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 $n_i = \frac{1}{2}\left(\sigma_i^z + \mathbb{1}\right)$. The hamiltonian then becomes the following.

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

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 similarly 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.

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

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

Loop formation rules should follow the TFIM SSE loop formation rules. We can perform off-diagonal updates in the same way, as well (I think!): form loops, flip them with probability $\frac{1}{2}$ (vanilla SW procedure). Since the applicability of the SW procedure to a MC simulation only cares about if we can write the partition function as a sum of weighted cluster configurations (exactly what SSE is!) that are independent of each other (i.e. clusters don't "overlap"), then flipping said clusters with probability $\frac{1}{2}$ (or, really, any probability if you're feeling fancy) is totally fine.