Stochastic Series Expansion by Yuanda Liao

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1 The general formalism

Stochastic Series Expansion (SSE) is a Monte Carlo flavor that does not use discrete path integral and therefore has no Trotter error. Consider the partition function

$$Z = \operatorname{Tr} \mathrm{e}^{-\beta H}.$$

We use the basis $\{\alpha\}$, and by Taylor series we have

$$\begin{aligned} Z &= \sum_{\alpha} \langle \alpha | \sum_{n=0}^{\infty} \frac{1}{n!} (-\beta)^n H^n | \alpha \rangle \\ &= \sum_{\{\alpha_i\}} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle \alpha_0 | -H | \alpha_1 \rangle \langle \alpha_1 | -H | \alpha_2 \rangle \cdots \langle \alpha_{n-1} | -H | \alpha_0 \rangle . \end{aligned}$$

In the equation above we find for the nth term we have n matrix element factors. Suppose we stop at the Mth term, and to make the terms look more symmetric, we rephrase the partition function into

$$Z = \sum_{\alpha_1, \ldots, \alpha_M} \sum_{n=0}^{\infty} \frac{\beta^n (M-n)!}{M!} \sum_{\{A_i\}} \prod_{i=1}^{M} \langle \alpha_{i-1} | A_i | \alpha_i \rangle , \tag{1}$$

where $\alpha_0 = \alpha_M$, and there are n $(-H)$ operators in the $\{A_i\}$ series, the rest being the unit operator.

Now we consider a piecewise Hamiltonian

$$H = -\sum_a \sum_b H_{a,b}, \tag{2}$$

where the a index refers to the operator type, which may be null operator, diagonal operator and off-diagonal operator. The b index is the site index. For example for a 2D $L \times L$ square lattice, b runs over 1 to L^2. We denote (a, b) as S, and now

$$Z = \sum_{S_1, \ldots, S_M} \sum_{\alpha_1, \ldots, \alpha_M} \sum_{n=0}^{\infty} \frac{\beta^n (M-n)!}{M!} \prod_{i=1}^{M} \langle \alpha_{i-1} | (H_i)_{a,b} | \alpha_i \rangle . \tag{3}$$

Now we see the configuration space: each configuration is to put

2 The 1D Heisenberg chain

We consider the example of Heisenberg model. The diagonal operator is

$$H_{1,b} = \frac{1}{4} - S^z_{\boldsymbol{i}} S^z_{\boldsymbol{j}}, \tag{4}$$

and the off-diagonal operator is

$$H_{2,b} = \frac{1}{2} (S^+_{\boldsymbol{i}} S^-_{\boldsymbol{j}} + \text{h.c.}). \tag{5}$$

The Hamiltonian is

$$H = -\sum_b (H_{1,b} - H_{2,b}) + \frac{N}{4}. \tag{6}$$

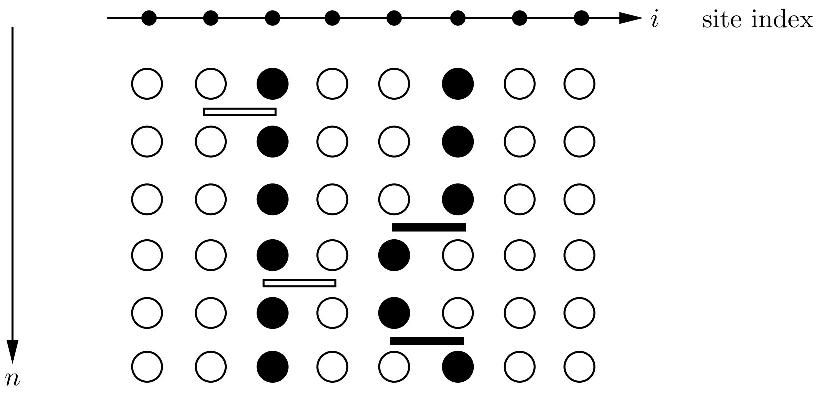

Figure 1: An SSE configuration with $M = 6$

The basis can be chose as

$$|\alpha\rangle = |\uparrow\downarrow\rangle\,, |\uparrow\uparrow\rangle\,, |\downarrow\downarrow\rangle\,, |\downarrow\uparrow\rangle\,. \tag{7}$$

We find that

$$\langle\alpha|-H_{2,b}|\alpha\rangle = -\frac{1}{2},$$

which means (3) has sign problem. What we really deal with is the model

$$H = J\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle}(S^z_{\boldsymbol{i}}S^z_{\boldsymbol{j}} - S^x_{\boldsymbol{i}}S^x_{\boldsymbol{j}} - S^y_{\boldsymbol{i}}S^y_{\boldsymbol{j}}) = -\sum_b (H_{1,b} + H_{2,b}) + \frac{N}{4}. \tag{8}$$

We consider a 1D Heisenberg chain. Figure 1 on page 2 gives a schematic configuration. The update scheme is the follows:

1. Sampling α_0.
2. Diagonal update
3. Non-diagonal update.