Documentation for the General QMC code

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1 Definition of the model Hamiltonian

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

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

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 specifially 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 $i = 1, \cdots N_{sites}$ and $\sigma = 1, \cdots N_{sun}$, so

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

- 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 $\boldsymbol{T}$ and $\boldsymbol{V}^{(k)}$ 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.

1.1 Structure of the hopping matrix T and the interaction matrices $\mathbf{V}^{(k)}$

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 $[z_1, \cdots z_{N_{eff}}]$ and define it to contain only vertices for which an interaction term is defined:

$$V^{(k)}_{xy} \neq 0 \quad \text{only if} \quad x, y \in [z^{(k)}_1, \cdots z^{(k)}_{N^{(k)}_{eff}}] . \tag{3}$$

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

$$(P^{(k)}_V)_{i,z} = \delta_{z^{(k)}_i, z} , \tag{4}$$

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

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

and

$$V^{(k)}_{xy} = (P^{(k)}_V)_{ix} \left[O^{(k)}_V \right]_{ij} (P^{(k)}_V)_{jy} = \sum_{i,j}^{N^{(k)}_{eff}} \delta_{z^{(k)}_i, x} \left[O^{(k)}_V \right]_{ij} \delta_{z^{(k)}_j, y} . \tag{6}$$

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 $[z_1^{(k)}, \cdots z_{N_{eff}^{(k)}}^{(k)}]$
- the interaction strenghts U_k
- the numbers α_k.

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

1.2 The Hubbard-Stratonovich decomposition

2 Implementation of a model Hamiltonian

We only have to write the subroutine for the Hamiltonian. A template is given by `Hamiltonian_template.f90`. Existing model subroutines are `Hamiltonian_Hubb.f90`.

2.1 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 $\boldsymbol{P}_V$,
- the matrix $\boldsymbol{O}_V$,
- 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.

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 correct?

Table 1: Components of the `Operator` structure variable `Op_V`.

2.2 The observables

2.3 The lattice

3 Input and output files

4 Walkthrough: the $SU(2)$-Hubbard model on a square lattice

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

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

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

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

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

4.1 Hopping term

The hopping matrix is implemented as follows. We allocate an array of dimension 1×1, 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 $\boldsymbol{P}_T = \mathbb{1}$ and $\boldsymbol{O}_T = \boldsymbol{T}$. Although a checkerboard decomposition is not yet used for the Hubbard model, in principle it can be implemented.

4.2 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 $\boldsymbol{P}_V^{(i)}$ 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: $\boldsymbol{O}_V^{(i)} = 1$.

Name of variable in the code	Description
`Ndim`	Spacial dimension of the lattice (total number of sites) what about the N_{sun}?
`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.

4.3 Definition of the square 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.

4.4 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.

5 Tutorial: set up a model Hamiltonian

based on the (not yet existing) template `Hamiltonian_template.f90`.