Notes on SSE for Rydberg

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1 Introduction

This is motivated by our need to make an SSE for the Rydberg hamiltonian.

$$H = -\Omega \sum_{i=1}^{N} \sigma_i^x - h \sum_{i=1}^{n} n_i - \sum_{\langle i,j \rangle} V_{ij} n_i n_j$$

Here, n_i is simply an occupation number (i.e. either 0 or 1). We can therefore trivially map this to spin-$\frac{1}{2}$ with $n_i = \frac{1}{2}(\sigma_i^z + \mathbb{1})$. The hamiltonian then becomes the following.

$$\begin{aligned} H =& -\Omega \sum_{i=1}^{N} \sigma_i^x - \frac{h}{2} \sum_{i=1}^{N} (\sigma_i^z + \mathbb{1}) - \sum_{\langle i,j \rangle} V_{ij} (\sigma_i^z + \mathbb{1}) \left(\sigma_j^z + \mathbb{1}\right) \\ =& -\Omega \sum_{i=1}^{N} \sigma_i^x - \frac{h}{2} \sum_{i=1}^{N} (\sigma_i^z + \mathbb{1}) - \sum_{\langle i,j \rangle} V_{ij} \left(\sigma_i^z \sigma_j^z + \sigma_i^z + \sigma_j^z + \mathbb{1}\right) \end{aligned}$$

This is extremely similar to a LTFIM (general J_{ij} for all pairs, assuming $J_{ij} > 0 \quad \forall \quad i, j$ as in the Rydberg case since $V_{ij} = \frac{C}{R_{ij}^6}$).

$$H = -\Omega \sum_{i=1}^{N} \sigma_i^x - h \sum_{i=1}^{N} \sigma_i^z + \sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z \qquad \text{LTFIM}$$

In the SSE formalism, we can decompose the Rydberg hamiltonian similarily to how we would for a regular TFIM as follows. Note that we will ignore the shift of $Nh/2$ in the Rydberg hamiltonian. To calculate observables, this can simply be added back after the fact.

$$\begin{aligned} H_{0,0} =& \mathbb{1} \\ H_{-1,a} =& \Omega \sigma_i^x \\ H_{0,a} =& \frac{h}{2} (\sigma_i^z + \mathbb{1}) \\ H_{1,a} =& V_{ij} \left(\sigma_i^z \sigma_j^z + \sigma_i^z + \sigma_j^z + \mathbb{1}\right) \end{aligned}$$

Also note that in the vanilla TFIM SSE formalism, the decomposition of the hamiltonian had $H_{0,a} = \Omega$ instead, which was convenient simply for cluster forming / flipping in the off-diagonal update procedure since the only non-zero matrix element of $H_{0,a}$ and $H_{-1,a}$ are both equal to Ω. In the Rydberg hamiltonian, their only non-zero matrix element is $2h$ and Ω, respectively. It's not obvious to me how to make these matrix elements equal to each other... I think it's not possible unless some other decomposition of the hamiltonian is thought of... Even then I'm not sure that it is possible.

$$\begin{aligned}\langle\uparrow|H_{-1,a}|\downarrow\rangle &= \langle\downarrow|H_{-1,a}|\uparrow\rangle = \Omega \\ \langle\uparrow|H_{0,a}|\uparrow\rangle &= h \\ \langle\uparrow\uparrow|H_{1,a}|\uparrow\uparrow\rangle &= 4V_{ij}\end{aligned}$$

All other matrix elements are zero. Notice that there are two less non-zero matrix elements that in the regular TFIM SSE formalism. So, the importance sampling of operators should be an easier task.

2 Diagonal Updates (Finite T)

The diagonal update proceeds similarily to that for the regular TFIM. Traverse the list of all M operators in the propagatin sequence, ignore off-diagonal operators (still only the $H_{-1,a}$ operator), and perform this MH procedure.

1. If a diagonal operator is encountered ($H_{0,a}$ or $H_{1,a}$), remove it with probability

$$P = \min\left(\frac{M-n+1}{\beta\left[Nh + 4\sum_{\langle i,j\rangle} V_{ij}\right]}, 1\right)$$

2. If the null operator, $H_{0,0}$, is encountered, insert a diagonal operator with the following procedure.

   - Decide whether or not to insert a diagonal operator with the probability

$$P = \min\left(\frac{\beta\left[Nh + 4\sum_{\langle i,j\rangle} V_{ij}\right]}{M-n}, 1\right).$$

   - If it was decided to insert a diagonal operator, choose the operator to insert with probabilities

$$\begin{aligned}P_{H_{0,a}} &= \frac{Nh}{Nh + 4\sum_{\langle i,j\rangle} V_{ij}}, \\ P_{H_{1,a}} &= \frac{4\sum_{\langle i,j\rangle} V_{ij}}{Nh + 4\sum_{\langle i,j\rangle} V_{ij}}.\end{aligned}$$

- If a site operator is chosen (i.e. it was decided to insert $H_{0,a}$), then choose a random site (probability $1/N$) to put the operator. If the chosen site is not $\uparrow$, reject the insertion altogether.

  If a bond operator is chosen ($H_{1,a}$), then choose a random bond (k,l) to put the operator with probability

  $$P = \frac{V_{kl}}{\sum_{\langle i,j\rangle} V_{ij}}.$$

  If the chosen bond has spins that are anti-parallel or both spin-down, reject the insertion altogether.

3 Off-Diagonal Updates and Forming Loops

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4.1 Off-Diagonal Updates

Diagonal updates are performed by forming loops in the $D+1$ simulation cell and proposing that the spins in each loop are flipped with a certain probability (thus changing the diagonal operators in each loop to off-diagonal ones). We will discuss loop-forming for the Rydberg hamiltonian shortly.

Firstly, as with the vanilla TFIM SSE QMC formalism, spins associated to bond operators, $H_{1,a}$, cannot ever be flipped since there are no corresponding off-diagonal bond operators. The spins we are allowed to flip in the simulation cell are those associated to site operators since we have a diagonal site operator, $H_{0,a}$, and an off-diagonal site operator, $H_{-1,a}$. However, the big difference between the vanilla TFIM and Rydberg hamiltonian is that the weights associated to the diagonal and off-diagonal site operators are not all the same. Thus, constructed loops *cannot* be flipped with probability $1/2$ (simple SW flipping procedure).

Once the loops have been formed (more later on how they're formed), the new configuration of spins after the proposed flip of one loop will have a weight $W(x')$. This weight is proportional to the product of the matrix elements, $B^i_{\sigma\sigma'}$, within this loop of which there are n_l matrix elements.

$$W(x') \propto \prod_{i=1}^{n_l} B^i_{\sigma\sigma'}$$

If there are $N^f_{H_{-1,a}}$ off-diagonal operators in the flipped loop and $N^f_{H_{0,a}}$ diagonal operators in the flipped loop, then

$$W(x') \propto \Omega^{N^f_{H_{-1,a}}} (2h)^{N^f_{H_{0,a}}}.$$

If there are $N_{H_{-1,a}}$ off-diagonal operators in the flipped loop and $N_{H_{0,a}}$ diagonal operators in the loop (pre-flip), then the weight of this configuration is

$$W(x) \propto \Omega^{N_{H_{-1,a}}} (2h)^{N_{H_{0,a}}}.$$

Note that $N_{H_{-1,a}} + N_{H_{0,a}} = N^f_{H_{-1,a}} + N^f_{H_{0,a}} = n_l$. Thus, the flipped loop is accepted with probability

$$P_{flip} = \frac{W(x')}{W(x') + W(x)}$$

$$= \frac{\Omega^{N^f_{H_{-1,a}}} (2h)^{N^f_{H_{0,a}}}}{\Omega^{N^f_{H_{-1,a}}} (2h)^{N^f_{H_{0,a}}} + \Omega^{N_{H_{-1,a}}} (2h)^{N_{H_{0,a}}}}$$

Note that in the case of $\Omega = 2h$ (the vanilla TFIM case),

$$\begin{aligned} P_{flip} =& \frac{\Omega^{N^f_{H_{-1,a}} + N^f_{H_{0,a}}}}{\Omega^{N^f_{H_{-1,a}} + N^f_{H_{0,a}}} + \Omega^{N_{H_{-1,a}} + N_{H_{0,a}}}} \\ =& \frac{\Omega^{n_l}}{\Omega^{n_l} + \Omega^{n_l}} \\ =& \frac{1}{2}, \end{aligned}$$

and we recover the simple SW flipping procedure.

4.2 Forming Loops

We just demonstrated what to do when loops in the $D+1$ simulation cell are formed. Flipping formed loops has the dual effect of sampling the off-diagonal and diagonal site operators, $H_{0,a}$ and $H_{-1,a}$, and also sampling the spin configurations (as before with the vanilla TFIM SSE QMC). How do we go about forming the loops?

1. Loops are not allowed to be formed that, if flipped, give a matrix element that is zero.
2. Bond operators $H_{1,a}$ must still belong to one cluster as before with vanilla TFIM SSE QMC.
3.