content

Notes on XY model

2019 年 8 月 21 日

1 Discription

The Hamiltonian of XY model is:

$$\mathcal{H} = -J\sum_i (S_i^+ S_{i+1}^- + c.c) - B\sum_i S_i^z, \tag{1}$$

For the sake of simplicification, I set $B = 0$.

2 Symmetry

It's easy to verify that $\mathcal{H}$ commutes with $\sum_i S_i^z$, that is $[\mathcal{H}, \sum_i S_i^z] = 0$. What's more, even a magnetic field is applied to direction z, system still has $U(1)$ symmetry, which means the rotation on the X-Y plane. If we let $M + 1 = 1$(M is the total number of spins), then system also has translation symmetry, which means operator P commutes with $\mathcal{H}$.

3 Exact Diagonalization

It's a good method to classify the state according to the value of $\sum_i S_i^z$, $\sum_i S_i^z \in \{-M/2, \ldots, M/2\}$. We use the spin to mark the state, so every state has a definate $\sum_i S_i^z$. Come to computation, I use a bool variable to represent the spin on site. As a result, a state can be represented by a binary number. $\sum_i S_i^z$ equals to $2L - M$(L is the number of 1 in the binary number). The total number of the states is 2^M, which can be represented by $\{0, 1, \ldots, 2^M - 1\}$. Fistly, we can calculate $\sum_i S_i^z$ of all states and divide them into different classes. After these process, we divide the Hilbert space into M+1 subspaces. Then, we can calculate the matrix form of Hamiltonian in every subspace. Finally, we just diagonal the $M + 1$ Hamiltonian matrix and get the eigen energy. The biggest subspace has dimension of $C_{2^{M/2}}^{2^M}$. With M increasing, diagonalization becomes harder and harder, whcih means ED can just apply to small system. But that does not mean ED is useless, it gives us some meaningful result to compare with other method.

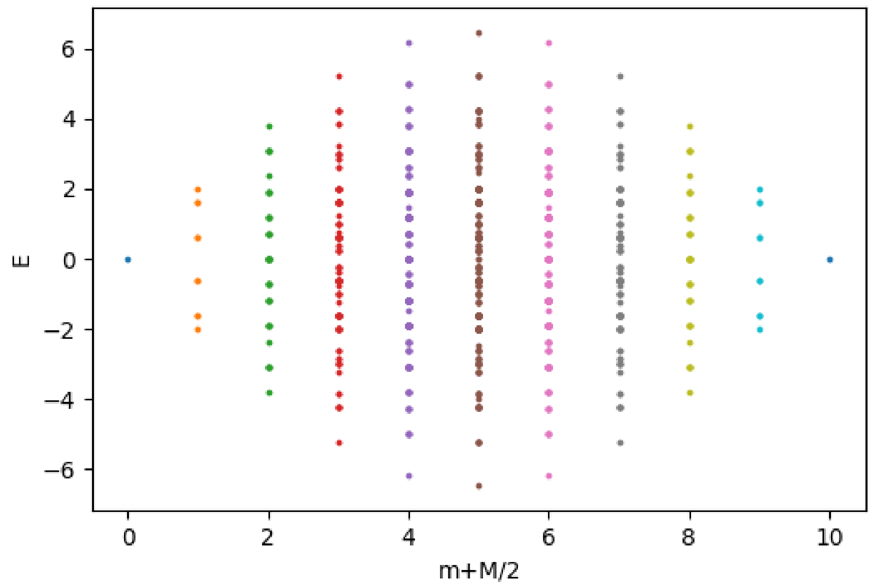


figure 1: ED result(set J=1,M=10)

The figure shows that ground state is in the subspace where $\sum_i S_i^z = 0$.

4 Analytical Method

4.1 Jordan-Wignar transform

The spin operator on different sites commute, and all commutation relations are: $[S_i^\alpha, S_j^\beta] = i\delta_{ij}\epsilon_{\alpha\beta\gamma}S_i^\gamma$. The main idea of J-W transform is to represent spin operators with fermion operators. The transform details are as below:

$$S_i^+ = e^{i\pi\sum_{j<i} c_j^+ c_j} c_i, \tag{2a}$$

$$S_i^- = e^{i\pi\sum_{j<i} c_j^+ c_j} c_i^+, \tag{2b}$$

$$S_i^z = \frac{1}{2} - c_i^+ c_i \tag{2c}$$

I don't want to discuss the algebra knowledge under J-W transform here.

4.2 Hamiltonian

Under the periodic boundary condition, the Hamiltonian is :

$$\mathcal{H} = -J\sum_{i=1}^{M-1}(S_i^+ S_{i+1}^- + c.c) - J(S_M^+ S_1^- + c.c) - B\sum_i S_i^z, \tag{3}$$

By using J-W transform, Hamiltonian can be rewritten as:

$$\mathcal{H} = J\sum_{i=1}^{M-1}(c_i c_{i+1}^{+} + c.c) - J(e^{i\pi\sum_j c_j^{+}c_j} c_M c_1^{+} + c.c) + B\sum_i c_i^{+}c_i - B\frac{M}{2}, \tag{4}$$

The parity operator has two different eigen values, so we calssify the Hilbert space according to this.

4.2.1 even sector

If we set $c_{M+1} = -c_1$, then the Hamiltonian is :

$$\mathcal{H} = J\sum_{i=1}^{M}(c_i c_{i+1}^{+} + c.c) + B\sum_i c_i^{+}c_i - B\frac{M}{2}, \tag{5}$$

let:$c_i = \frac{1}{\sqrt{M}}\sum_k e^{ikn_i}c_k$, $k = \frac{(2m+1)\pi}{M}$, where $m = \{-\frac{M}{2}, \ldots, \frac{M}{2} - 1\}$(we set M an even number).

Then the Hamiltonian can be simplified as:

$$\mathcal{H} = -2J\sum_k cosk c_k^{+}c_k + B\sum_k c_k^{+}c_k - const, \tag{6}$$

Because $S_i^z = \frac{1}{2} - c_i^{+}c_i$, $\sum_i S_i^z = \frac{M}{2} - \sum_i c_i^{+}c_i = \frac{M}{2} - \sum_k c_k^{+}c_k$. As a result, $\sum_k c_k^{+}c_k = -(\sum_i S_i^z - \frac{M}{2}) = M - (\sum_i S_i^z + \frac{M}{2})$, and parity needs $\sum_k c_k^{+}c_k$ is an even number. So we can calculate the eigen energy in the subspace where $\sum_i S_i^z + \frac{M}{2} = 0, 2, \ldots, M$. To compare with the ED results, we can calculate the ground state of subspace which satisfy the condition mentioned before(M=10). For example, when $(\sum_i S_i^z + \frac{M}{2}) = 0$, $\sum_k c_k^{+}c_k = M$, so ground state energy is 0....

4.2.2 odd sector

The Hamiltonian is the same as equ.6, the thing that only change is that $k = \frac{2m\pi}{M}$.

4.3 Result

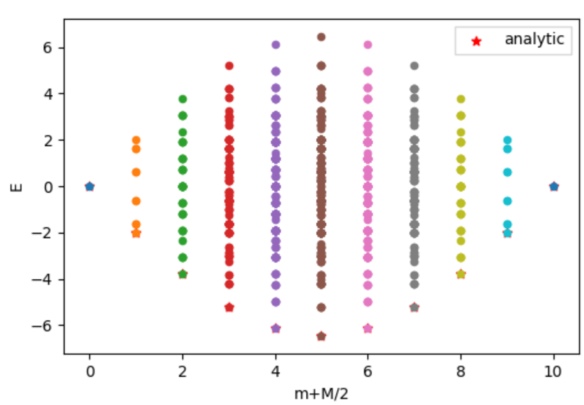


figure 2: ED result and analytical ground energy(set J=1,M=10)

5 Correlation Function of ground state

Because the $U(1)$ symmetry, it's the same to calculate $< S_i^x S_j^x >$ as $< S_i^y S_j^y >$, and owing to translation symmetry, all correlation can be expressed as $< S_0^x S_j^x >$. Since $S_0^x S_i^x = \frac{1}{4}(S_0^+ + S_0^-)(S_i^+ + S_i^-)$ and for ground state $< S_0^+ S_i^+ >=< S_0^- S_i^- >= 0$, so $< S_0^x S_i^x >= \frac{1}{4}(< S_0^+ S_i^- > + < S_0^- S_i^+ >)$.

5.1 Majorana fermion

Put a transform on c_i, c_i^+, which is :

$$\alpha_i = c_i^+ + c_i, \tag{7a}$$

$$\beta_i = c_i^+ - c_i, \tag{7b}$$

α_i becomes a pure real operator while β_i becomes a pure image operator. It seems that one fermion is devided to two half fermions. We will see why this transform is so important next subsection. From equ.7b, it's easy to varify that $\alpha_i \alpha_i = \beta_i \beta_i = 1$ and $\alpha_i \beta_i = 1 - 2c_i^+ c_i$.

5.2 Simplification

$$< S_0^+ S_i^- >=< c_0 c_i^+ e^{i\pi \sum_{j<i} c_j^+ c_j} >, \tag{8}$$

It's a hard way to calculate equ.8 directly. But if we use the transform metioned before, equ.8 could be simplified as:

$$S_0^x S_i^x = \frac{1}{4}(S_0^+ + S_0^-)(S_i^+ + S_i^-) = \frac{1}{4} < \beta_0 \ldots \alpha_{i-1} \beta_{i-1} \alpha_i >, \tag{9}$$

5.3 Pfaffian

The Pfaffian for a $2n \times 2n$ skew-symmetric matrix is defined as:

$$Pf(A) = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} sgn(\sigma) \prod_i^n a_{\sigma(2i-1),\sigma(2i)}, \tag{10}$$

Because swap between $2i-1$ and $2i$, $a_{\sigma(2i-1),\sigma(2i)}$ will give a minus. But $sgn(\sigma)$ gives another minus, so the value stay unchanged. The parameter 2^n is to eliminate this repeat. $n!$ is to eliminate the swap between $\{\sigma(2i-1), \sigma(2i)\}$ and $\{\sigma(2j-1), \sigma(2j)\}$.By using wick theorem, equ.9 can be written as a Pfaffian of a matrix. That is:

$$S_0^x S_i^x = \frac{1}{4} Pf \begin{pmatrix} 0 & < \beta_0 \alpha_1 > & < \beta_0 \beta_1 > & \ldots & \ldots \\ * & 0 & < \alpha_1 \beta_1 > & < \alpha_1 \alpha_2 > & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix} \tag{11}$$

Further, for an arbitrary $2n \times 2n$ real or complex matrix B:

$$Pf(BAB^T) = det(B)Pf(A) \tag{12}$$

For a tridiagonal matrix, Pfaffian is :

$$Pf\begin{pmatrix} 0 & a_1 & & & & & & \\ -a_1 & 0 & b_1 & & & & & \\ & -b_1 & 0 & a_2 & & & & \\ & & -a_2 & \ddots & \ddots & & & \\ & & & \ddots & 0 & b_{n-1} & & \\ & & & & -b_{n-1} & 0 & a_n \\ & & & & & -a_n & 0 \end{pmatrix} = \prod_i a_i \tag{13}$$

Every $2n \times 2n$ skew matrix can be transformed into tridiagonal matrix by using elementary transformations.

5.3.1 Guassian elimination

A $n \times n$ matrix of the form:

$$M_k = E_n - \alpha_k (e_k^{(n)})^T, \tag{14}$$

where E_n is the $n \times n$ identity matrix and $e_k^{(n)}$ the k-th unit vector in $\mathcal{C}^n$, is called a Guass transformation. A Gauss transformation can thus be used to zero the entries in a column or row of A below a chosen point k. In order to avoid divisions by a small number of zero, a permutation P_k interchangeing entry k with another nonzero, typically the largest entry in the k+1...n is performed.

$$T = M_{n-1}P_{n-1} \dots M_2 P_2 A P_2^T M_2^T \dots P_{n-1}^T M_{n-1}^T, \tag{15}$$

where T is a tridiagonal matrix and P represents the pivot matrix and it's not hard to verify that $det(P) = -1$,$det(M) = 1$.

6 Result

The main work is to calculate $< \beta_i \alpha_j >, < \alpha_i \beta_j >, < \beta_i \beta_j >, < \alpha_i \alpha_j >$ for $i \leq j$. Because $\beta_i \alpha_j = (c_i^+ - c_i)(c_j^+ + c_j) = c_i^+ c_j - c_i c_j^+$, the problem becomes calculating $< c_i^+ c_j >$ and $< c_i c_j^+ >$.c_i, c_i^+ has the form:

$$c_i = \frac{1}{\sqrt{M}} \sum_k c_k e^{ikn_i}, \tag{16a}$$

$$c_i^+ = \frac{1}{\sqrt{M}} \sum_k c_k^+ e^{-ikn_i}, \tag{16b}$$

So,

$$c_i^+ c_j = \frac{1}{M} \sum_{k,k'} c_k^+ c_{k'} e^{-ikn_i} e^{ik'n_j}, \tag{17a}$$

$$c_i c_j^+ = \frac{1}{M} \sum_{k,k'} c_k c_{k'}^+ e^{-ikn_i} e^{ik'n_j}, \tag{17b}$$

Because the ground state has a definate particle number, the items of $k \neq k'$ equal to zero. That means result in equ.18a could be simplified as:

$$< \beta_i \alpha_j > = \frac{1}{M} \sum_k c_k^+ c_k 2cos[k(n_i - n_j)] - \frac{1}{M} \sum_k e^{ik(n_i - n_j)}, \tag{18a}$$

$$< \beta_i \beta_j > = \frac{1}{M} \sum_k c_k^+ c_k (2i) sin[k(n_i - n_j)] - \frac{1}{M} \sum_k e^{ik(n_i - n_j)}, \tag{18b}$$

$$< \alpha_i \alpha_j > = \frac{1}{M} \sum_k c_k^+ c_k (-2i) sin[k(n_i - n_j)] + \frac{1}{M} \sum_k e^{ik(n_i - n_j)}, \tag{18c}$$

$$< \alpha_i \beta_j > = \frac{1}{M} \sum_k c_k^+ c_k (-2) cos[k(n_i - n_j)] + \frac{1}{M} \sum_k e^{ik(n_i - n_j)}. \tag{18d}$$

For equ.18a,b and c,$j > i$ so $\frac{1}{M} \sum_k e^{ik(n_i - n_j)} = 0$. For equ.18d, when $j > i$, $\frac{1}{M} \sum_k e^{ik(n_i - n_j)} = 0$; when $j = i, \frac{1}{M} \sum_k e^{ik(n_i - n_j)} = 1$. More analyse shows that 18b,18c equal to zero because k is symmetric about origin. Equ.6 in odd sector shows that $c_k^+ c_k = 1$ only for $k \in [-[M/4], [M/4]]$. If we choose M equals to a odd number multiples 2, then the ground state is unique. So all the nonzero entries are listed as below.

$$< \beta_i \alpha_j > = (1 + 2 \times re.(\frac{e^{i\pi 2d/M}(1 - e^{i\pi d/2}) \times e^{-i\pi d/M}}{1 - e^{i\pi 2d/M}})) \times 2/N, j > i \tag{19a}$$

$$< \alpha_i \beta_j > = 0, i = j \tag{19b}$$

$$< \alpha_i \beta_j > = -(1 + 2 \times re.(\frac{e^{i\pi 2d/M}(1 - e^{i\pi d/2}) \times e^{-i\pi d/M}}{1 - e^{i\pi 2d/M}})) \times 2/N, j > i \tag{19c}$$

6.1 Some Hints

Let matrix in equ.11 is A. It's such an astonishing thing that we do not need pivot operation when get the Pfaffian of matrix A, which gives us lots of convenience. For example, the size of the system is M, then we just need calculate Pfaffian once for matrix $A_{2(M-1),2(M-1)}$. All corelations could be found in the submatrix of A. As a result, the normal complexity is M^4(M^3 for Pfaffian and calculate M times) and under this condition the complexity is M^3.

6.2 Correlations

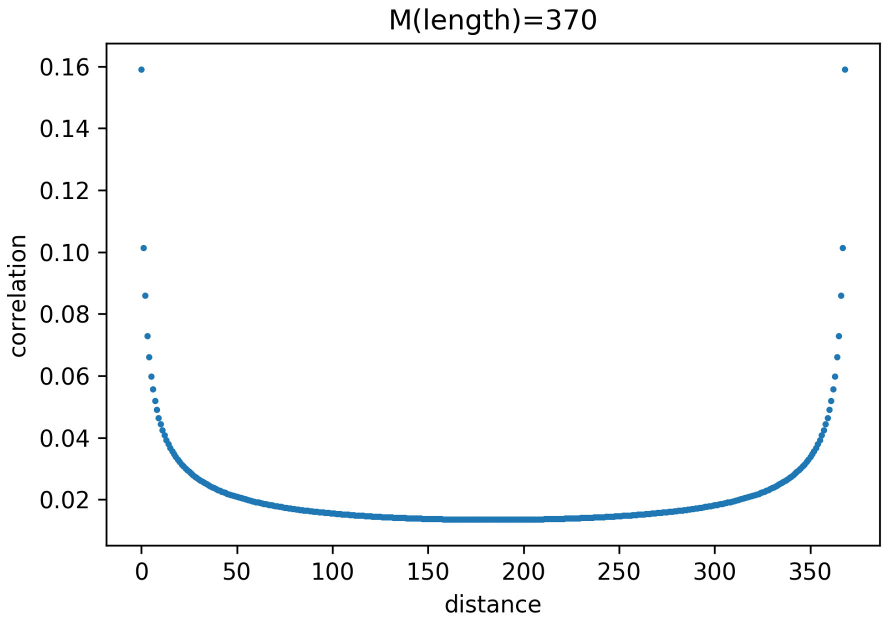


figure 3: correlation function

The scaling law tells us that $correlation \sim d^{-\alpha}$,that is $log(correlation) \sim -\alpha log(d)$. So I print a new figure according to this relation.

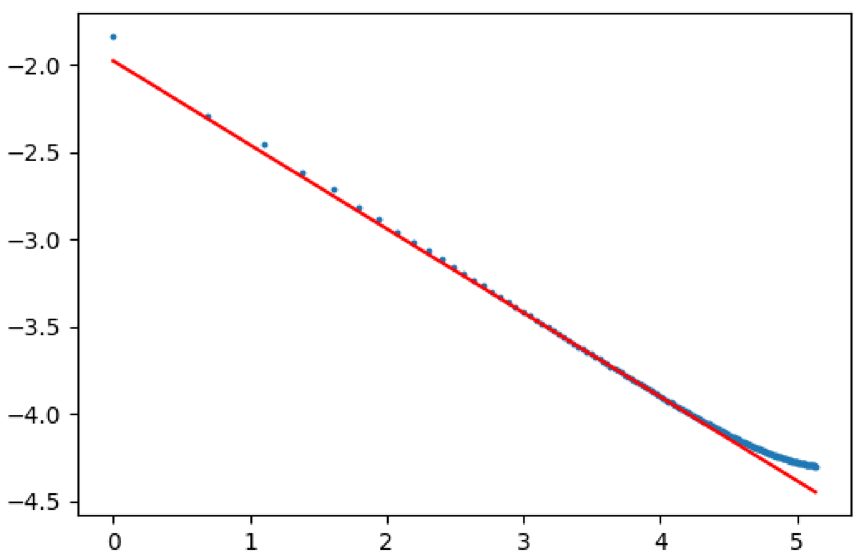


figure 4: correlation function

The figure shows it's not a strict linear relation. So, what's the problem? The problem is that the system is still not large enough. What's more, we use periodic boundary condition so it will be inaccurate when near the boundary. How to handle this problem? Here are two different methods.

6.2.1 Conformal theory

We can modify the defination of the distance. A good way is $d' = \frac{M}{\pi} sin(\pi d/M)$. The figure below shows it's a good defination.

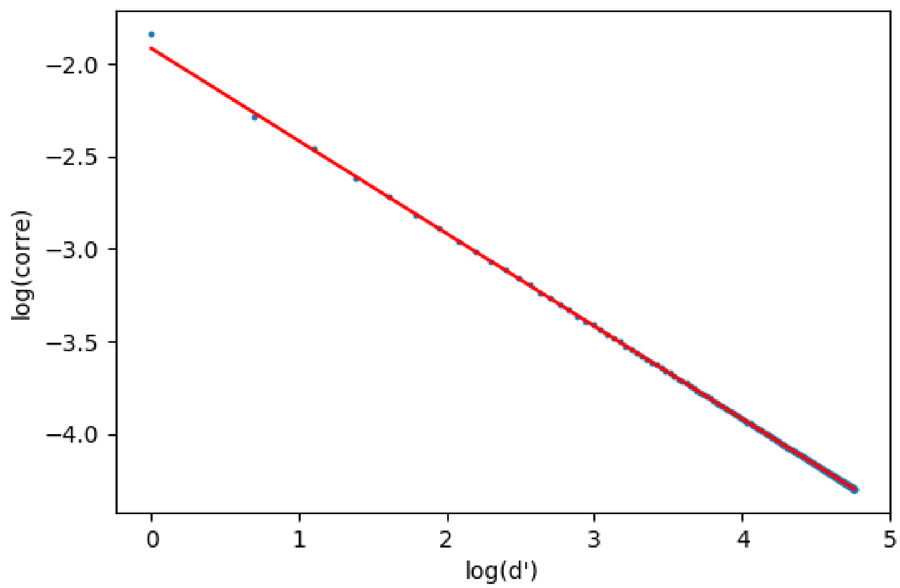


figure 5: correlation function

The figure gives $\alpha = 0.5$ which is consistent with analytical result.

6.2.2 Enlarge M

From the calculation process before, the complexity has no relation with M. In fact, the complexity is just realted to the longest correlation we want. So we can just enlarge M but mantain the longest correlation. For example, I set $M = 55555555 \times 2$ and I calculate the former 270 spin correlations.

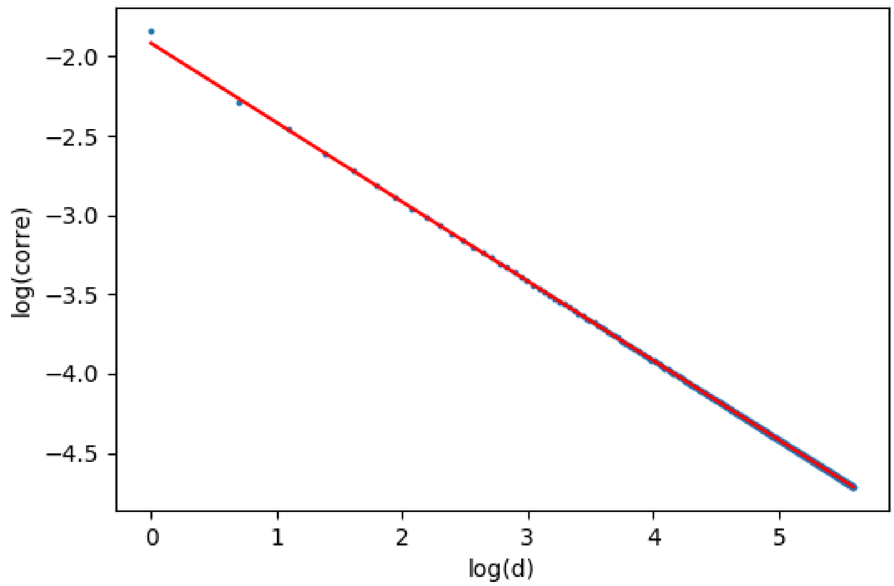


figure 6: correlation function

The result also shows $\alpha = 0.5$.

7 Finite Tmeperature

At finite temperature, $< S_0^x S_n^x >= \frac{Tr(S_0^x S_n^x e^{-\beta H})}{Tr(e^{-\beta H})}$. The Hamiltonian itself is not free fermion, the more convenient form is:

$$\begin{aligned} Tr(S_0^x S_n^x e^{-\beta H}) &= Tr(S_0^x S_n^x e^{-\beta H_{even}} \frac{e^{i\pi N}+1}{2}) + Tr(S_0^x S_n^x e^{-\beta H_{odd}} \frac{-e^{i\pi N}+1}{2}) \\ &= \frac{1}{2} Tr(S_0^x S_n^x e^{-\beta H_{even}}) + \frac{1}{2} Tr(S_0^x S_n^x e^{-\beta H_{even}} e^{i\pi N}) + \frac{1}{2} Tr(S_0^x S_n^x e^{-\beta H_{odd}}) - \frac{1}{2} Tr(S_0^x S_n^x e^{-\beta H_{odd}} e^{i\pi N}) \end{aligned} \tag{20}$$

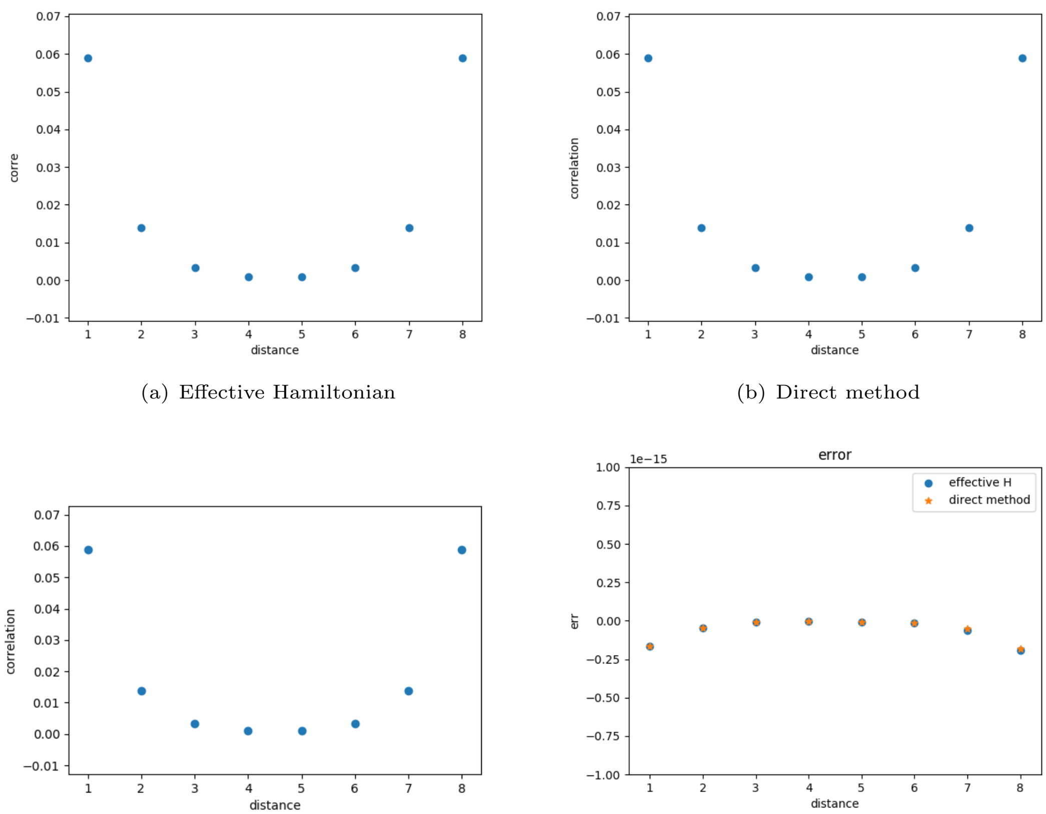
It's also important to calculate the partition function:

$$\begin{aligned} Tr(e^{-\beta H}) &= \frac{1}{2} Tr(e^{-\beta H_{even}}) + \frac{1}{2} Tr(e^{-\beta H_{even}} e^{i\pi N}) + \frac{1}{2} Tr(e^{-\beta H_{odd}}) - \frac{1}{2} Tr(e^{-\beta H_{odd}} e^{i\pi N}) \\ &= \frac{1}{2}(Z_{even} + \overline{Z}_{even} + Z_{odd} - \overline{Z}_{odd}), \end{aligned} \tag{21}$$

7.1 Effective Hamiltonian

I set $\overline{H}_{even/odd} = H_{even/odd} - \frac{i\pi N}{\beta}$. Then the new Hamiltonian gives a distribution:

$$f(E) = \frac{1}{-e^{\beta E}+1} = -n_B(E), \tag{22}$$



(a) Effective Hamiltonian

(b) Direct method

(c) Exact solution

(d) error

figure 7: Results of three different methods for M=9 and T=2

$c_k^+ c_k$ in equ.18 equals to $f(E)$ which is the distribution function of each Hmailtonian. Equ.20 also equals to:

$$Equ.20 = \frac{1}{2} < S_0^x S_n^x >_{e,n} Z_{even} + \frac{1}{2} < S_0^x S_n^x >_{e,s} \overline{Z}_{even} + \frac{1}{2} < S_0^x S_n^x >_{o,n} Z_{even} - \frac{1}{2} < S_0^x S_n^x >_{o,s} \overline{Z}_{even}, \quad (23)$$

which could be solved by wick theorem and equ.18. Here is a detail I want to state. Under the condition that $\epsilon_k = 0$ and $n_i = n_j$, the entry $< \alpha_i \beta_i >$ diverges. But it does not violet the basic theory. Because under this condition the partition function is zero. So perhaps their product converges. To avoid this condition, we can set the size of the system $M = odd$.

7.2 Direct Method

By using the representation:

$$e^{i\pi N} = \alpha_1 \beta_1 \dots \alpha_M \beta_M. \quad (24)$$

And the pfaffian of some matrixs gives the correlation at finite temperature.

7.3 Result

From the figure above, all these methods are consistent with each other.

7.3.1 Large Size

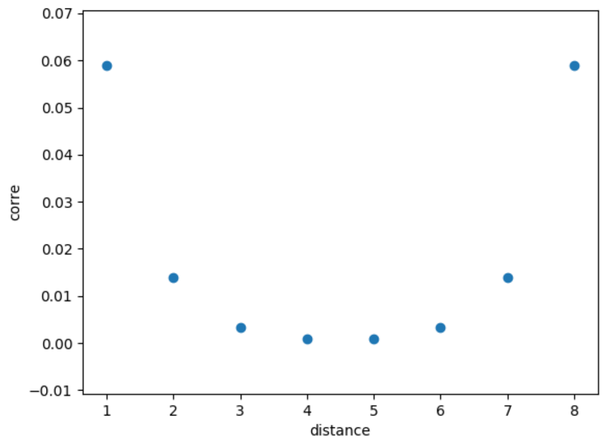


figure 8: correlation at finite T=1 and M=109

8 Time Evolution at ground state

We are interested in the correlation on time direction, more precisely, $< S_n^x S_n^x(t) >_0$. Because S_n^x change the parity of the state, things become too complicated if we use periodic boundary condition. So I use open boundary condition. For an given Hamiltonian H which now has no translation symmetry. Here exists a matrix P which transform H to a diagonal matrix. That is, $P^+HP = \mathcal{H}$, in which $\mathcal{H}$ is a diagonal matrix. We set the diagonal entries are $e_1, e_2, \ldots$. Note that H is a matrix not the true Halmiltonian operator. The Hamitonian in fact is $\hat{H} = C^+HC$, where $C^+ = (c_1^+ c_2^+ \ldots)$. The transformtion means the Hamiltonian could be transformed as a free fermion. The transformation also gives $D = P^+C$.

It just needs a few lines of calculate to obtain:

$$< S_n^x S_n^x(t) >_0 = \frac{1}{4} < \alpha_1\beta_1 \ldots \alpha_n \alpha_1(t)\beta_1(t) \ldots \alpha_n(t) >_0, \tag{25}$$

The Pfaffian matrix could be divided into four part.

$$\begin{pmatrix} A_{(2n-1)\times(2n-1)} & B_{(2n-1)\times(2n-1)} \\ C_{(2n-1)\times(2n-1)} & D_{(2n-1)\times(2n-1)} \end{pmatrix} \tag{26}$$

The Pfaffian matrix needs $C = -B^T$ and it's easy to verify $A = D$ and all entries in A are known in previous section. So the most important thing is to calculate B, more precisely, $< \alpha_i\beta_j(t) >_0, < \alpha_i\alpha_j(t) >_0$ $, < \beta_i\alpha_j(t) >_0, < \beta_i\beta_j(t) >_0$. Before listing all results, we can construct a matrix. $R_{ij} = e^{-ie_it}\Theta(-e_i)\delta_{ij}$ and

$Q_{ij} = e^{ie_i t}\Theta(e_i)\delta_{ij}$. Then:

$$matrix(< \alpha_i\alpha_j(t) >) = (PRP^*)^T + (PQP^*), \quad (27a)$$
$$matrix(< \alpha_i\beta_j(t) >) = -(PRP^*)^T + (PQP^*), \quad (27b)$$
$$matrix(< \beta_i\alpha_j(t) >) = (PRP^*)^T - (PQP^*), \quad (27c)$$
$$matrix(< \beta_i\beta_j(t) >) = -(PRP^*)^T - (PQP^*). \quad (27d)$$

Then, just as before, the Pfaffian of matrix.26 gives the correlations.

9 Result

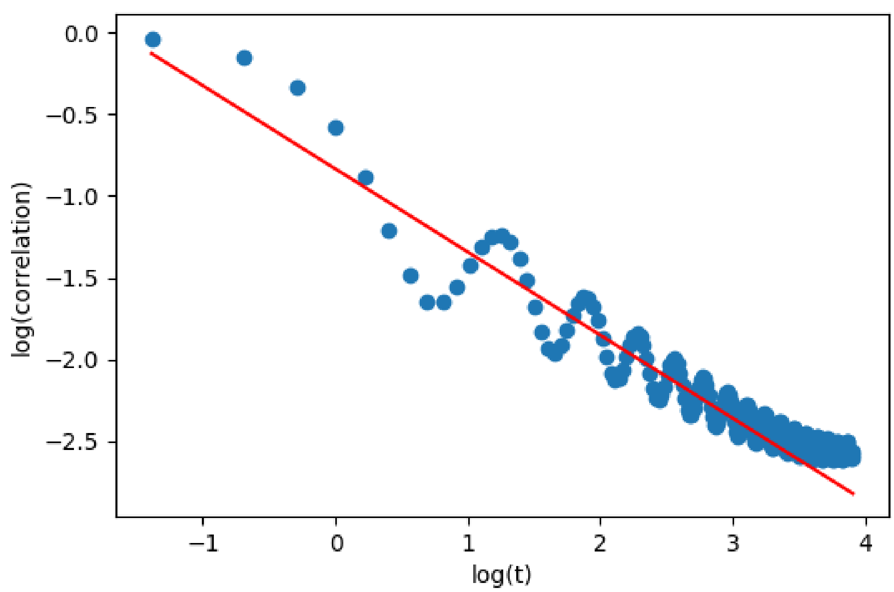


figure 9: time revolution correlation function

The k of the line in fig.9 is 0.5, Which gives that $\alpha = 0.5$ along time direction.