

Green Function for a small step in Paramagnetic spin model

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Problem:

N spins forming a 1-D spin chain and they act independently.

σ_i is the i^{th} spin and σ_i can be $\begin{cases} 1 & \text{up} \\ 0 & \text{down} \end{cases}$

The configuration of the system is $\tilde{\sigma} = (\sigma_1, \sigma_2, \dots, \sigma_N)$.

Master equation

$$\begin{aligned}
 \frac{d}{dt}P_t(\tilde{\sigma}) &= -\sum_{\tilde{\sigma}''} W(\tilde{\sigma} \rightarrow \tilde{\sigma}'')P_t(\tilde{\sigma}) + \sum_{\tilde{\sigma}'} W(\tilde{\sigma}' \rightarrow \tilde{\sigma})P_t(\tilde{\sigma}') \\
 &= -\sum_{\tilde{\sigma}'} \sum_{\tilde{\sigma}''} W(\tilde{\sigma}' \rightarrow \tilde{\sigma}'')P_t(\tilde{\sigma}')\delta_{\tilde{\sigma}', \tilde{\sigma}} + \sum_{\tilde{\sigma}'} W(\tilde{\sigma}' \rightarrow \tilde{\sigma})P_t(\tilde{\sigma}') \\
 &= \sum_{\tilde{\sigma}'} \left(W(\tilde{\sigma}' \rightarrow \tilde{\sigma}) - \delta_{\tilde{\sigma}', \tilde{\sigma}} \sum_{\tilde{\sigma}''} W(\tilde{\sigma}' \rightarrow \tilde{\sigma}'') \right) P_t(\tilde{\sigma}') \\
 &= \sum_{\tilde{\sigma}'} L(\tilde{\sigma}' \rightarrow \tilde{\sigma})P_t(\tilde{\sigma}')
 \end{aligned}$$

By definition,

$$W(\tilde{\sigma} \rightarrow \tilde{\sigma}) = 0 \tag{1}$$

and

$$W(\tilde{\sigma}' \rightarrow \tilde{\sigma}) = \sum_{i=1}^N W_i(\tilde{\sigma}' \rightarrow \tilde{\sigma}) \tag{2}$$

and

$$W_i(\sigma' \rightarrow \sigma) = (c\alpha\delta_{\sigma_i 1}\delta_{\sigma'_i 0} + (1-c)\alpha\delta_{\sigma_i 0}\delta_{\sigma'_i 1}) \prod_{j \neq i} \delta_{\sigma_j \sigma'_j} \quad (3)$$

And we have

$$L(\sigma' \rightarrow \sigma) = W(\sigma' \rightarrow \sigma) - \delta_{\sigma', \sigma} \sum_{\sigma''} W(\sigma' \rightarrow \sigma'') \quad (4)$$

Then we can substitute (2) and (3) into (4) , which will give us

$$L(\sigma' \rightarrow \sigma) = \sum_{i=1}^N [c\alpha\delta_{\sigma'_i 0}(\delta_{\sigma_i 1} - \delta_{\sigma_i \sigma'_i}) + (1-c)\alpha\delta_{\sigma'_i 1}(\delta_{\sigma_i 0} - \delta_{\sigma_i \sigma'_i})] \prod_{j \neq i} \delta_{\sigma_j \sigma'_j} \quad (5)$$

Let's go back to the master equation, by setting $dt = \epsilon$

$$\frac{P_{t+\epsilon}(\sigma) - P_t(\sigma)}{\epsilon} = \sum_{\sigma'} L(\sigma' \rightarrow \sigma) P_t(\sigma')$$

Then

$$\begin{aligned} P_{t+\epsilon}(\sigma) &= P_t(\sigma) + \sum_{\sigma'} \epsilon L(\sigma' \rightarrow \sigma) P_t(\sigma') \\ &= \sum_{\sigma'} [\delta_{\sigma \sigma'} + \epsilon L(\sigma' \rightarrow \sigma)] P_t(\sigma') \end{aligned}$$

Compared with

$$P_{t+\epsilon}(\sigma) = \sum_{\sigma'} G(\sigma' \rightarrow \sigma; \epsilon) P_t(\sigma')$$

So the green function for this small step ($t \rightarrow t + \epsilon$) is

$$\begin{aligned} G(\sigma' \rightarrow \sigma; \epsilon) &= \delta_{\sigma \sigma'} + \epsilon L(\sigma' \rightarrow \sigma) \\ &= \sum_{i=1}^N \frac{1}{N} \delta_{\sigma_i \sigma'_i} \prod_{j \neq i} \delta_{\sigma_j \sigma'_j} + \epsilon L(\sigma' \rightarrow \sigma) \\ &= \sum_{i=1}^N \left[\frac{1}{N} \delta_{\sigma_i \sigma'_i} + c\epsilon\alpha\delta_{\sigma'_i 0}(\delta_{\sigma_i 1} - \delta_{\sigma_i \sigma'_i}) + (1-c)\epsilon\alpha\delta_{\sigma'_i 1}(\delta_{\sigma_i 0} - \delta_{\sigma_i \sigma'_i}) \right] \prod_{j \neq i} \delta_{\sigma_j \sigma'_j} \end{aligned}$$

If a and b are just 1 or 0, we can write down

$$\delta_{ab} = 1 + 2ab - a - b.$$

By using this trick, we can simplify the green function. Finally, we will have

$$\begin{aligned} & G(\underset{\sim}{\sigma}' \rightarrow \underset{\sim}{\sigma}; \epsilon) \\ &= \sum_{i=1}^N \left[\left(\frac{1}{N} - c\epsilon\alpha \right) + \left(\frac{2}{N} - 2\epsilon\alpha \right) \sigma_i \sigma'_i - \left(\frac{1}{N} - 2c\epsilon\alpha \right) \sigma_i - \left(\frac{1}{N} - \epsilon\alpha \right) \sigma'_i \right] \\ & \quad \prod_{j \neq i} (1 + 2\sigma_j \sigma'_j - \sigma_j - \sigma'_j) \\ &= \sum_{i=1}^N (A + B\sigma_i \sigma'_i - C\sigma_i - D\sigma'_i) \prod_{j \neq i} (1 + 2\sigma_j \sigma'_j - \sigma_j - \sigma'_j) \end{aligned}$$

where

$$\begin{aligned} A &= \frac{1}{N} - c\epsilon\alpha \\ B &= \frac{2}{N} - 2\epsilon\alpha \\ C &= \frac{1}{N} - 2c\epsilon\alpha \\ D &= \frac{1}{N} - \epsilon\alpha \end{aligned}$$

Now I am still trying to change the form of this green function so that I could easily calculate the green function for a given path. And probably I could use other tricks instead of $\delta_{ab} = 1 + 2ab - a - b$. Please tell me if you have any ideas or questions, we can discuss and I really appreciate it!

References

- [1] R. van Zon and J. Schofield, J. Chem. Phys. 122, 194502 (2005)