AFQMC_METROPLIS note.

Hao Shi

* use second order trotter breakup:

$$e^{-\tau \hat{H}} = e^{-\tau \hat{K}/2}\ e^{-\tau \hat{V}}\ e^{-\tau \hat{K}/2}$$

set: $e^{-\tau \hat{K}/2} = \square$, $e^{-\tau \hat{V}} = 0$

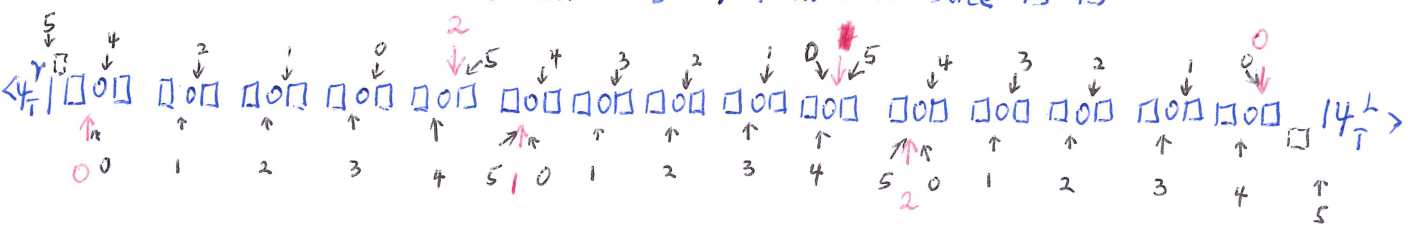
$$e^{-\tau \hat{H}}\ e^{-\tau \hat{H}} = e^{-\tau \hat{K}/2}\ e^{-\tau \hat{V}} \boxed{e^{-\tau \hat{K}/2}\ e^{-\tau \hat{K}/2}\ e^{-\tau \hat{V}}}\ e^{-\tau \hat{K}/2}$$

always apply $e^{-\tau \hat{K}/2}\ e^{-\tau \hat{K}/2}\ e^{-\tau \hat{V}}$ together.

□ 0 □ □ 0 □ □ 0 □ ... □ 0 □ □ 0 □ □ 0 □ $|\psi_T\rangle$

* blk_size and blk_num

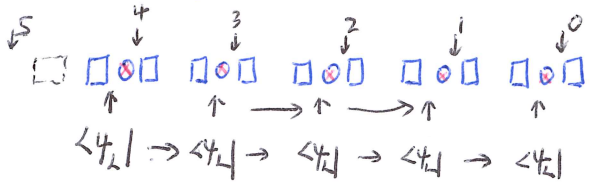
set blk_size = 5, blk_num = 3 , total time slice is 15.



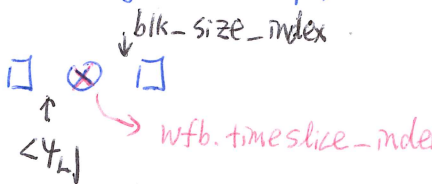
wf_blk_num is only stored from 0~2. (red color)

wf_blk_size is stored from 0~5. (black color), and 0, 5 is one blk_num wave function.

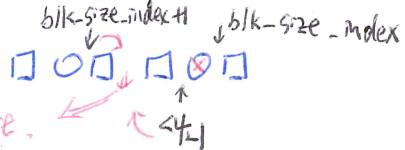
* In one block, update to right. (actually, left and right are symmetric)



each time, during update_to_right_one_step, we have:

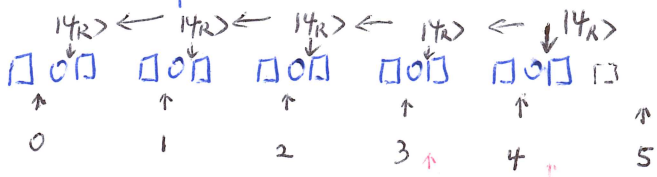


for measure:



⇒ always use $\langle\psi_L|$ and blk-size_index+1 to measure.

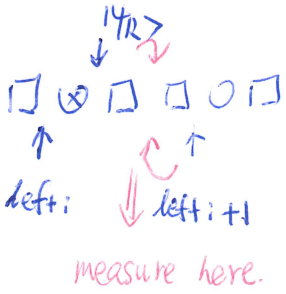
* In one block, update to left.



during update_to_left_one_step.

timeslice_blk_size − 1 − blk_size_index

5 − 1 − blk_size_index.



move $|\psi_R\rangle$ to right half step to measure.

* reweight.

$$|\psi_R'\rangle \xleftarrow{e^{-\tau k} e^{-\tau v}} |\psi_R\rangle$$

$$|\hat{\psi}_R\rangle = e^{-\tau k} e^{-\tau v} |\psi_R\rangle$$

$$|\hat{\psi}_R\rangle = |\psi_R'\rangle \times \text{reweight}.$$

$$\langle \psi_L | \hat{\psi}_R \rangle = \langle \psi_L | e^{-\tau k} e^{-\tau v} | \psi_R \rangle = \langle \psi | \psi_R' \rangle \times \text{reweight}.$$

Only need to time is reweight if we want to move to next step.