

# Documentation for the General QMC code

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## 1 Theory part

### 1.1 Definition of the physical Hamiltonian and its implementation

The physical Hamiltonians that we can simulate have the general form:

$$\mathcal{H} = \sum_{s=1}^{N_{fl}} \sum_{x,y} c_{xs}^\dagger T_{xy} c_{ys} - \sum_{k=1}^M U_k \left[ \sum_{s=1}^{N_{fl}} \sum_{x,y} \left( c_{xs}^\dagger V_{xy}^{(k)} c_{ys} - \alpha_k \right) \right]^2. \quad (1)$$

Note, that we introduced *two* different labels to address spin degrees of freedom:

- The number of spin flavours is set by  $N_{fl}$ .
- The number  $N_{sun}$  also labels spin states and specifically sets the symmetry group of the fermions, namely the dimension of the special unitary group  $SU(N_{sun})$ .

And the following labels specify the lattice sites:

- The indices  $x, y$  are multi-indices that label degrees of freedom, containing lattice sites and spin states:  $x = (i, \sigma)$ , where  $i = 1, \dots, N_{sites}$  and  $\sigma = 1, \dots, N_{sun}$ , so

$$\sum_{x,y} \equiv \sum_{i=1, j=1}^{N_{sites}} \sum_{\sigma=1, \sigma'=1}^{N_{sun}}. \quad (2)$$

- The number of correlated sites which is a subset of all sites, is labelled by  $M$  ( $M \leq N_{sites}$ ).
- Let us further define  $N_{dim} = N_{sun} N_{sites}$  such that the matrices  $\mathbf{T}$  and  $\mathbf{V}^{(k)}$  are of dimension  $N_{dim} \times N_{dim}$
- $N_{sites}$  is the total number of spacial vertices:  $N_{sites} = N_{unit\ cell} N_{orbital}$ , where  $N_{unit\ cell}$  is the number of unit cells of the underlying Bravais lattice and  $N_{orbital}$  is the number of (spacial) orbitals per unit cell **Check the definition of  $N_{orbital}$  in the code.**

### 1.2 Structure of the matrices $\mathbf{T}$ and $\mathbf{V}^{(k)}$ and their implementation

In general, the matrices  $\mathbf{T}$  and  $\mathbf{V}^{(k)}$  are sparse matrices. This property is used to minimize computational cost and storage. In the following, we discuss the implementation of the single-particle matrix representation  $\mathbf{V}^{(k)}$  of the interaction operator. The same logic applies for the hopping matrix  $\mathbf{T}$ .

We denote a subset of  $N_{eff}$  (**in the code,  $N_{eff}$  is called just  $N$** ) degrees of freedom by the set  $[z_1, \dots, z_{N_{eff}}]$  and define it to contain only vertices for which an interaction term is defined:

$$V_{xy}^{(k)} \neq 0 \quad \text{only if} \quad x, y \in [z_1^{(k)}, \dots, z_{N_{eff}}^{(k)}]. \quad (3)$$

We define the projection matrices  $\mathbf{P}_V^{(k)}$  of dimension  $N_{eff}^{(k)} \times N_{dim}$ :

$$(P_V^{(k)})_{i,z} = \delta_{z_i^{(k)},z}, \quad (4)$$

where  $i \in [1, \dots, N_{eff}^{(k)}]$  and  $z \in [1, \dots, N_{dim}]$ . The matrix operator  $\mathbf{P}_V^{(k)}$  picks out the non-vanishing entries of  $\mathbf{V}^{(k)}$ , which are contained in the  $(N_{eff}^{(k)} \times N_{eff}^{(k)})$  - dimensional matrix  $\mathbf{O}_V^{(k)}$ :

$$\mathbf{V}^{(k)} = \mathbf{P}_V^{(k)T} \mathbf{O}_V^{(k)} \mathbf{P}_V^{(k)}, \quad (5)$$

and

$$V_{xy}^{(k)} = (P_V^{(k)})_{ix} \left[ O_V^{(k)} \right]_{ij} (P_V^{(k)})_{jy} = \sum_{i,j}^{N_{eff}^{(k)}} \delta_{z_i^{(k)},x} \left[ O_V^{(k)} \right]_{ij} \delta_{z_j^{(k)},y}. \quad (6)$$

**Comment that the P matrices have only one non-vanishing entry per column.** To set the interaction part, we therefore have to specify the following:

- the matrix elements  $\left[ O_V^{(k)} \right]_{ij}$
- the set  $[z_1^{(k)}, \dots, z_{N_{eff}^{(k)}}^{(k)}]$
- the interaction strenghts  $U_k$
- the numbers  $\alpha_k$ .

**Be more specific here what really has to be specified in the actual code.** The same logic also applies to the implementation of the hopping interaction **be more specific**.

### 1.3 The Hubbard-Stratonovich decomposition

#### 1.4 Implementation: the Operator variable

In the code implementation, we define a structure called **Operator**. This structure variable **Operator** bundles several components that are needed to define and use an operator matrix in the program. In Fortran a structure variable like this is called a derived type. The components it contains are:

- the projector  $\mathbf{P}_V$ ,
- the matrix  $\mathbf{O}_V$ ,
- the effective dimension  $N_{eff}$ ,
- and a couple of auxiliary matrices and scalars.

In general, we will not only have one structure variable **Operator**, but a whole array of these structures.

## 2 Tutorial to set up the $SU(2)$ -Hubbard model on a square lattice

The  $SU(2)$  symmetric Hubbard model is given by

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} \left( c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.c.} \right) + \frac{U}{2} \sum_i \left[ \sum_\sigma \left( c_{i\sigma}^\dagger c_{i\sigma} - 1/2 \right) \right]^2. \quad (7)$$

Name of variable in the code	Description
Op_V%N	effective dimension $N_{eff}$
Op_V%O	matrix $\mathbf{O}_V$
Op_V%U	matrix containing the eigenvectors of $\mathbf{O}_V$
Op_V%E	eigenvalues of $\mathbf{O}_V$
Op_V%P	projection matrix $\mathbf{P}_V$
Op_V%N_non_zero	number of non-vanishing eigenvalues of $\mathbf{O}_V$
Op_V%g	coupling strength in Hubbard-Stratonovich transformation
Op_V%alpha	constant, to set particle-hole symmetry <b>correct?</b>

Table 1: Components of the **Operator** structure variable **Op\_V**.

To bring Eq. (7) in the general form (1), we set

$$\begin{aligned}
N_{fl} &= 1 \\
N_{sun} &= 2 \\
T_{xy} &= -t\delta_{\langle i,j \rangle}\delta_{\sigma,\sigma'} \\
M &= N_{sites} \\
U_k &= -U/2 \\
V_{xy}^{(k)} &= \delta_{x,y}\delta_{i,k} = \delta_{i,j}\delta_{\sigma,\sigma'}\delta_{i,k} \\
\alpha_k &= 1/(N_{sites}N_{sun})^2 = 1/(2N_{sites})^2.
\end{aligned} \tag{8}$$

In the following, we skip the  $N_{sun}$ -spin degree of freedom which is present in the multi-indices  $x, y$  of the matrices  $\mathbf{T}$  and  $\mathbf{V}^{(k)}$ . So  $N_{dim} = N_{sites}$ .

**What is the role of the  $N_{sun}$  index in the code?**

- it appears in the coupling  $g$  in the **Operator** structure.
- it appears as a normalization constant in the definition of observables
- it appears as exponent in the calculation of the phase factor and the update ratio

**Is the code limited to  $SU(N)$  symmetric models with respect to the  $N_{sun}$  degree of freedom?**

Note that in this example  $N_{dim} = Latt\%N$  since there is only one spacial orbital per unit cell of the underlying Bravais lattice.

## 2.1 Hopping term

The hopping matrix is implemented as follows. We allocate an array of dimension  $1 \times 1$ , called **Op\_T**. It therefore contains only a single **Operator** structure. We set the effective dimension (here,  $N_{eff} = N_{dim}$ ), and allocate and initialize this structure by a single call to the subroutine **Op\_make**:

```
call Op_make(Op_T(1,1),Ndim)
```

Since the effective dimension is identical to the total dimension, it follows trivially, that  $\mathbf{P}_T = \mathbf{1}$  and  $\mathbf{O}_T = \mathbf{T}$ . **Although a checkerboard decomposition is not yet used for the Hubbard model, in principle it can be implemented.**

## 2.2 Interaction term

To implement this interaction, we allocate an array of **Operator** structures. The array is called **Op\_V** and has dimensions  $N_{dim} \times N_{fl} = N_{sites} \times 1$ . We set the effective dimension,  $N_{eff} = 1$ , and allocate and initialize this array of structures by repeatedly calling the subroutine **Op\_make**:

```

N_sites = Latt%N
N_fl = 1
N_eff = 1

do nf = 1, N_FL
do i = 1, Latt%N
call Op_make(Op_V(i,nf),N_eff)
enddo
enddo

```

For each lattice site  $i$ , the projection matrices  $\mathbf{P}_V^{(i)}$  are of dimension  $1 \times N_{dim}$  and have one non-vanishing entry:  $(P_V^{(i)})_{1j} = \delta_{ij}$ . The effective matrices are again trivial:  $\mathbf{O}_V^{(i)} = 1$ .

Name of variable in the code	Description
Ndim	Spacial dimension of the lattice (total number of sites) <i>what about the <math>N_{sun}</math>?</i>
Latt%N	Number of unit cells of the underlying Bravais lattice
Op.T	Array of structure variables that bundles all variables needed to define the hopping operator.
Op.V	Array of structure variables that bundles all variables needed to define the two-particle interaction operator.
N_sun	Number of spin states of the $SU(N_{sun})$ -symmetric fermions
N_fl	Number of spin flavors

Table 2: Common variables that are set in the Hamiltonian, operator and lattice modules of the code.

## 2.3 Definition of the lattice

This is set in the subroutine `Ham_latt`. The square lattice is already implemented. In principle, one can specify other lattice geometries and use them by specifying the keyword `Lattice_type` in the parameter file.

## 2.4 Observables for the Hubbard model

To do next:

- dicuss the measurements: what observables exit and how do I add a new one?
- discuss the implementation of the lattice.
- discuss the Hubbard-Stratonovich decompositions (this is related to the coupling in the operator structure), discuss also the spin-symmetry-breaking HS-decomposition for the Hubbard model.

# 3 Tutorial to set up a lattice

# 4 Tutorial to define observables

## 5 Input and output of the code

### 5.1 The parameter file

## 6 Using the code

*Example simulation, tutorial: where to find and how to start*

### 6.1 Parameter files

*describe the input parameters, give sample values for the stabilization parameters*

### 6.2 Analysis files

*how the analysis of Monte Carlo data is done*

## 7 List of files

*all files that constitute the code, with a brief description*

### 7.1 `cgr1.f90` & `cgr2.f90`

Stable computation of the physical single-particle equal time Green function  $G(\tau)$ .

## 7.2 control\_mod.f90

Includes a set of auxiliary routines, regarding the flow of the simulation. Examples are initialization of performance variables, precision tests and controlled termination of the code.



### 7.3 gperp.f90

## 7.4 Hamiltonian\_Hub.f90

Here, the physical simulation parameters (the model parameters) and the lattice parameters are read in. The lattice, the non-interacting and the interacting part of the Hubbard Hamiltonian are set according to the parameters and the chosen Hubbard-Stratonovich decomposition.

## 7.5 Hop\_mod.f90

## 7.6 inconfc.f90

The auxiliary-field QMC method is based on a Hubbard-Stratonovich decomposition of the interaction term. This decomposition introduces a space-time array of (discrete) configurations of auxiliary fields, i.e. Ising spins. In this routine, an existing configuration is read in, checks on its dimensionality are made and, in case no prior configuration exists, a random configuration of Ising spins is set up.

## 7.7 main.f90

Top-level part of the program. Here, the program flow which consists of initialization, sweeps through the space-time lattice, and finalizing the program, is coded.

## 7.8 nranf.f90

Auxiliary routine controlling the evaluation of random numbers.

## 7.9 Operator.f90

The algorithm is centered around evaluation of single-particle operators, represented as square matrices. In this routine, the abstract type `Operator` is defined, including information on the coupling strength, the sites that participate in the single-particle hopping process, and the type of Hubbard-Stratonovich transformation. This routine collects all program relevant operations that are applied to the type `Operator`, like initializations or multiplications.

## 7.10 outconfc.f90

Description in plain text:

At the end of the simulation, the last configuration of Hubbard-Stratonovich variables, together with the last set of random numbers is written to the file confout.

Prior to the start of a new simulation of the identical space-time dimesion, one can (manually) copy the file confout to the file confin and make the new run use the old configuration.

Doing this saves warmup time compared to a complete random (unphysical) configuration.

Input/output variables

in:

inout:

inout:

out:

Dependencies

include: mpif.h

modules: Hamiltonian

interfaces:

global variables: ntrot, nsigma

subroutines: MPI\_COMM\_RANK, MPI\_COMM\_SIZE, Get\_seed\_Len, Ranget

Things to check:

Rename subroutine to confout.f90 for consistency



## 7.11 print\_bin\_mod.f90

Description in plain text:

Here the way to write the measure bins to the respective output files is coded.

A bin is an average over many individual measurements.

The bin defines the unit of Monte Carlo time.

Dependencies

include:

modules:

interfaces: Print\_bin

Contains

subroutines: Print\_bin\_c, Print\_bin\_r, Print\_scal, Print\_bin\_tau

Things to check:

### 7.11.1 Print\_bin\_C

Description in plain text:

Input/output variables

in: Latt, type(Lattice)

in: Phase\_bin\_tmp, complex

in: File\_pr, character(Len=64)

in: nob, integer

inout: Dat\_eq(:, :, :), complex

inout: Dat\_eq0(:), complex

out:

Dependencies

include: mpif.h

modules: Lattices\_v3

interfaces:

global variables: TYPE(LATTICE), N, listk, b1\_p, b2\_p

subroutines: MPI\_COMM\_RANK, MPI\_COMM\_SIZE, MPI\_REDUCE, Fourier\_R\_to\_k

Things to check:

STATUS(MPI\_STATUS\_SIZE), integer, needed?

### 7.11.2 Print\_bin\_R

Description in plain text:

Input/output variables

in: Latt, type(Lattice)

in: Phase\_bin\_tmp, complex

in: File\_pr, character(Len=64)

in: nob, integer

inout: Dat\_eq(:, :, :), real

inout: Dat\_eq0(:), real

out:

Dependencies

include: mpif.h

```

modules: Lattices_v3
interfaces:
global variables:  TYPE(LATTICE), N, listk, b1_p, b2_p
subroutines:  MPI_COMM_RANK, MPI_COMM_SIZE, MPI_REDUCE, Fourier_R_to_k

Things to check:
STATUS(MPI_STATUS_SIZE), integer,  needed?

```

### 7.11.3 Print\_scal

Description in plain text:

```

Input/output variables
in: File_pr, character(Len=64)
in: nobs, integer
inout: Obs,:), complex
out:

```

```

Dependencies
include: mpif.h
interfaces:
global variables:
subroutines:  MPI_COMM_RANK, MPI_COMM_SIZE, MPI_REDUCE

```

```

Things to check:
STATUS(MPI_STATUS_SIZE), integer,  needed?
change subroutine name to print_bin_scal for consistency

```

### 7.11.4 Print\_bin\_tau

Description in plain text:

```

Input/output variables
in: Latt, type(Lattice)
in: Phase_bin, complex
in: File_pr, character(Len=64)
in: nobs, integer
in: dtau, real
inout: Dat_tau(:, :, :, :), complex
inout, optional: Dat0_tau(:, :, :), complex
out:

```

```

Dependencies
include: mpif.h
modules: Lattices_v3
interfaces:
global variables:  TYPE(LATTICE), N, listk, b1_p, b2_p
subroutines:  MPI_COMM_RANK, MPI_COMM_SIZE, MPI_REDUCE, Fourier_R_to_k

```

```

Things to check:
STATUS(MPI_STATUS_SIZE), integer,  needed?

```

## 7.12 tau\_m.f90

Description in plain text:

module tau\_m\_mod, with several subroutines

Dependencies

include:

modules: Hamiltonian, Operator\_mod, Precdef, Control, Hop\_mod

Contains

subroutines: tau\_m, propr, proprm1

Things to check:

change file name to tau\_m\_mod.f90 for consistency

### 7.12.1 TAU\_M

Description in plain text:

Input/output variables

in: nstm, integer

in: nwrap, integer

in: ust(ndim,ndim; nstm,n\_fl), complex

in: vst(ndim,ndim,nstm,n\_fl), complex

in: dst(ndim,nstm,n\_fl), complex

in: GR(ndim,ndim,n\_fl), complex

in: phase, complex

in: stab\_nt(0:nstm), integer

inout:

inout:

out:

Dependencies

include:

modules:

interfaces: wrapul, cgr2\_1, cgr2\_2, cgr2

global variables: ndim, n\_fl, cone, ltrot

subroutines: obsert, initd, propr, proprm1, wrapur, cgr2\_2, Control\_Precision

Things to check:

cone?

### 7.12.2 propr

Description in plain text:

Input/output variables

in: nt

inout: Ain(ndim,ndim,n\_fl)

inout:

out:

Dependencies

include:

modules:

interfaces:  
global variables: ndim, n\_fl, op\_v, nsigma, Phi, type  
subroutines: Hop\_mod\_mmthr, Op\_mmultR

Things to check:

### 7.12.3 proprml

Description in plain text:

Input/output variables

in: nt

inout: Ain(ndim,ndim,n\_fl)

inout:

out:

Dependencies

include:

modules:

interfaces:

global variables: ndim, n\_fl, op\_v, nsigma, Phi, type

subroutines: Hop\_mod\_mmthl, Op\_mmultL

Things to check:

### 7.13 UDV\_WRAP.f90

Description in plain text:

UDV\_Wrap\_mod is a module file, containing subroutines on the stabilization of matrix computations.

Dependencies

modules: MyMats, Files\_mod

Contains

subroutines: UDV\_Wrap\_Pivot, UDV\_Wrap

Things to check:

change file name to UDV\_Wrap\_mod.f90 for consistency

#### 7.13.1 UDV\_Wrap\_Pivot

Description in plain text:

Input/output variables

in: A(:, :), complex

in: ncon, integer

in: n1, integer

in: n2, integer

inout: U(:, :), complex

inout: V(:, :), complex

inout: D(), complex

out:

Dependencies

include:

modules:

interfaces:

global variables:

subroutines: UDV\_Wrap, MMULT, Compare

Things to check:

#### 7.13.2 UDV\_Wrap

Description in plain text:

Input/output variables

in: A(:, :), complex

in: ncon, integer

inout: U(:, :), complex

inout: V(:, :), complex

inout: D(), complex

out:

Dependencies

include: mpif.h

modules:

interfaces:

global variables:

subroutines: MPI\_COMM\_SIZE, MPI\_COMM\_RANK, QR, SVD, MMULT

Things to check:

STATUS(MPI\_STATUS\_SIZE), integer: not used

## 7.14 upgrade.f90

Description in plain text:

The update of the Hubbard-Stratonovich configuration is done sequentially for each point in the space-time lattice, i.e. one Hubbard-Stratonovich Ising spin after the other. In this routine, an update (i.e. a spin flip) is accepted or rejected. The decision is made using the Metropolis method of importance sampling.

Input/output variables

in: N\_op, integer  
in: nt, integer  
in: OP\_dim, integer  
inout: GR(ndim,ndim,n\_fl), complex  
inout: Phase, complex  
out:

Dependencies

include:  
modules: Hamiltonian, Random\_wrap, Control, Precdef  
interfaces:  
global variables: ndim, n\_fl, op\_v, nflipl, Phi, n\_non\_zero, Gaml, P, nsigma, g, alpha, type, E  
subroutines: zgemm, control\_upgrade

Things to check:

nranf, integer, external (where is external fct. defined)  
log, logical (reserved name)  
alpha: both a local and a global variable. CHECK!!

## 7.15 wrapgrdo.f90

Description in plain text:

Single-particle equal-time Green functions are the central object of the code.

The physical single-particle equal-time Green function  $G(\tau)$  is updated in wrapgrdo.f90 (down propagation, from  $\tau=LTROT$  to  $\tau=0$ ).

The update is sequentially, over all (interacting) lattice sites or lattice bonds.

Input/output variables

in: ntau, integer

inout: gr (ndim,ndim,n\_fl), complex

inout: phase, complex

out:

Dependencies

include:

modules: Hamiltonian, MyMats, Hop\_mod

interfaces: upgrade

global variables: op\_v, phi, nsigma, ndim, n\_fl

subroutines: Hop\_mod\_mmthl, Hop\_mod\_mmthr\_m1, Op\_Wrapdo, Upgrade

Things to check:



## 7.16 wrapgrup.f90

Description in plain text:

Single-particle equal-time Green functions are the central object of the code.

The physical single-particle equal-time Green function  $G(\tau)$  is updated in wrapgrup.f90 (up propagation, from  $\tau=0$  to  $\tau=L\tau_{\text{ROT}}-1$ ).

The update is sequentially, over all (interacting) lattice sites or lattice bonds.

Input/output variables

in: ntau, integer

inout: gr (ndim,ndim,n\_fl), complex

inout: phase, complex

out:

Dependencies

include:

modules: Hamiltonian, Hop\_mod

interfaces: upgrade

global variables: op\_v, phi, nsigma, ndim, n\_fl

subroutines: Hop\_mod\_mmthr, Hop\_mod\_mmthl\_m1, Op\_Wrapup, Upgrade

Things to check:

## 7.17 wrapul.f90

Description in plain text:

To stabilize the simulation at the time slice  $\tau_2 = i n_{\text{stab}}$ , the Green function has to be recomputed regularly, based on the stable matrices at an earlier stabilization point,  $\tau_1 = (i-1) n_{\text{stab}}$ . These stable matrices result from a singular-value-decomposition of the propagation matrix. They are computed in wrapul.f90 (down propagation).

Input/output variables

in: ntau1, integer  
in: ntau, integer  
inout: ulup (ndim,ndim,n\_fl), complex  
inout: dlup (ndim,n\_fl), complex  
inout: vlup (ndim,ndim,n\_fl), complex  
out:

Dependencies

include:  
modules: Hamiltonian, Hop\_mod, UDV\_Wrap\_mod  
interfaces:  
global variables: ndim, n\_fl, Op\_V, Phi, nsigma,  
subroutines: initd, Op\_mmultL, Hop\_mod\_mmthl, mmult, UDV\_Wrap

Things to check:

## 7.18 wrapur.f90

Description in plain text:

To stabilize the simulation at the time slice  $\tau_2 = i n_{\text{stab}}$ , the Green function has to be recomputed regularly, based on the stable matrices at an earlier stabilization point,  $\tau_1 = (i-1) n_{\text{stab}}$ . These stable matrices result from a singular-value-decomposition of the propagation matrix. They are computed in wrapur.f90 (up propagation).

Input/output variables

in: ntau1, integer  
in: ntau, integer  
inout: ur (ndim,ndim,n\_fl), complex  
inout: dr (ndim,n\_fl), complex  
inout: vr (ndim,ndim,n\_fl), complex  
out:

Dependencies

include:  
modules: Hamiltonian, Hop\_mod, UDV\_Wrap\_mod  
interfaces:  
global variables: ndim, n\_fl, Op\_V, Phi, nsigma,  
subroutines: initd, Op\_mmultR, Hop\_mod\_mmtlr, mmult, UDV\_Wrap

Things to check:

Description in plain text:

Input/output variables

in:

inout:

inout:

out:

Dependencies

include:

modules:

interfaces:

global variables:

subroutines:

Things to check:

## 8 Module Hamiltonian

*Detailed description of the module Hamiltonian since it will be modified by the users*

The module contains the following subroutines:

### 8.1 ham\_set

It calls the subroutines

- ham\_latt
- ham\_hop
- ham\_v

It reads in the file

- parameters

It sets the variables `ltrot`, `n_fl`, `n_sun`. If compiled as a MPI-program, it broadcasts all variables that define the lattice, the model and the simulation process.

### 8.2 ham\_latt

It sets the lattice, by calling the subroutine

- make\_lattice(l1\_p, l2\_p, a1\_p, a2\_p, latt)

### 8.3 ham\_hop

Setup of the hopping amplitudes between the vertices of the graph (lattice sites and unit cell orbitals). It calls the subroutines

- op\_make(op\_t(nc,n),ndim
- op\_set(op\_t(nc,n))

## 8.4 ham\_v

It calls the subroutines

- op\_make(op\_v(i,nf),1)
- op\_set( op\_v(nc,nf) )

## 8.5 s0(n,nt)

It is defined as  $s0(n, nt) = 1.d0$ . Why? It is superfluous.

## 8.6 alloc\_obs(ltau)

Allocation of equal time and time-resolved quantities.

## 8.7 init\_obs(ltau)

Initializes equal time and time-resolved quantities with zero.

## 8.8 obser(gr,phase,ntau)

Includes the definition of all equal-time observables (scalars and correlation functions) that are built from the single-particle Green function based on Wick's theorem.

## 8.9 pr\_obs(ltau)

Output (print) of the observables.

## 8.10 obsert(nt,gt0,g0t,g00,gtt,phase)

Includes the definition of time-resolved observables that are built from the time-resolved single-particle Green function based on Wick's theorem.

# 9 Installation

## 9.1 Dependencies

*which software and libraries are needed and which version*

- libraries: LAPACK, BLAS, EISPACK, NAG *They are included in the package, but NAG is not public-domain (?)*
- tools: cmake
- compiler: gfortran or ifort

## 9.2 Build the GQMC program from source code

*configuration, compile and Installation* In the top level directory, where the README file resides, do:

```
mkdir build
cd build
cmake ..
make
```

## **10 Reference manual**

## **11 License**

Use of the GQMC code requires citation of the paper ... The GQMC code is available for academic and non-commercial use under the terms of the license ... For commercial licenses, please contact the GQMC development team.

## **12 ideas**

FAQ, walkthroughs,