# Short overview over the general operator module for kwant

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These few pages are meant to help to understand the working flow of the general operator module. I know that lots of aspects are still superficial and not very precise and that many details are not correct in this manuscript, but I hope that it still helps to understand the bigger picture working flow. At the moment, we want to calculate objects of the form

$$\psi_a^* M_a O_{ab} M_b O_{bc} \dots O_{xy} M_y \phi_y, \tag{1}$$

where $[O_{ab}, O_{bc}, \dots, O_{xy}]$ and $[M_a, M_b, \dots, M_y]$ are the user-defined lists for the hopping operator and the onsite matrices, respectively.

## I. KWANT.OPERATOR._LOCALOPERATOR

To begin with, let me summarize the important steps in the kwant.operator._LocalOperator such that it is easier to see the differences and extensions for the general operator.

**__init__():**

- store class variables
- normalize where to a unified format

**__call__():**

- create result_array (numpy array)
- call _operate

**_operate (at the example of Current, but similar in other cases):**

- preparation: create 1-2 (one for the hopping=hamiltonian and maybe one for the onsite if it is not unique) instances of BlockSparseMatrix (BSM), H_ab_blocks and M_a_blocks, which contains all the information needed for the calculation:
  - BSM.get(w): returns the operator matrix which belongs to the element 'w' of the where-list
  - BSM.block_shapes(w,0/1): returns number of orbitals of the corresponding site 'where[w,0/1]'
  - BSM.block_offsets(w,0/1): returns the first index which belongs to the corresponding site 'where[w,0/1]' in the wave function
- loop over all 'where'-elements and calculate the expectation value. For the chosen 'where'-element 'w'...
  - ... get the number of orbitals, a_norbs and b_norbs, via H_ab_blocks.block_shapes(w,0/1)
  - ... get the wave function start_index, a_s and b_s, via H_ab_blocks.block_offsets(w,0/1)
  - ... get the explicit hopping matrix H_ab via H_ab_blocks.get(w)
  - ... get the explicit onsite matrix M_a via M_a_blocks.get(w)
  - ... sum over all orbitals:

$$\sum_{i,j=1}^{a_{norbs}} \sum_{k=1}^{b_{norbs}} \psi^*(a_s + i) M_a(i,j) H_{ab}(j,k) \phi(b_s + k) \tag{2}$$

for the given wave functions $\psi$ and $\phi$. $i$, $j$ and $k$ are orbital indexes.

## II. GENERAL OPERATOR

### A. The calculation of the matrix element in _operate

There is one major differences for the general operator compared to the kwant.operator: there are more (arbitrary number of) onsite and hopping operators, which is why we need lists of most objects, see the following tabular.

| kwant.operator(.Current)._operate() | general.Operator._operate() |
|---|---|
| · create 2 BlockSparseMats | · create list of BlockSparseMats (for each operator) |
| · get a_norbs, b_norbs | · get list x_norbs (for each hopping site) |
| · get the explicit matrix $M_a$ | · get a list of onsite mats |
| · get the explicit matrix $H_{ab}$ | · get a list of hopping mats |
| · get wave function start indexes a_s and b_s | · get wave function start indexes bra_start and ket_start |

Since we do not know how many operators there are, the looping over all needed sites and filling the lists for one given site combinations is handled by recursive functions.

$$\sum_{o1_a,o2_a,o1_b,o2_b,\ldots} \underbrace{\psi^*(bra\_start + o1_a)M[0](o1_a,o2_a)}_{\text{pre rec funcs}} \underbrace{\times O[0](o2_a,o1_b)M[1](o1_b,o2_b)}_{\text{rec func step}} \times \ldots \times \underbrace{\times O[N-1](o2_x,o1_y)M[N](o1_y,o2_y)}_{\text{rec func step}} \underbrace{\times \phi(ket\_start + o2_y)}_{\text{rec func end}} \tag{3}$$

In the code so far, there are actually 2 recursive functions, one for looping over all sites and filling the lists for a given site combinations (sitesum_recfunc) and one for doing the actual sum over the orbitals (orbsums_recfunc). It would be possible to combine them in one function, but for me it seems to be more clear having separated the two steps.

### B. The problem of the wherelist

The only conceptual problem is how to tell the different operator for which sites/hoppings they are nonzero (or where they are supposed to be calculated). In the current state of implementation, a list of list of hoppings is given:

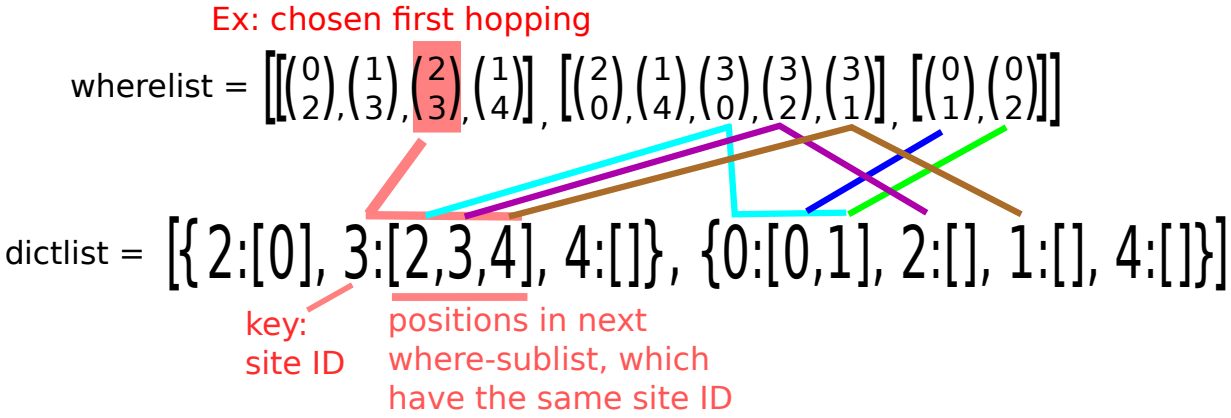
$$\text{wherelist} = \left[\left[\begin{pmatrix} a_1 \\ b_1 \end{pmatrix}, \begin{pmatrix} \cdot \\ \cdot \end{pmatrix}, \ldots \text{a-b-hops}\right], \left[\begin{pmatrix} \cdot \\ \cdot \end{pmatrix}, \ldots \text{b-c-hops}\right], \ldots\right]. \tag{4}$$

We only want to consider "connected" hoppings in the sense that for a given 'a-b-hopping', e.g. ($a_{10}$,$b_4$), only 'b-c-hoppings' should be considered which have the same b-site, e.g. ($b_4$,$c_7$) or ($b_4$,$c_{105}$). The same is true for all the other hoppings. Note that the wherelist above contains all the information needed, not only for the hopping operator but also for the onsite matrices.

To manage to calculate only the appropriate terms, we create in genOp.__init__() a list of dicts which has the site-IDs as keys and returns a list of the positions of all hoppings in the next hopping-level whose first element is this particular site:

$$\begin{aligned} \text{dictlist} = \Big[ &\{b_1 : [5, 3, 42, \ldots \text{(positions in wherelist[1] whose b-site is } b_1)], b_2 : [\ldots], \ldots\}, \\ &\{c_1 : [7, 13, \ldots \text{(positions in wherelist[2] whose c-site is } c_1)], c_2 : [\ldots], \ldots\}, \\ &\{\ldots\}, \ldots \Big] \end{aligned} \tag{5}$$

Since I know which Site is under consideration at the moment, I can find out all the related hoppings of the next operator (in the next where-sublist) with the help of dict_list and wherelist — that's all I need. Here is an example of how the dictlist looks like for a given wherelist and how to find the related hoppings in the next where-sublist:




Note that for efficiency reasons, instead of the dicts, we use two auxiliary 1d-arrays, (wherepos_neigh and posaux_list). Moreover, the wherelist is also flattened to 1d-arrays of hoppings together with one auxiliary list (auxwhere_list) which tells the starting positions of the prior sublists in the flattened where. At the moment I will not discuss the creation and the details of the auxiliary lists here, since these details are not necessary to understand the working mechanism of the general operator.

To finish, let me summarize the steps which happen in the **general.operator.__init__():**

- store class variables
- normalize where-sublists and flatten 'where' to 1d-array of hoppings
- create dictlist (and create two auxiliary lists to be used instead of dictlist for efficiency reasons)
- create list of all site combinations. This is used to be able to find out which output data belongs to which site-combination
- normalize hopping operators and onsite operators
- (initialize BlockSparseMat-lists)

**general.operator.__call__():**

- create result_array (numpy array)
- call _operate

As a last comment, I want to state that the result array is not directly obvious as opposed to the kwant.operators, in which the result array is directly related to 'where'. Since in the general operator case, all the site paths first have to be precomputed from the given wherelist, not even the result length is predetermined. For that reason, in genOp.__init__(), a list of all site-paths is created (self.sitechains) which has the same structure as the result array. This list directly tells which result in the output-array belongs to which site path.