFFLAGS_SP) $(MKLFLAGS)
```

The variables MKLLIBS, MKLINC, GFFLAGS, GFFLAGS_SP and MKLFLAGS are defined in the file Makefile. The environmental variables INCLUDE_OPENMMF and LIB_OPENMMF indicate the paths to the include and library directories of the openMMF library. Compilation of C++ source code follows the same formula, using the additional flag -lgfortram and the corresponding compiler g++. For an explicit example of usage in this case see the building script under examples/CPP/Makefile.

When running applications that use the MKL-intel library, the environmental variable LD_LIBRARY_PATH must indicate the path to such a library, which can be done with the shell command:

export LD_LIBRARY_PATH="/opt/intel/compilers_and_libraries_2017/linux/mkl/lib/intel64

which assumes that the library is installed in the default folder corresponding to the MKL version installed in the system.

3 What does the library calculate and how?

The library can be used to calculate the time-evolution operator, U(t',t), t' > t, of systems whose Hamiltonian has the form:

$$H = \sum_{i,j}^{D} E_{i,j} |i\rangle \langle j| + \sum_{i,j}^{D} \sum_{\ell=1}^{N} \sum_{n \in \mathbb{Z}} V_{i,j}^{\ell,n} e^{in\omega_{\ell}t} |i\rangle \langle j| + \text{h.c.}$$

$$\tag{1}$$

where D is the dimension of the Hilbert space, $E_{i,j}$ defines a static component of H, $V_{i,j}^{\ell,n}$ is the coupling between the states i and j oscillating at frequency $n\omega_{\ell}$ (i.e. the n-th harmonic of the ℓ -th fundamental frequency ω_{ℓ}) and N is the number of incommensurate frequencies.

To calculate the time-evolution operator we generalise the Rotating (or Resonant) Wave Approximation (RWA), taking into account the complex time dependence of Eq. (1). For this, we rephrase the problem in terms of building a time-dependent unitary transformation, $U_F(t)$ to a new basis $\{|\bar{i}\rangle\}$, that leads to a time-independent and diagonal Hamiltonian, \bar{H} . The operator $U_F(t)$ is called the micromotion operator and the new basis is a generalised multimode definition of the dressed basis. After applying the standard quantum-mechanical transformation rule to the Schrödinger equation [?, ?], this condition becomes:

$$U_F^{\dagger}(t) \left[H(t) - i\hbar \partial_t \right] U_F(t) = \sum_{\bar{i}} \bar{E}_{\bar{i}} \left| \bar{i} \right\rangle \left\langle \bar{i} \right| \tag{2}$$

where $\bar{E}_{\bar{i}}$ is the eigen-energy of the dressed state $|\bar{i}\rangle$, which is an eigenstate of the static Hamiltonian \bar{H} .

Importantly, in the basis of states defined by this transformation the time evolution operator is diagonal and has the form:

$$\bar{U}(t',t) = \sum_{\bar{i}} e^{-i\bar{E}_{\bar{i}}(t'-t)} |\bar{i}\rangle \langle \bar{i}|$$
(3)

which let us to calculate the time evolution operator in the original basis $\{|i\rangle\}$, just by inverting the transformation $U_F(t)$, according to [?]:

$$U(t',t) = U_F(t')\bar{U}(t',t)U_F(t) \tag{4}$$

To formulate a fully defined computational problem, we express the unitary transformation $U_F(t)$ as the multifrequency Fourier series [?]:

$$U_F(t) = \sum_{\vec{i}} U_{i,\vec{i}}^{\vec{n}} e^{-i\vec{\omega}\cdot\vec{n}t} |i\rangle \langle \bar{i}|$$
 (5)

where $\vec{\omega} = (\omega_1, \omega_2, \dots, \omega_N)$ and \vec{n} is a N-dimensional vector of integers. After plugging this expansion in Eq. (2) and performing an integral over time, we obtain a fully defined eigenproblem for the eigenvalues $\bar{E}_{\bar{i}}$ and Fourier components of the unitary transformation $U_{i.\bar{E}}^{\vec{n}}$:

$$\sum_{j} (E_{i,j} - \hbar \vec{n} \cdot \vec{\omega}) U_{j,\bar{i}}^{\vec{n}} + \sum_{j} \sum_{\vec{m}} \left[V_{i,j}^{\vec{m}} U_{j,\bar{i}}^{\vec{n}+\vec{m}} + V_{ji}^{\vec{m}*} U_{j,\bar{i}}^{\vec{m}-\vec{n}} \right] = \bar{E}_{\bar{i}} U_{i,\bar{i}}^{\vec{n}}$$
(6)

where $\vec{n}_{\ell,m} = \vec{n} + mP_{\ell}$ with $P_{\ell} = (0, \dots, 1, \dots, 0)$ the projector at the ℓ -th position. To obtain a finite matrix representation of this problem we truncate the sum over the number of modes of the Fourier expansion Eq. (5).

This formulation to calculate the time-evolution operator is equivalent to the multimode Floquet representation of the Hamiltonian that introduces an extended Hilbert space $|E_i, \vec{n}\rangle$ [?, ?]. However, the semiclassical description presented here makes emphasis in the physically accessible states.

4 Use of the library

Here we illustrate the use of the library's functionality considering a qubit driven by two harmonic forces. The Hamiltonian of this system has the form:

$$H = \hbar\omega_0 S_z + \hbar\Omega_1 \cos(\omega_1 t) S_x + \hbar\Omega_{2,x} \cos(\omega_2 t) S_x + \hbar\Omega_{2,y} \cos(\omega_2 t) S_z \tag{7}$$

The Fortran and C++ source codes to find the time-evolution operator are in the files:

- examples/FORTRAN/main_DressedQubit.f90 .
- examples/CPP/main_dressedqubit.cpp .

4.1 Declaration of the Hamiltonian

First of all, we should declare the two derived types:

```
TYPE(ATOM) ID
TYPE(MODE), DIMENSION(:), ALLOCATABLE :: FIELDS
```

The variable ID contains information about the type of system, such as the number of levels and their energy spectrum (see the declaration of TYPE(ATOM) in Section 11). The derived type FIELDS stores information required to build the components of the Hamiltonian as well as the explicit matrix representation of the couplings.

In this concrete example, the components of ID are initialised by calling the subroutine:

```
CALL FLOQUETINIT(ID, 'qubit', INFO)
```

The second argument indicates the type of system (here 'qubit'), which, is sufficient to initialise the variable ID :

```
ID%id_system = 1
ID%D_BARE = 2
```

where ID%D_BARE indicates the dimension of the Hilbert space.

Additional options of the function FLOQUETINIT are presented in section 5, which are useful for initialising some frequently used physical systems with default parameters. When dealing with a general quantum system (i.e. with an arbitrary energy spectrum), there is no need to call this function and the values of a variable of TYPE(ATOM) must be initialised explicitly.

In the source code, the next relevant instruction is the definition of an integer vector that provides information about the number of driving frequencies. The integer array MODES_NUM is allocated with size 3, indicating that the system will be driven by two fundamental frequencies (corresponding to $\ell=1,2$ in Eq. 1), since the first component is reserved to the static part of the Hamiltonian. The values of the elements of this array indicate the number of driving harmonics of each frequency, which here we set to 1 (making n=1 in Eq. 1).

The total number of driving frequencies is equal to the sum of all elements of the array MODES_NUM. The user then should allocate sufficient memory space to store each one of the matrix representations of the couplings $V^{\ell,n}$. This is done with the sequence of instructions:

```
TOTAL_FREQUENCIES = SUM(MODES_NUM,1)
ALLOCATE(FIELDS(TOTAL_FREQUENCIES))
DO m=1,TOTAL_FREQUENCIES
   ALLOCATE(FIELDS(m)%V(ID%D_BARE,ID%D_BARE))
END DO
```

By default the first element of the array of FIELDS is reserved for the static component of the Hamiltonian, which includes the spectrum of the static system as diagonal elements of the matrix FILEDS(1)%V. The next step then consist in defining all components of the Hamiltonian. For a quantum system with arbitrary energy spectrum, each one of the matrices FIELDS(m)%V must be declared explicitly.

When dealing with spin systems, as in the present example, each component of the Hamiltonian can be written as:

$$V^{\ell,n} = e^{\phi_x} X S_x + e^{\phi_y} Y S_y + e^{\phi_z} Z S_z \tag{8}$$

where S_i is the angular momentum operator. Therefore, we need only six parameters (three phases and three amplitudes) to define the coupling matrices.

These six parameters should be declared explicitly for each one of the the driving modes, along with the frequency (omega) and the corresponding number of modes to be included in the Fourier expansion of the evolution operator (N_Floquet). The values of these parameters are initialised as follows:

Source code	Parameter in Eq. (8)
FIELDS(1)%X=0.0	X
FIELDS(1)%Y=0.0	Y
FIELDS(1)%Z=1.0	Z
FIELDS(1)%phi_x=0.0	ϕ_z
FIELDS(1)%phi_y=0.0	ϕ_z
FIELDS(1)%phi_z=0.0	ϕ_z
FIELDS(1)%omega=0.0	ω
FIELDS(1)%N_Floquet= 0	N

where we have a direct correspondence with Eq. (8). This set of instructions is repeated for each one of the driving fields, as can be seen in the source code.

4.2 Hamiltonian components

The instructions detailed before let us to build the matrix representation of the terms in Eq. (8). This is done simply by calling the subroutine:

CALL SETHAMILTONIANCOMPONENTS(ID, size(modes_num, 1), total_frequencies, MODES_NUM, FIELDS, INFO)

which results in storing the coupling $V^{\ell,n}$ in the set of matrices FIELDS(r)%V, with r=1,total_frequencies.

We remind the user that when the system of interest is not one of the default types defined in section 4.1, the user must define explicitly and in full all the coupling matrices. For an example of this situation, see the source file example/FORTRAN/main_lattice.f90.

4.3 Multimode Floquet matrix and diagonalisation

Once the components of the Hamiltonian are defined (i.e the complete set of matrices FIELDS(r)%V has been initialised), the multimode Hamiltonian can be calculated calling the function:

```
CALL MULTIMODEFLOQUETMATRIX(ID, size(modes_num, 1), total_frequencies, MODES_NUM, FIELDS, INFO)
```

As a result of this call, the system stores the full multimode Floquet matrix on the left-hand side of Eq. (6) in the matrix H_FLOQUET. This matrix is defined in the module ARRAYS and can be accessed (and modified!) by all computational routines that include this module. The size of this matrix is calculated internally and stored in the parameter h_floquet_size, which is also a global variable.

The library includes a subroutine to evaluate a sparse representation of this matrix, which results after invoking:

Setting INFO = 0, this instruction produces the representation of the Floquet matrix H_FLOQUET in the three array variation of the Compressed Sparse Row (CSR) storage format. With INFO=6, we get the matrix stored as three arrays of equal length, corresponding to values, rows and columns positions. The non-zero values of the matrix are stored in the complex array VALUES, and the information about their location is encoded in the integer arrays COLUMN and ROW_INDEX. The size of these three arrays are evaluated internally.

The library includes wrappers to diagonalisation subroutines from the Lapack and the MKL-intel (for the sparse CSR representation) libraries. These functions are called using:

Lapack:

```
CALL LAPACK_FULLEIGENVALUES(U_F,SIZE(H_FLOQUET,1),E_FLOQUET,INFO)
```

MKL:

```
CALL MKLSPARSE_FULLEIGENVALUES(D_MULTIFLOQUET,SIZE(VALUES,1),VALUES,ROW_INDEX,

COLUMN,E_L,E_R,E_FLOQUET,U_F,INFO)
```

In both cases, the eigenvalues are stored in the array E_FLOQUET and the eigenvectors are stored as columns of the matrix U_F. Remember that these eigenvectors correspond to the coefficients of the multimode Fourier decomposition of the micromotion operator Eq. (5). Invoking the MKL subroutine requires two additional parameter E_L and E_R: the lower and upper bounds of the interval to be searched for eigenvalues, respectively. The user is responsible to set meaningful values of both parameters.

The MKL sparse solvers requires the use of the variation of the Compressed sparse row (CSR) representation of the matrix, which is produced by sorting the array of ROW position, in such a way that all non-zero values of a given row become stored consecutively. This sorting is done using a QUICK_SORT algorithm by Robert Renka (OAK Ridge Natl. Lab, US) accessible from the Alan Miller's Fortran Software website [?]. Alternatively, calling the function MULTIMODEFLOQUETMATRIX_SP with the variable INFO=6, the user obtains the extended Hamiltonian represented by the three arrays of value,column,row, which can be used with a different eigenvalue solver for sparse matrices.

4.4 Time-evolution operator

With the full spectrum of H_FLOQUET, the time evolution operator between T1 and T2, corresponding to Eq. (4), can be evaluated calling the function:

```
CALL MULTIMODETIMEEVOLUTINOPERATOR(SIZE(U_F,1),SIZE(MODES_NUM,1),MODES_NUM,U_F,E_FLOQUET, ID%D_BARE,FIELDS,T1,T2,U_AUX,INFO)
```

which produces the matrix representation of the operator in Eq. (4). The time evolution operator is stored in the complex matrix U_AUX, whose size is equal to the number of bare states ID%D_BARE.

4.5 Micromotion operator

The micromotion operator is the time-dependent unitary transformation between the basis and the basis of state where the Hamiltonian is time-independent. Since we know the Fourier decomposition of this transformation via the diagonalisation of H_FLOQUET, we can evaluate the instantaneous transformation, e.g. at time T1, using the subroutine:

```
CALL MULTIMODEMICROMOTION(ID,SIZE(U_F,1),NM,MODES_NUM,U_F,E_FLOQUET,ID%D_BARE, FIELDS_,T1,U_F1,INFO)
```

which produces the matrix representation of the operator in Eq. (5). This micromotion operator is stored in the square matrix U_F1 of size ID%D_BARE.

4.6 Identifying the dressing modes

In several applications is useful to define a dressed basis of states and the openMMF library includes functions to simplify the evaluation of the evolution operator in this basis. For this, first the user should identify the subset of driving fields that define the dressed states. This is done using an integer array with as a many components as dressing fields. The elements of this array indicate the indices of the fields corresponding to the array modes_num. For example, if there is only one dressing field and it corresponds to the second component of the array MODES_NUM, then the array that indicates the dressing field, DRESSINFIELDS_INDICES, must be:

```
INTEGER, DIMENSION(2) :: DRESSINGFIELDS_INDICES
DRESSINGFIELDS_INDICES(1) = 1 ! THE STATIC COMPONEN
DRESSINGFIELDS_INDICES(2) = 2 ! THE FIRST DRIVING FIELD, WHICH DRESSES THE SYSTEM
```

With this, the Fourier decomposition of the micromotion operator defining the dressed basis in Eq. (5), can be obtained simply by calling the function:

```
CALL MICROMOTIONFOURIERDRESSEDBASIS(ID, DRESSINGFIELDS_INDICES, MODES_NUM, FIELDS, U_FD, E_DRESSED, INFO)
```

The Fourier components $U_{i,\bar{i}}^{\bar{n}}$ are stored in the matrix U_FD and the spectrum of dressed energies, $\bar{E}_{\bar{i}}$, are stored in the array E_DRESSED. With these two elements, we can calculate the micromotion operator of the dressed basis using the subroutine:

```
CALL MICROMOTIONDRESSEDBASIS(ID, MODES_NUM, DRESSINGFIELDS_INDICES, FIELDS, U_FD, E_DRESSED, T1, U_FD_1, INFO)
```

The micromotion operator at T1 is then stored as the square matrix U_FD_1. This set of instructions let us to evaluate the time-evolution operator in the dressed basis using the sequence:

5 Default system types

The openMMF library defines three different system types by default. These are Qubit, Spin and the ground state of several alkali atoms. A general system with D energy leveles can be defined using the "spin" type and setting by hand all coupling matrices.

5.1 Qubit

This type represents a two level system, where the couplings with the oscillating field are of the form

$$V^{\ell,n} = XS_x e^{\phi_{\ell,x}} + YS_y e^{\phi_{\ell,y}} + YS_z e^{\phi_{\ell,z}}$$

$$\tag{9}$$

with S_i , $i \in x, y, z$ the set of spin 1/2 angular momentum operators with $\hbar := 1$.

The corresponding derived type is initialised with the instruction:

FLOQUET_INIT(ID, 'qubit', INFO)

5.2 Spin of total angular momentum S_z

This type represents a system with $2S_z + 1$ equally space energy levels, where the couplings with oscillating fields are of the form:

$$V^{\ell,n} = X S_x e^{\phi_{\ell,x}} + Y S_y e^{\phi_{\ell,y}} + Y S_z e^{\phi_{\ell,z}}$$
(10)

with $S_i, i \in x, y, z$ the set of angular momentum operators with total spin S_z .

The corresponding derived type is initialised with the instruction:

```
FLOQUET_INIT(ID,'spin',2*Sz,INFO)
```

where the third argument is a DOUBLEPRECISION variable equal to the double of the projection of the total angular momentum.

5.3 Ground state Alkali atoms.

The effective model of an alkali atom consist of an electron with zero orbital angular momenta interacting with a static nucleus. These two particles interact via their magnetic moments, which define two manifolds of states corresponding to the total angular momenta $F = I \pm 1/2$. The library can be used to study interaction and intra manifold dynamics.

For example, to study the dynamics with focus on the manifold with total angular momentum F = I - 1/2 ('L', for lower), the corresponding ID can be obtained by invoking:

CALL FLOQUET_INIT(ID, SPECIE_NAME, 'L', INFO)

and the Hamiltonian components are built assuming the form:

$$V^{\ell,n} = \frac{\mu_B g_{I-1/2} B_x}{4} F_x e^{\phi_{\ell,x}} + \frac{\mu_B g_{I-1/2} B_y}{4} F_y e^{\phi_{\ell,y}} + \frac{\mu_B g_{I-1/2} B_z}{4} F_z e^{\phi_{\ell,z}}$$
(11)

Similarly, to study the dynamic of the manifold with F = I + 1/2 ('U', for upper), the system is initialised using:

CALL FLOQUET_INIT(ID, SPECIE_NAME, 'U', INFO)

which assumes couplings of the form

$$V^{\ell,n} = \frac{\mu_B g_{I+1/2} B_x}{A} F_x e^{\phi_{\ell,x}} + \frac{\mu_B g_{I+1/2} B_y}{A} F_y e^{\phi_{\ell,y}} + \frac{\mu_B g_{I+1/2} B_z}{A} F_z e^{\phi_{\ell,z}}$$
(12)

where

$$g_{I\pm 1/2} = \tag{13}$$

Finally, when both manifolds are of interest, we should use:

CALL FLOQUET_INIT(ID, SPECIE_NAME, 'B', INFO)

which prepares the system to initialise couplings of the form:

$$V^{\ell,n} = \frac{\mu_B B_x}{A} (g_J J_x + g_I I_x) e^{\phi_{\ell,x}} + \frac{\mu_B B_y}{A} (g_J J_y + g_I I_y) e^{\phi_{\ell,y}} + \frac{\mu_B B_z}{A} (g_J J_z + g_I I_z) e^{\phi_{\ell,z}}$$
(14)

In all these cases, after invoking the initialisation routine <code>FLOQUET_INIT</code> and defining the parameters of the couplings using the derived data type <code>TYPE(MODES)::FIELDS</code>, the matrix representation of each component of the Hamiltonian can be obtained with a single call to the subroutine:

CALL SETHAMILTONIANCOMPONENTS(ID, size(modes_num, 1), total_frequencies, MODES_NUM, FIELDS, INFO)

where total_frequencies is the total number of driving fields (including a static component). For a complete example see the source code at examples/FORTRAN/main_87Rb.f90.

6 C++ wrappers

The library includes C++ interfaces for each one of the subroutines defined. These interfaces are declared in files with the same name as the ones containing the Fortran declarations, but with the particle _C appended before the ending extension .f90. Similarly, wrapper subroutine are named using the corresponding Fortran names and appending the particle _c at the end of the name. For example, the file MultimodeFloquetTE_C.f90 is paired with the file MultimodeFloquet.f90 and defines the subroutine MULTIMODETIMEEVOLUTIONOPERATOR_C, which is used in c++ using multimodetimeevolutionoperator_c_ followed by the declared list of arguments (see example at examples/CPP/main_qubit.cpp.

The prototype of all function enabled for C++ are declared in the header file include/MultimodeFloquet.h. This scheme lets us to establish a line-by-line correspondence between the Fortran and C++ source codes.

7 Python wrappers

The library includes an interface to Python, which is implemented using CTYPES. Similarly to the C++ wrappers, for Python we define a function for each one of the functionalities of the library. This set of functions is declared in the file src/openmmf.py, which should be copied to the python working directory. The Python wrappers call the C++ wrappers which are compiled in the file library library. The user should make sure that the correct path to this file is set in src/openmmf.py.

The python wrapper requires to define the equivalent of the atomand mode derived data types, which are:

```
class atom_c_T(ctypes.Structure):
    _fields_ = [
                ("id_system", c_int),
                ("d_bare", c_int)
           ]
and
class mode_c_T(ctypes.Structure):
    c_dcmplx = ctypes.c_double*2
    _fields_ = [
                ("omega",
                            c_double),
                ("x",
                            c_dcmplx),
                ("y",
                            c_dcmplx),
                ("z",
                            c_dcmplx),
                ("phi_x",
                          c_double),
                ("phi_y",
                             c_double),
                ("phi_z",
                             c_double),
                ("N_Floquet", c_int)
            ]
```

respectively.

Each python wrapper function in **src/openmmf.py** takes numpy input parameters and define the set of ctype pointers required to call the corresponding C++ wrapper function. Let's examine the instruction to build the multimode Floquet Hamiltonian:

def multimodefloquetmatrix(id,modes_num,fields,info):

```
= ctypes.pointer(id)
 id_p
{\tt nm}
                   = c_int(modes_num.size)
 total_frequencies = c_int(np.sum(modes_num))
 info
                   = c_int(info)
modes_num_p
                   = modes_num.ctypes.data_as(POINTER(c_int))
fields_p
                   = ctypes.pointer(fields)
h_floquet_size =
 openmmfC.multimodefloquetmatrix_c_python_(id_p,ctypes.byref(nm),
              ctypes.byref(total_frequencies),
modes_num_p,fields_p,ctypes.byref(info))
return h_floquet_size
```

The input parameter mode_num is an numpy array of integers that, as before, defines the number of driving mode and harmonics. Alos, the input parameter info is a numpy integer. id is an instance of the class atom_c_T and fields is an instance of the class modes_c_T. This functions calls openmmfC.multimodefloquetmatrix_c_p passing all parameters by reference.

The ctypes wrappers rely on the equivalence between the data types in Fortran, C++ and Python, which should be observed rigourosly following the Table 1

Fortran	C++	ctypes	numpy
integer	int	$ctypes.c_int$	numpy.int32
double precision	double	$ctypes.c_double$	numpy.double
complex*16	std::;complex¿	$c_d cmplx = ctypes.c_double * 2$	np.complex

Table 1: Equivalence between the numerical data types in Fortran, C++, Ctypes and numpy.

8 Bugs and known limitations

If you find any bug please contact the developing team using the github hosting link https://github.com/openMMF/

9 Acknowledgements

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10 MODULES

In this section we provide the header of each one of the subroutines of the library, including the argument declaration, to help the user to identify the type of variable expected by each function.

10.1 Physical Constants

The module physical_constants defines the default values of commonly used parameters defining the Hamiltonian of atomic systems. The user can modify these values accessing the file in src/Modules.f90.

```
MODULE physical_constants
 IMPLICIT NONE
 DOUBLE PRECISION, PARAMETER :: pi
                                            = 4.0*ATAN(1.0)
 DOUBLE PRECISION, PARAMETER :: e
                                            = 1.602176462D-19
 DOUBLE PRECISION, PARAMETER :: h_P
                                            = 6.62606957D-34
 DOUBLE PRECISION, PARAMETER :: hbar
                                            = h_P/(2.0*4.0*ATAN(1.0))
 DOUBLE PRECISION, PARAMETER :: mu_B
                                            = 9.27400968D-24
 DOUBLE PRECISION, PARAMETER :: k_B
                                            = 1.3806488D-23
 DOUBLE PRECISION, PARAMETER :: mu_cero = 12.566370614D-7
 DOUBLE PRECISION, PARAMETER :: epsilon_cero = 8.854187817D-12
 DOUBLE PRECISION, PARAMETER :: amu = 1.660538921D-27
 DOUBLE PRECISION, PARAMETER :: g_t
                                            = 9.8D0
 DOUBLE PRECISION, PARAMETER :: SB_ct
                                            = 5.6704D-8
 COMPLEX*16,
               PARAMETER :: J_IMAG
                                            = DCMPLX(0.0D0, 1.0D0)
 DOUBLE PRECISION, PARAMETER :: speedoflight = 299792458.0D0
 DOUBLE PRECISION
                             :: TOTAL_TIME
END MODULE physical_constants
```

10.2 Arrays

The module ARRAYS provides global definitions of matrices. When using the module, the user cannot define variables using any of the names declared in this module.

```
MODULE ARRAYS

DOUBLE PRECISION, DIMENSION(:,:), ALLOCATABLE :: Identity,j_x,j_y,j_z,I_x,I_y,I_z

COMPLEX*16, DIMENSION(:,:), ALLOCATABLE :: H_IJ,HAMILTONIAN

COMPLEX*16, DIMENSION(:,:), ALLOCATABLE :: H_FLOQUET,H_FLOQUET_COPY

COMPLEX*16, DIMENSION(:,:), ALLOCATABLE :: U_ZEEMAN

END MODULE ARRAYS
```

To deallocate these arrays, the user can invoke the call:

```
CALL DEALLOCATEALL(ID)
```

where the variable TYPE(ATOM) ID defines the type of problem.

10.3 Atomic properties

The ATOMIC_PROPERTIES module defines the default physical parameters of common alkali atomic species used in the context of ultracold atomic physics.

```
MODULE ATOMIC_PROPERTIES

USE physical_constants

IMPLICIT NONE

DOUBLE PRECISION :: L=0.0D0, S = 0.5D0

DOUBLE PRECISION :: mass_at = 87*amu

DOUBLE PRECISION :: I,g_I,g_J

DOUBLE PRECISION :: J,F,gf,mf

DOUBLE PRECISION :: gF_2,gF_1,G_F

DOUBLE PRECISION :: A,a_s,alpha_E

INTEGER :: Fup,Fdown,Ftotal

INTEGER :: Total_states_LSI

CHARACTER(LEN=7) :: ID_name
```

```
!87Rb
 DOUBLE PRECISION :: I_87Rb = 1.5D0
 DOUBLE PRECISION :: J_87Rb = 0.5D0
 DOUBLE PRECISION :: gJ_87Rb = 2.0D0
 DOUBLE PRECISION :: gI_87Rb = -0.000995D0
 DOUBLE PRECISION :: A_87Rb = 2*pi*hbar*3.417341D9
 DOUBLE PRECISION :: a_s_87Rb = 5.77D-9
 DOUBLE PRECISION :: alpha_E_87Rb = 2*pi*hbar*0.0794*1D-4
 INTEGER :: Fup_87Rb = 2
INTEGER :: Fdown_87Rb = 1
 CHARACTER(LEN=7) :: ID_name_87Rb = "87Rb"
  !6Li
 DOUBLE PRECISION :: I_6Li = 1.0D0
 DOUBLE PRECISION :: J_6Li = 0.5D0
 DOUBLE PRECISION :: gJ_6Li = 2.0D0
 DOUBLE PRECISION :: gI_6Li = -0.000995D0
 DOUBLE PRECISION :: A_6Li = 2*pi*hbar*152.137D6
 DOUBLE PRECISION :: a_s_6Li = 5.77D-9
 DOUBLE PRECISION :: alpha_E_6Li = 2*pi*hbar*0.0794*1D-4
 INTEGER :: Fup_6Li = 1
INTEGER :: Fdown_6Li = 1
 CHARACTER(LEN=7) :: ID_name_6Li = "6Li"
 DOUBLE PRECISION :: I_qubit = 0.0D0
 DOUBLE PRECISION :: J_qubit = 0.0D0
 DOUBLE PRECISION :: gJ_qubit = 1.0D0
 DOUBLE PRECISION :: gI_qubit = 0.0D0
 DOUBLE PRECISION :: A_qubit = 1.0D0
 DOUBLE PRECISION :: a_s_qubit = 0.0D0
 DOUBLE PRECISION :: alpha_E_qubit = 0.0D0
 CHARACTER(LEN=7) :: ID_name_qubit = "qubit"
  !spin
 DOUBLE PRECISION :: I_spin = 0.0D0
 DOUBLE PRECISION :: J_spin = 0.0D0
 DOUBLE PRECISION :: gJ_spin = 1.0D0
 DOUBLE PRECISION :: gI_spin = 0.0D0
 DOUBLE PRECISION :: A_spin = 1.0D0
 DOUBLE PRECISION :: a_s_spin = 0.0D0
 DOUBLE PRECISION :: alpha_E_spin = 0.0D0
 INTEGER :: Fup_spin = 1
 INTEGER
                :: Fdown_spin = 1
 CHARACTER(LEN=7) :: ID_name_spin = "spin"
 !lattice
 CHARACTER :: PERIODIC
 CHARACTER(LEN=7) :: ID_name_lattice = "lattice"
END MODULE ATOMIC_PROPERTIES
10.4 MKL
MODULE FEAST
```

integer fpm(128) real*8 Emin, Emax

```
real*8     epsout
integer     loop
integer     M0 ! initial guess
integer     M1 ! total number of eigenvalues found
integer     info_FEAST
real*8,     DIMENSION(:),     ALLOCATABLE :: E, RES ! vector of eigenvalues
complex*16, DIMENSION(:,:), ALLOCATABLE :: X     ! matrix with eigenvectore
END MODULE FEAST
```

11 DERIVED TYPES (src/modes.f90)

The derived type defined

```
MODULE TYPES
```

```
TYPE :: MODE
  DOUBLE PRECISION :: OMEGA
   COMPLEX*16
              :: X,Y,Z
  DOUBLE PRECISION :: phi_x,phi_y,phi_z
             :: N_Floquet
   COMPLEX*16, DIMENSION(:,:), ALLOCATABLE :: V
   COMPLEX*16, DIMENSION(:), ALLOCATABLE :: VALUES
   INTEGER, DIMENSION(:), ALLOCATABLE :: ROW, COLUMN
END TYPE MODE
TYPE :: ATOM
  INTEGER
INTEGER
                 :: id_system
                  :: D_BARE
  DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: E_BARE
END TYPE ATOM
TYPE :: HARMONIC_FACTORS
  COMPLEX*16,DIMENSION(:,:), ALLOCATABLE :: U,U_r,U_AVG
   INTEGER, DIMENSION(:), ALLOCATABLE :: n
END type HARMONIC_FACTORS
```

END MODULE TYPES

12 COMPUTATIONAL SUBROUTINES

```
MODULE FLOQUETINITINTERFACE
  INTERFACE FLOQUETINIT
     MODULE PROCEDURE FLOQUETINIT_QUBIT, FLOQUETINIT_SPIN,FLOQUETINIT_ALKALI
 END INTERFACE FLOQUETINIT
contains
 SUBROUTINE FLOQUETINIT_QUBIT(ID,atomicspecie,INFO)
    ! ATOMICSPECIE: 87Rb,6Li,Cs,41K,qubit,lattice, SPIN
    ! MANIFOLD : "U" UPPER HYPERFINE MANIFOLD, "L" LOWER HYPERFIND MANIFOLD, "B" BOTH
    ! JTOTAL : IF ATOMICSPECIE .EQ. SPIN THEN JTOTAL IS THE TOTAL ANGULAR MOMENTUM OF THE SPIN
                 IF ATOMICSPECIE .EQ. LATTICE, THEN JTOTAL IS THE NUMBER OF SITES
    ! calculate the dimenson of the Hilbert space
    ! initialize all the matrices required for a full Floquet calcuations
    ! Calculate the nuclear, electron and total angular momentum operators
                    INTENT(INOUT) :: ID
 CHARACTER (LEN=*), INTENT(IN) :: ATOMICSPECIE
 INTEGER,
                   INTENT(INOUT) :: INFO
```

. . .

```
SUBROUTINE FLOQUETINIT_SPIN(ID, atomicspecie, jtotal, info)
  ! ATOMICSPECIE: 87Rb,6Li,Cs,41K,qubit,lattice, SPIN
  ! MANIFOLD : "U" UPPER HYPERFINE MANIFOLD, "L" LOWER HYPERFIND MANIFOLD, "B" BOTH
  ! JTOTAL : IF ATOMICSPECIE .EQ. SPIN THEN JTOTAL IS THE TOTAL ANGULAR MOMENTUM OF THE SPIN
                IF ATOMICSPECIE .EQ. LATTICE, THEN JTOTAL IS THE NUMBER OF SITES
  ! calculate the dimenson of the Hilbert space
  ! initialize all the matrices required for a full Floquet calcuations
  ! Calculate the nuclear, electron and total angular momentum operators
 IMPLICIT NONE
 TYPE(ATOM),
                   INTENT(INOUT) :: ID
 CHARACTER (LEN=*), INTENT(IN) :: ATOMICSPECIE DOUBLE PRECISION, intent(in) :: jtotal
 INTEGER, INTENT(INOUT) :: INFO
SUBROUTINE FLOQUETINIT_ALKALI(ID, atomicspecie, manifold, info)
  ! ATOMICSPECIE: 87Rb,6Li,Cs,41K,qubit,lattice, SPIN
  ! MANIFOLD : "U" UPPER HYPERFINE MANIFOLD, "L" LOWER HYPERFIND MANIFOLD, "B" BOTH
  ! JTOTAL : IF ATOMICSPECIE .EQ. SPIN THEN JTOTAL IS THE TOTAL ANGULAR MOMENTUM OF THE SPIN
               IF ATOMICSPECIE .EQ. LATTICE, THEN JTOTAL IS THE NUMBER OF SITES
  ! calculate the dimenson of the Hilbert space
  ! initialize all the matrices required for a full Floquet calcuations
  ! Calculate the nuclear, electron and total angular momentum operators
 TYPE(ATOM),
                   INTENT(INOUT) :: ID
 CHARACTER (LEN=*), INTENT(IN) :: ATOMICSPECIE
 CHARACTER (LEN=1), INTENT(IN) :: MANIFOLD
 INTEGER, INTENT(INOUT) :: INFO
END MODULE FLOQUETINITINTERFACE
SUBROUTINE SETHAMILTONIANCOMPONENTS(ID, NM, NF, MODES_NUM, FIELD, INFO)
 ! ID tYPE OF ATOM
  ! MODES_NUM, VECTOR. THE SIZE OF THE VECTOR TELL US THE NUMBER OF
             FREQUENCIES, AND THE VALUE OF EACH COMPONENT INDICATES
             THE NUMBER OF HARMONICS OF EACH FREQUENCI
  ! FIELDS : IN AND OUTPUT THE MATRICES
  ! INFO
 USE ARRAYS
 USE ATOMIC_PROPERTIES
 USE TYPES
 USE SUBINTERFACE_LAPACK ! write_matrix interface
 IMPLICIT NONE
                            INTENT(IN) :: NM,NF
 INTEGER,
                            INTENT(IN)
 TYPE(ATOM),
                                        :: MODES_NUM
 INTEGER, DIMENSION(NM), INTENT(IN)
 TYPE(MODE), DIMENSION(NF), INTENT(INOUT) :: FIELD
  INTEGER,
                            INTENT(INOUT) :: INFO
```

```
SUBROUTINE F_representation(Fx,Fy,Fz,Ftotal)
 USE FUNCIONES
 IMPLICIT NONE
 DOUBLE PRECISION, DIMENSION(:,:), INTENT(OUT):: Fx,Fy,Fz
 DOUBLE PRECISION, INTENT(IN) :: Ftotal
  !INTEGER, INTENT(IN) :: Ftotal_
  !DOUBLE PRECISION
 INTEGER k,p,N_k
 double precision k_!,Ftotal
 Fx = 0.0
 Fy = 0.0
 Fz = 0.0
SUBROUTINE I_{and_J}representations(j_x, j_y, j_z, I_x, I_y, I_z, I, S, I)
 USE FUNCIONES
 IMPLICIT NONE
 DOUBLE PRECISION, DIMENSION(:,:),INTENT(INOUT) :: j_x,j_y,j_z,I_x,I_y,I_z
 DOUBLE PRECISION, INTENT(IN) :: L,S,I
SUBROUTINE MULTIMODETIMEEVOLUTINOPERATOR(D,NM,MODES_NUM,U_F_MODES,E_MULTIFLOQUET,
                                               D_BARE, FIELD, T1, T2, U, INFO)
  ! TIME EVOLUTION OPERATOR OF A MULTIMODE DRESSED SYSTEM.
  ! THE EVOLUTION OPERATOR IS WRITEN IN THE BASIS USED TO EXPRESS THE
 ! MULTIMODE FLOQUET HAMILTONIAN
 ! U : MATRIX OF AMPLITUED OF PROBABILITIES FOR TRANSITIONS BETWEEN T1 TO T2
!!$ D
                  (IN) : DIMENSION OF THE EXTENDED HILBERT SPACE
!!$
                           (SIZE OF THE MULTIMODE FLOQUET MATRIX)
!!$ NM
                   (IN) : NUMBER OF MODES
!!$ MODES_NUM
                 (IN) : VECTOR (NM) INDICATING THE NUMBER OF HARMONICS OF EACH MODE
!!$ U_F_MODES (IN) : TRANSFORMATION, DIMENSOON (D,D)
!!$ E_MULTIFLOQUET (IN) : MULTIMODE FLOQUET SPECTRUM
!!$ D_BARE (IN) : DIMENSION OF THE BARE HILBERT SPACE
!!$ FIELD
                  (IN) : STRUCTURE DESCRIBING THE COUPLINGS
!!$ T1
                         : INITIAL TIME
                   (IN)
!!$ T2
                  (IN) : FINAL TIME
                  (OUT) : TRANFORMATION BETWEEN THE EXTENDED BARE BASIS AND
!!$ U
!!$
                            THE FLOQUET STATES, DIMENSION (D_BARE,D)
              (INOUT): (POSSIBLE) ERROR FLAG
!!$ INFO
 USE TYPES
 USE SUBINTERFACE_LAPACK
 IMPLICIT NONE
 INTEGER,
                                             INTENT(IN) :: D,D_BARE,NM
                                             INTENT(INOUT) :: INFO
  INTEGER,
```

13

```
DIMENSION(D_BARE,D_BARE), INTENT(OUT) :: U
SUBROUTINE MULTIMODEFLOQUETMATRIX(ATOM_,NM,NF,MODES_NUM,FIELD,INFO)
 !ID, size(modes_num, 1), total_frequencies, MODES_NUM, FIELDS, INFO
 ! USE FLOQUET
 !ATOM_ type atom, -> dimension of the bare Hilbert space
 !NM -> number of modes
 !NF -> Number of Fields
 !MODES_NUM -> number of harmonics of each mode
 !FIELD -> Field couplings
 !INFO
 USE ARRAYS
 USE ATOMIC_PROPERTIES
 USE TYPES
 USE SUBINTERFACE_LAPACK
 IMPLICIT NONE
 INTEGER,
                         INTENT(IN) :: NM,NF
 INTEGER,
                         INTENT(INOUT) :: INFO
 INTEGER, DIMENSION(NM), INTENT(IN) :: MODES_NUM
 TYPE(MODE), DIMENSION(NF), INTENT(IN) :: FIELD
 TYPE(ATOM),
                         INTENT(IN) :: ATOM_
SUBROUTINE MULTIMODEFLOQUETMATRIX_SP(ATOM__,NM,NF,MODES_NUM,FIELDS,VALUES_,ROW_INDEX_,COLUMN_,INFO)
! ATOM_
          (IN) : type of quantum system
! NM
          (IN) : number of modes
!NF
         (IN) : number of driving fields
!MODES_NUM (IN) : vector indicating the number of harmonics of each driving field (mode)
!FIELDS (IN)
                 : Fields
!VALUES_ (OUT) : Hamiltonian values
!INFO
         (INOUT) : error flag. INFO=0 means there is no error
 USE TYPES
                 !(modes.f90)
 USE MERGINGARRAYS ! (utils.f90)
 IMPLICIT NONE
 INTEGER
                                    INTENT(IN) :: NM,NF
 TYPE(MODE), DIMENSION(NF),
                                    INTENT(INOUT) :: FIELDS
 TYPE(ATOM),
                                    INTENT(IN) :: ATOM__
          DIMENSION(NM),
 INTEGER,
                                   INTENT(IN) :: MODES_NUM
                                    INTENT(INOUT) :: INFO
 COMPLEX*16, DIMENSION(:), ALLOCATABLE, INTENT(OUT) :: VALUES_
 INTEGER, DIMENSION(:), ALLOCATABLE, INTENT(OUT) :: COLUMN_
          DIMENSION(:), ALLOCATABLE, INTENT(OUT) :: ROW_INDEX_
 INTEGER,
```

INTENT(IN) :: MODES_NUM

INTENT(IN) :: U_F_MODES

INTENT(IN) :: E_MULTIFLOQUET

INTENT(IN) :: FIELD

INTENT(IN) :: T1,T2

INTEGER,

TYPE(MODE),

COMPLEX*16,

DOUBLE PRECISION,

DOUBLE PRECISION, DIMENSION(D),

COMPLEX*16, DIMENSION(D,D),

DIMENSION(NM),

DIMENSION(NM),

```
SUBROUTINE MULTIMODEFLOQUETTRANSFORMATION(D,NM,MODES_NUM,U_F_MODES,E_MULTIFLOQUET, D_BARE,FIELD,T1,U,INFO)
```

```
! TIME-DEPENDENT TRANSFORMATION BETWEEN THE EXTENDED BARE BASIS AND THE FLOQUET STATES
  ! U(T1) = sum_ U^n exp(i n omega T1)
!!$ D
                         (IN) : DIMENSION OF THE EXTENDED HILBERT SPACE (SIZE OF THE MULTIMODE FLOQUET
!!$ NM
                        (IN) : NUMBER OF MODES
!!$ MODES_NUM (IN) : VECTOR (NM) INDICATING THE NUMBER OF HARMONICS OF EACH MODE !!$ U_F_MODES (IN) : TRANSFORMATION, DIMENSOON (D,D)
!!$ E_MULTIFLOQUET (IN) : MULTIMODE FLOQUET SPECTRUM
!!$ D_BARE (IN) : DIMENSION OF THE BARE HILBERT SPACE
!!$ FIELD

(IN) : STRUCTURE DESCRIBING THE COUPLINGS

!!$ T1

(IN) : TIME. THE BARE 2 DRESSED TRANSFORMATINO IS TIME DEPENDENT

!!$ U

(OUT) : TRANFORMATION BETWEEN THE EXTENDED BARE BASIS AND THE FLOQUET STATES,

DIMENSION (D_BARE,D)

!!$ INFO

(INOUT): (POSSIBLE) ERROR FLAG
  USE TYPES
  IMPLICIT NONE
  INTEGER,
                                                          INTENT(IN) :: D,D_BARE,NM
                                                           INTENT(INOUT) :: INFO
  INTEGER,
  INTEGER,
  INTEGER, DIMENSION(NM), TYPE(MODE), DIMENSION(NM),
                                                          INTENT(IN) :: MODES_NUM
INTENT(IN) :: FIELD
                                                          INTENT(IN) :: T1
  DOUBLE PRECISION.
  DOUBLE PRECISION, DIMENSION(D), INTENT(IN) :: E_MULTIFLOQUET COMPLEX*16, DIMENSION(D,D), INTENT(IN) :: U_F_MODES COMPLEX*16, DIMENSION(D_BARE,D), INTENT(OUT) :: U
SUBROUTINE MULTIMODEMICROMOTION(ID,D,NM,MODES_NUM,U_F_MODES,E_MULTIFLOQUET,D_BARE,FIELD,T1,U,INFO)
  ! TIME-DEPENDENT TRANSFORMATION BETWEEN THE EXTENDED BARE BASIS AND THE FLOQUET STATES
  ! U(T1) = sum_ U^n exp(i n omega T1)
  - !
!!$ D
                         (IN) : DIMENSION OF THE EXTENDED HILBERT SPACE (SIZE OF THE MULTIMODE FLOQUET
!!$ NM
                         (IN) : NUMBER OF MODES
!!$ MODES_NUM(IN): VECTOR (NM) INDICATING THE NUMBER OF HARMONICS OF EACH MODE!!$ U_F_MODES(IN): TRANSFORMATION, DIMENSOON (D,D)!!$ E_MULTIFLOQUET (IN): MULTIMODE FLOQUET SPECTRUM
!!$ D_BARE (IN) : DIMENSION OF THE BARE HILBERT SPACE
!!$ FIELD

(IN): STRUCTURE DESCRIBING THE COUPLINGS

!!$ T1

(IN): TIME. THE BARE 2 DRESSED TRANSFORMATINO IS TIME DEPENDENT

!!$ U

(OUT): TRANFORMATION BETWEEN THE EXTENDED BARE BASIS AND THE FLOQUET STATES, D

!!$ INFO

(INOUT): (POSSIBLE) ERROR FLAG
  !USE TYPES_C
  USE TYPES
  !USE MODES_4F
  USE SUBINTERFACE_LAPACK
  USE ATOMIC_PROPERTIES
  IMPLICIT NONE
  TYPE(ATOM),
                                    INTENT(IN) :: ID
  INTEGER.
                                                            INTENT(IN) :: D,D_BARE,NM
```

INTENT(INOUT) :: INFO

INTENT(IN) :: FIELD

15

INTENT(IN) :: MODES_NUM

INTEGER,

INTEGER,

DIMENSION(NM),

TYPE(MODE), DIMENSION(NM),

```
COMPLEX*16, DIMENSION(D,D), INTENT(IN) :: U_
COMPLEX*16, DIMENSION(D_BARE,D_BARE), INTENT(OUT) :: U
                                                   INTENT(IN) :: U_F_MODES
SUBROUTINE MICROMOTIONFOURIERDRESSEDBASIS(ID, DRESSINGFIELDS_INDICES, MODES_NUM, FIELDS,
                                                                                     U_FD,E_DRESSED,INFO)
                       :: TYPE(ATOM) system ID
              (in)
! DRESSINGFIELDS_INDICES (in) :: integer array indicating the indices of the dressing modes
!\ {\tt MODES\_NUM}\ ({\tt in}) \qquad ::\ {\tt integer}\ {\tt array}\ {\tt indicating}\ {\tt the}\ {\tt number}\ {\tt of}\ {\tt harmonics}\ {\tt of}\ {\tt all}\ {\tt driving}\ {\tt modes}
                       :: Array of TYPE(MODE) of dimension
! FIELDS (in)
              (out) :: complex*16 matrix fourier decomposition of the micromotion operator of the dr
! U_FD
! E_DRESSED (out) :: dressed energies
         (inout) :: error flag
! INFO
  USE TYPES
  TYPE(ATOM).
                                         INTENT(IN) :: ID
  INTEGER, DIMENSION(:), INTENT(IN) :: DRESSINGFIELDS_INDICES
INTEGER, DIMENSION(:), INTENT(IN) :: MODES_NUM

TYPE(MODE), DIMENSION(:), INTENT(IN) :: FIELDS

COMPLEX*16, DIMENSION(:,:), ALLOCATABLE, INTENT(OUT) :: U_FD
  DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE, INTENT(OUT) :: E_DRESSED
SUBROUTINE MICROMOTIONDRESSEDBASIS(ID, MODES_NUM, DRESSINGFIELDS_INDICES, FIELDS,
                                                                  U_F_MODES,E_MULTIFLOQUET,T1,U,INFO)
! ID (in)
                   :: TYPE(ATOM) system ID
! MODES_NUM (in) :: integer array indicating the number of harmonics of each driving mode
! DRESSINFIELDS_INDICES :: integer array indicating the indices of the dressing modes
! FIELDS :: Array of TYPE(MODES) with NM components (all driving fields)
! U_F_MODES :: complex*16 matrix of dimension DxD. Fourier decomposition of the micromotion ope
! E_MULTIFLOQUET :: dressed energies
! T1 :: double precision, time
                   :: complex*16 matrix of dimension D_BARE x D_BARE. micromotion operator at time T1
! U
! INFO
                   :: error flag
  USE TYPES
  IMPLICIT NONE
  TYPE(ATOM), INTENT(IN) :: ID

INTEGER, DIMENSION(:), INTENT(IN) :: MODES_NUM

INTEGER, DIMENSION(:), INTENT(IN) :: DRESSINGFIELDS_INDICES

COMPLEX*16, DIMENSION(:,:), INTENT(IN) :: U_F_MODES
  DOUBLE PRECISION, DIMENSION(:), INTENT(IN) :: E_MULTIFLOQUET
  TYPE(MODE), DIMENSION(:), INTENT(IN) :: FIELDS
  DOUBLE PRECISION ,
                                          INTENT(IN) :: T1
  COMPLEX*16, DIMENSION(:,:), INTENT(OUT) :: U
  INTEGER,
                                           INTENT(INOUT) :: INFO
```

INTENT(IN) :: T1

INTENT(IN) :: E_MULTIFLOQUET

DOUBLE PRECISION,

DOUBLE PRECISION, DIMENSION(D),

```
AVERAGE TIME EVOLUTION OPERATOR OF A MULTIMODE DRESSED SYSTEM.
11$
!!$ THE AVERAGE EVOLUTION OPERATOR IS WRITEN IN THE BASIS USED TO EXPRESS THE
!!$ MULTIMODE FLOQUET HAMILTONIAN
!!$ U : MATRIX OF AVERAGE TRANSITION PROBABILITIES
!!$
                  (IN) : DIMENSION OF THE EXTENDED HILBERT SPACE
!!$ D
                              (SIZE OF THE MULTIMODE FLOQUET MATRIX)
!!$
!!$ NM (IN) : NUMBER OF MODES
!!$ MODES_NUM (IN) : VECTOR (NM) INDICATING THE NUMBER OF HARMONICS OF EACH MODE
!!$ U_F_MODES (IN) : TRANSFORMATION, DIMENSOON (D,D)
!!$ E_MULTIFLOQUET (IN) : MULTIMODE FLOQUET SPECTRUM
!!$ D_BARE(IN) : DIMENSION OF THE BARE HILBERT SPACE!!$ U(OUT) : MATRIX OF AVERAGE TRANSITION PROBABILITIES!!$ INFO(INOUT): (POSSIBLE) ERROR FLAG
  USE TYPES
  IMPLICIT NONE
  TYPE(MODE),DIMENSION(NM), INTENT(IN) :: FIELD INTEGER, DIMENSION(NM), INTENT(IN) :: MODES_NUM
  INTEGER,
                                                   INTENT(IN) :: D,D_BARE,NM
  INTEGER,
                                                   INTENT(INOUT) :: INFO
  DOUBLE PRECISION, DIMENSION(D_BARE,D_BARE), INTENT(OUT) :: U
```

DRIVER SUBROUTINES

```
SUBROUTINE DRESSEDBASIS(D,ID,NM,MODES_NUM,FIELDS,U_FD,E_DRESSED,INFO)
 !!$ THIS SUBROUTINES CALCULATES THE FOURIER COMPONENTS OF THE
 !!$ TRANSFORMATION BETWEEN THE BARE BASIS TO THE DRESSED BASIS DEFINDED
 !!$ BY THE FULL SET OF DRIVING FIELDS.
 !!$
 !!$ D
                                              : DIMENSION OF THE MULTIMODE EXTENDED HILBERT SPACE
 !!$ ID (IN)
                                              : TYPE OF QUANTUM SYSTEM
::$ MODES_NUM
!!$ FIELDS (IN)
!!$ U_FD (OUT)
!!$ E_DRESSED (OUT)
!!$ INFO (INOUT)
                                       : NUMBER OF MODES == NUMBER OF DRIVING FIELDS
: VECTOR INDICATING THE NUMBER OF HARMONICS OF EACH DRESSING FIELD
: AMPLITUDE, FREQUENCY AND PHASES OF ALL DRIVING FIELDS
: THIS IS THE TRANSFORMATION WE ARE LOOKING FOR
: DRESSED ENERGIES
                                              : INFO = O MEANS SUCESS
   USE ATOMIC_PROPERTIES
```

```
USE TYPES
USE SUBINTERFACE
USE SUBINTERFACE_LAPACK
USE FLOQUETINIT_
USE ARRAYS
IMPLICIT NONE
INTEGER, DIMENSION(NM), INTENT(IN) :: MODES_NUM
COMPLEX*16, DIMENSION(D,D), INTENT(OUT) :: U_FD
```

DOUBLE PRECISION, DIMENSION(D), INTENT(OUT) :: E_DRESSED 17

INTEGER, INTENT(IN) :: NM,D INTENT(INOUT) :: INFO

INTEGER, SUBROUTINE DRESSEDBASIS_SP(D,ID,NM,MODES_NUM,FIELDS,U_FD,E_DRESSED,INFO) !!\$ THIS SUBROUTINES CALCULATES THE TRANSFORMATION BETWEEN THE BARE !!\$ BASIS TO THE DRESSED BASIS DEFINDED BY THE FULL SET OF DRIVING FIELDS. II\$ D : DIMENSION OF THE MULTIMODE EXTENDED HILBERT SPACE !!\$ ID (IN) : TYPE OF QUATUM SYSTEM !!\$ NM (IN) : NUMBER OF MODES == NUMBER OF DRIVING FIELDS : VECTOR INDICATING THE NUMBER OF HARMONICS OF EACH DRESSING FIELD
: AMPLITUDE, FREQUENCY AND PHASES OF ALL DRIVING FIELDS
: THIS IS THE TRANSFORMATION WE ARE LOOKING FOR
: DRESSED ENERGIES
: INFO = O MEANS SUCESS !!\$ MODES_NUM !!\$ FIELDS (IN)
!!\$ U_FD (OUT)
!!\$ E_DRESSED (OUT) !!\$ INFO (INOUT) USE ATOMIC_PROPERTIES USE TYPES USE SPARSE_INTERFACE USE SUBINTERFACE USE SUBINTERFACE_LAPACK USE FLOQUETINIT_ USE ARRAYS IMPLICIT NONE TYPE(MODE), DIMENSION(NM), INTENT(INOUT) :: FIELDS TYPE(ATOM), INTENT(IN) :: ID INTEGER, DIMENSION(NM), INTENT(IN) :: MODES_NUM
COMPLEX*16, DIMENSION(D,D), INTENT(OUT) :: U_FD DOUBLE PRECISION, DIMENSION(D), INTENT(OUT) :: E_DRESSED INTENT(IN) INTEGER, :: NM,D INTEGER, INTENT(INOUT) :: INFO SUBROUTINE TIMEEVOLUTIONOPERATOR(ID, D_BARE, NM, MODES_NUM, FIELD, T1, T2, U, INFO) ! TIME EVOLUTION OPERATOR OF A MULTIMODE DRESSED SYSTEM. THE EVOLUTION ! OPERATOR IS WRITEN IN THE BASIS USED TO EXPRESS THE ! MULTIMODE FLOQUET HAMILTONIAN ! U : MATRIX OF AMPLITUED OF PROBABILITIES FOR TRANSITIONS BETWEEN T1 TO T2 !!\$ NM (IN) : NUMBER OF MODES !!\$ MODES_NUM (IN) : VECTOR (NM) INDICATING THE NUMBER OF HARMONICS OF EACH MODE !!\$ D_BARE (IN) : DIMENSION OF THE BARE HILBERT SPACE (IN) : STRUCTURE DESCRIBING THE COUPLINGS !!\$ FIELD !!\$ T1 : INITIAL TIME (IN) (IN) : FINAL TIME !!\$ T2 (OUT) : TRANFORMATION BETWEEN THE EXTENDED BARE BASIS AND !!\$ U !!\$ THE FLOQUET STATES, DIMENSION (D_BARE,D) !!\$ INFO (INOUT): (POSSIBLE) ERROR FLAG USE ATOMIC_PROPERTIES USE TYPES

USE SUBINTERFACE

USE SUBINTERFACE_LAPACK

USE FLOQUETINIT

USE ARRAYS

```
IMPLICIT NONE
    TYPE(ATOM) ,
                                                    INTENT(IN) :: ID
    INTEGER,
                                                   INTENT(IN) :: D_BARE
                                                  INTENT(IN) :: NM
    INTEGER,
                                                 INTENT(IN) :: MODES_NUM
INTENT(IN) :: FIELD
    INTEGER, DIMENSION(NM), TYPE(MODE), DIMENSION(NM),
                                                                  :: T1
    DOUBLE PRECISION.
                                                   INTENT(IN)
    DOUBLE PRECISION,
                                                                  :: T2
                                                    INTENT(IN)
    COMPLEX*16, DIMENSION(D_BARE,D_BARE), INTENT(OUT) :: U
    INTEGER,
                                                    INTENT(INOUT) :: INFO
SUBROUTINE MICROMOTIONFOURIERDRESSEDBASIS (ID, DRESSINGFIELDS_INDICES,
                                              MODES_NUM,FIELDS, U_FD,E_DRESSED,INFO)
! THIS SUBROUTINE CALCULATES THE FOURIER COMPONENTS (U_FD) AND PHASES (E_DRESSED)
! OF THE MICROMOTION OPERATOR OF SUBSET OF DRIVING MODES
           (in) :: TYPE(ATOM) system ID
! DRESSINGFIELDS_INDICES (in) :: integer array indicating the indices of the dressing modes
! MODES_NUM (in) :: integer array indicating the number of harmonics of all driving modes :: Array of TYPE(MODE) of dimension
! U_FD (out) :: complex*16 matrix fourier decomposition of the micromotion
                    operator of the dressed basis
! E_DRESSED (out) :: dressed energies
! INFO (inout) :: error flag
  USE TYPES
  IMPLICIT NONE
 TYPE(ATOM), INTENT(IN) :: ID

INTEGER, DIMENSION(:), INTENT(IN) :: DRESSINGFIELDS_INDICES

INTEGER, DIMENSION(:), INTENT(IN) :: MODES_NUM

TYPE(MODE), DIMENSION(:), INTENT(IN) :: FIELDS

COMPLEX*16, DIMENSION(:,:), ALLOCATABLE, INTENT(OUT) :: U_FD
  DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE, INTENT(OUT) :: E_DRESSED
  INTEGER, INTENT(INOUT) :: INFO
END SUBROUTINE MICROMOTIONFOURIERDRESSEDBASIS
SUBROUTINE MICROMOTIONDRESSEDBASIS(ID, MODES_NUM, DRESSINGFIELDS_INDICES, FIELDS,
                                                    U_F_MODES,E_MULTIFLOQUET,T1,U,INFO)
! THIS SUBROUTINE CALCULATES U: THE TIME-DEPENDENT MICROMOTION OPERATOR OF
! A SUBSET OF THE DRIVING MODES. U_F_MODES AND E_MULTIFLOQUET ARE THE ARRAYS
! CALCULATED WITH THE SUBROUTINE MICROMOTIONFOURIERDRESSEDBASIS
                  :: TYPE(ATOM) system ID
! MODES_NUM (in) :: integer array indicating the number of harmonics of each driving mode
! DRESSINFIELDS_INDICES :: integer array indicating the indices of the dressing modes
           :: Array of TYPE(MODES) with NM components (all driving fields)
! FIELDS
! U_F_MODES
                 :: complex*16 matrix of dimension DxD. Fourier decomposition of
                   the micromotion operator of the dressed basis
! E_MULTIFLOQUET :: dressed energies
! T1 :: double precision, time
! U
                 :: complex*16 matrix of dimension D_BARE x D_BARE. micromotion operator
                    at time T1
```

USE TYPES IMPLICIT NONE

:: error flag

!

! INFO

```
INTENT(IN) :: ID
 TYPE(ATOM),
 INTEGER,
                   DIMENSION(:),
                                  INTENT(IN) :: MODES_NUM
 INTEGER,
                 DIMENSION(:), INTENT(IN) :: DRESSINGFIELDS_INDICES
 COMPLEX*16, DIMENSION(:,:), INTENT(IN) :: U_F_MODES
 DOUBLE PRECISION, DIMENSION(:), INTENT(IN) :: E_MULTIFLOQUET
 TYPE(MODE), DIMENSION(:),
                                 INTENT(IN)
                                                :: FIELDS
 DOUBLE PRECISION , INTENT(IN) :: TO COMPLEX*16, DIMENSION(:,:), INTENT(OUT) :: U
                                                :: T1
                                   INTENT(INOUT) :: INFO
 INTEGER,
13.1 Utility subroutines
SUBROUTINE PACKINGBANDMATRIX(N,A,KD,AB,INFO)
! brute force packing of a banded matrix
 IMPLICIT NONE
 INTEGER, INTENT(INOUT) :: INFO
 INTEGER, INTENT(IN)
                      :: N,KD
 COMPLEX*16, DIMENSION(N,N) :: A
 COMPLEX*16, DIMENSION(KD+1,N) :: AB
SUBROUTINE LAPACK_FULLEIGENVALUES(H,N,W_SPACE,INFO)
!eigenvalues/vectors of matrix ab
!H, inout, packed banded matrix
! , out, eigenvectors
!N, in, matrix dimension
!W_space, out, eigenvalues
!INFO, inout, error flag
 !H is COMPLEX*16 array, dimension (N, N)
 ! 69 *>
                 On entry, the Hermitian matrix A. If UPLO = 'U', the
 ! 70 *>
                   leading N-by-N upper triangular part of A contains the
 ! 71 *>
                 upper triangular part of the matrix A. If UPLO = 'L',
                 the leading N-by-N lower triangular part of A contains
 ! 72 *>
 ! 73 *>
                 the lower triangular part of the matrix A.
 ! 74 *>
                 On exit, if JOBZ = 'V', then if INFO = 0, A contains the
 ! 75 *>
                   orthonormal eigenvectors of the matrix A.
 ! 76 *>
                   If JOBZ = 'N', then on exit the lower triangle (if UPLO='L')
 ! 77 *>
                   or the upper triangle (if UPLO='U') of A, including the
 ! 78 *>
                   diagonal, is destroyed.
 ! The eigenvector H(:,r) corresponds to the eigenvalue W_SPACE(r)
 IMPLICIT NONE
 INTEGER,
                                   INTENT(IN) :: N
 COMPLEX*16, DIMENSION(N,N), INTENT(INOUT) :: H
 DOUBLE PRECISION, DIMENSION(N), INTENT(INOUT) :: W_SPACE
 INTEGER,
                                   INTENT(OUT) :: INFO
SUBROUTINE LAPACK_FULLEIGENVALUESBAND(AB,Z,KD,N,W,INFO)
!eigenvalues/vectors of banded matrix ab
!AB, inout, packed banded matrix
!Z, out, eigenvectors
!KD out, calcuated eigenvectors
```

!N, in,matrix dimension
!W, out, eigenvalues

```
!INFO, inout, error flag
```

```
!H is COMPLEX*16 array, dimension (N, N)
  ! 69 *>
                    On entry, the Hermitian matrix A. If UPLO = 'U', the
  ! 70 *>
                    leading N-by-N upper triangular part of A contains the
  ! 71 *>
                    upper triangular part of the matrix A. If UPLO = 'L',
  ! 72 *>
                    the leading N-by-N lower triangular part of A contains
                    the lower triangular part of the matrix A.
  ! 73 *>
                    On exit, if JOBZ = 'V', then if INFO = 0, A contains the
  ! 74 *>
  ! 75 *>
                    orthonormal eigenvectors of the matrix A.
  ! 76 *>
                    If JOBZ = 'N', then on exit the lower triangle (if UPLO='L')
  ! 77 *>
                    or the upper triangle (if UPLO='U') of A, including the
  ! 78 *>
                    diagonal, is destroyed.
  !
  ! The eigenvector H(:,r) corresponds to the eigenvalue W_SPACE(r)
  IMPLICIT NONE
  INTEGER,
                                           INTENT(IN) :: N,KD
                    DIMENSION(KD+1,N), INTENT(INOUT) :: AB
  COMPLEX*16,
               DIMENSION(N,N),
                                          INTENT(INOUT) :: Z
  COMPLEX*16,
  DOUBLE PRECISION, DIMENSION(N),
                                          INTENT(INOUT) :: W
  INTEGER,
                                           INTENT(OUT) :: INFO
SUBROUTINE LAPACK_SELECTEIGENVALUES(H,N,W_SPACE,L1,L2,Z,INFO)
!selected eigenvalues/vectors of hermitian matrix
!H, inout, packed banded matrix
! , out, eigenvectors
!N, in, matrix dimension
!W_space, out, eigenvalues
!L1 ordinal lowest eigenvalue
!L2 ordinal highest eigenvlaue
!Z : eigenvectors
!INFO, inout, error flag
  !USE FLOQUET
  IMPLICIT NONE
  INTEGER,
                                  INTENT(IN) :: N,L1,L2
                                 INTENT(INOUT) :: H
  COMPLEX*16, DIMENSION(:,:),
                                INTENT(OUT) :: Z
  COMPLEX*16, DIMENSION(:,:),
  DOUBLE PRECISION, DIMENSION(:), INTENT(OUT) :: W_SPACE
  INTEGER,
                                   INTENT(OUT)
                                                :: INFO
SUBROUTINE MKLSPARSE_FULLEIGENVALUES(D,DV,VALUES,ROW_INDEX,COLUMN,E_L,E_R,E_FLOQUET,U_F,INFO)
!CALCULATES THE ENERGY SPECTRUM OF THE MATRIX REPRESENTED BY VALUES, ROW_INDEX AND COLUMN
! D (IN), MATRIX DIMENSION == NUMBER OF EIGENVALUES
! DV (IN), NUMBER OF VALUES != 0
! VALUES (IN) ARRAY OF VALUES
! ROW_INDEX (IN), ARRAY OF INDICES
! COLUMN (IN), ARRAY OF COLUMN NUMBERS
! E_L (IN), LEFT BOUNDARY OF THE SEARCH INTERVAL
! E_R (IN), RIGHT BOUNDARY OF THE SEARCH INTERVAL
! E_FLOQUET (OUT), ARRAY OF EIGENVALUES
```

! INFO (INOUT) ERROR FLAG and VERBOSITY FLAG

O display no information

!

```
1 DISPLAY INFORMAITON ABOUT THE SIZE OF THE ARRAYS
!
                  10 DISPLAY INFORMAITON ABOUT THE ARRAYS AND THE ARRAYS
  USE FEAST
  IMPLICIT NONE
                                      INTENT(IN) :: D,DV
  INTEGER,
 COMPLEX*16, DIMENSION(DV), INTENT(INOUT) :: VALUES
INTEGER, DIMENSION(DV), INTENT(INOUT) :: COLUMN
INTEGER, DIMENSION(D+1), INTENT(INOUT) :: ROW_INDEX
  DOUBLE PRECISION,
                                    INTENT(IN) :: E_L, E_R
  DOUBLE PRECISION, DIMENSION(D), INTENT(OUT) :: E_FLOQUET
  COMPLEX*16, DIMENSION(D,D), INTENT(OUT) :: U_F
  INTEGER,
                                     INTENT(INOUT) :: INFO
SUBROUTINE QUICK_SORT_INTEGERS(v,index_t,N)
  IMPLICIT NONE
  INTEGER, INTENT(IN) :: N
  INTEGER, DIMENSION(N), INTENT(INOUT) :: v
  INTEGER, DIMENSION(N),INTENT(INOUT) :: index_t
  INTEGER, PARAMETER :: NN=10000, NSTACK=8000
SUBROUTINE WRITE_MATRIX(A)
! it writes a matrix of doubles nxm on the screen
  DOUBLE PRECISION, DIMENSION(:,:) :: A
  CHARACTER(LEN=105) STRING
  CHARACTER(LEN=105) aux_char
  integer :: aux
SUBROUTINE WRITE_MATRIX_INT(A)
!it writes a matrix of integer nxm on the screen
  INTEGER, DIMENSION(:,:) :: A
SUBROUTINE COORDINATEPACKING(D,A,V,R,C,index,INFO)
  IMPLICIT NONE
  INTEGER, INTENT(IN):: D
  COMPLEX*16,DIMENSION(D,D),INTENT(IN) :: A
  COMPLEX*16, DIMENSION(D*D), INTENT(OUT) :: V
  INTEGER, DIMENSION(D*D), INTENT(OUT) :: R,C
  INTEGER, INTENT(OUT) :: index
  INTEGER, INTENT(INOUT) :: INFO
SUBROUTINE APPENDARRAYS(V,B,INFO)
  COMPLEX*16, DIMENSION(:), ALLOCATABLE, INTENT(INOUT) :: V
  COMPLEX*16, DIMENSION(:),INTENT(IN) :: B
                            INTENT(INOUT) :: INFO
  INTEGER,
```

```
SUBROUTINE APPENDARRAYSI(V,B,INFO)
 INTEGER, DIMENSION(:),ALLOCATABLE, INTENT(INOUT) :: V
 INTEGER, DIMENSION(:),INTENT(IN)
                            :: B
 INTEGER,
                    INTENT(INOUT) :: INFO
SUBROUTINE VARCRCPACKING(N,DIM,UPLO,zero,A,VALUES,COLUMNS,ROWINDEX,INFO)
 INTEGER,
                      INTENT(IN)
 INTEGER,
                      INTENT(INOUT) :: INFO,DIM
 CHARACTER,
                      INTENT(IN)
                              :: UPLO
 DOUBLE PRECISION,
                      INTENT(IN)
                                :: ZERO
 COMPLEX*16, DIMENSION(N, N), INTENT(IN)
                                :: A
 COMPLEX*16, DIMENSION(DIM), INTENT(OUT) :: VALUES
          DIMENSION(DIM), INTENT(OUT) :: COLUMNS
 INTEGER.
 INTEGER,
          DIMENSION(N+1), INTENT(OUT) :: ROWINDEX
14
    Python Wrappers prototypes
14.1
     Initialisation
deffloquetinit(id,*argsv,info): id is an instance of the class atom_cT, declared as id=openmmf.atom_cT().info
0 is an python integer.
  This function can be take several forms to define different physical systems.
  To declare a qubit type use openmmf.floquetinit(id, 'qubit', info=info).
  To declare an alkali atom and one option of the electronic ground state hyperfine manifold use openmmf.floquetinit(i
alkali_name taking any of the values '87Rb', '85Rb', '123Cs', '41K', '23Na', and manifold one of 'U', 'L', 'B'
, to define the Lower, Upper or Both hyperfine manifoldds of the electronic ground state, respectively.
  To define a spin of total angular momentum S, use openmmf.floquetinit(id,'spin',S,info=info)
  To define an arbitrary system with N energy levels use openmmf.floquetinit(id,'lattice',N,info=info)
  {\tt defsethamiltonian components}({\tt id}, {\tt modes}_n um, fields, info): idisaninstance of atom_{cT} modes_n umannum py. array fields, info)
def multimode floquet matrix (id, modes_num, fields, info):
  \operatorname{def} \operatorname{lapack}_{f} ulleigenvalues(U_{F}, h_{f} loguet_{s} ize, e_{f} loguet, in fo):
  ______
def multimodetransitionavg(h_f loquet_s ize, fields, modes_n um, U_F, e_f loquet, d_b are, p_a vg, info):
  ______
FOURIER COMPONENTS OF THE TRANSFORMATION BETWEEN THE DRESSED AND THE BARE
def multimode floquet transformation (modes_num, U_F, e_floquet, d_bare, fields, t1, U_B 2D, info):
  ______
def multimode micromotion(id, h_f loquet_size, modes_num, U_F, e_f loquet, d_bare, fields, t1, U_B2D, info):
  ______
COMP. ROUTINE: EVALUATE THE TIME EVOULUTION OPERATOR BETWEEN T1 AND T2 US-
ING THE FOURIER DECOMPOSITION OF THE MICROMOTION OPERATOR, WHICH IS STORE IN
```

def timeevolutionoperator(id, d_bare , $modes_num$, fields, t1, t2, U, info):

DRIVER ROUTINE: EVALUATE THE TIME EVOULUTION OPERATOR BETWEEN T1 AND T2

