Problem Set 4: Solution

1. **AKLT model** (2+2+3 points)

The ground state of the spin-1 AKLT-model in a periodic chain with N sites has the following matrix-product state (MPS) form:

$$|\Psi\rangle = \sum_{s_1,\dots,s_N} \mathrm{Tr}(A^{s_1}\dots A^{s_N})|s_1,\dots,s_N\rangle\,,$$

where $s_j = +1, 0, -1$ and

$$A^{+1} = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix},\quad A^0 = \frac{1}{2}\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix},\quad A^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 0\\ -1 & 0\end{pmatrix}.$$

(a) Compute the transfer matrix

$$T_{(\alpha_l,\alpha_l'),(\alpha_{l+1},\alpha_{l+1}')} = \sum_{s_l}(A^{s_l}_{\alpha_l',\alpha_{l+1}'})^* A^{s_l}_{\alpha_l,\alpha_{l+1}}\,,$$

and verify that its eigenvalues are $3/4$, $-1/4$, $-1/4$, $-1/4$.

(b) Compute the transfer matrices for $\hat{S}_z$ and $e^{i\pi\hat{S}^z}$, using

$$T^{\hat{O}}_{(\alpha_l,\alpha_l'),(\alpha_{l+1},\alpha_{l+1}')} = \sum_{s_l,s_l'}(A^{s_l}_{\alpha_l,\alpha_{l+1}})^* A^{s_l'}_{\alpha_l',\alpha_{l+1}'}\langle s_l|\hat{O}|s_l'\rangle\,.$$

(c) Calculate spin-spin and string correlation functions

$$C^{zz}_{ij} \equiv \frac{\langle\Psi|\hat{S}^z_i\hat{S}^z_j|\Psi\rangle}{\langle\Psi|\Psi\rangle},$$

$$C^{\mathrm{string}}_{ij} \equiv -\frac{\langle\Psi|\hat{S}^z_i\prod_{l=i+1}^{j-1}e^{i\pi\hat{S}^z_l}\,\hat{S}^z_j|\Psi\rangle}{\langle\Psi|\Psi\rangle}.$$

Note that the string correlation function characterizes the hidden "dilute" antiferromagnetic order. How do these correlation functions behave asymptotically ($\lim_{|j-i|\to\infty}\lim_{N\to\infty}$)?

Solution: (a) For the transfer matrix $T_{(\alpha_l,\alpha_l'),(\alpha_{l+1},\alpha_{l+1}')} = \sum_{s_l}(A^{s_l}_{\alpha_l',\alpha_{l+1}'})^* A^{s_l}_{\alpha_l,\alpha_{l+1}}$, it is convenient to view $(A^{s_l}_{\alpha_l',\alpha_{l+1}'})^* A^{s_l}_{\alpha_l,\alpha_{l+1}}$ as the matrix element $[A^{s_l}\otimes(A^{s_l})^*]_{(\alpha_l,\alpha_l'),(\alpha_{l+1},\alpha_{l+1}')}$ of the tensor product $T = \sum_{s_l}A^{s_l}\otimes(A^{s_l})^*$. The matrices A^{s_l} defining the AKLT state are real, so the tensor products needed for the transfer matrix are given by

$$A^{+1}\otimes A^{+1} = \frac{1}{2}\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}\otimes\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix} = \begin{pmatrix}0&0&0&\frac{1}{2}\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix},$$

$$A^0\otimes A^0 = \frac{1}{4}\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}\otimes\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix} = \begin{pmatrix}\frac{1}{4}&0&0&0\\0&-\frac{1}{4}&0&0\\0&0&-\frac{1}{4}&0\\0&0&0&\frac{1}{4}\end{pmatrix},$$

$$A^{-1}\otimes A^{-1} = \frac{1}{2}\begin{pmatrix}0 & 0\\ -1 & 0\end{pmatrix}\otimes\begin{pmatrix}0 & 0\\ -1 & 0\end{pmatrix} = \begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&0\\\frac{1}{2}&0&0&0\end{pmatrix}.$$

Then, the transfer matrix yields

$$T = A^{+1} \otimes A^{+1} + A^0 \otimes A^0 + A^{-1} \otimes A^{-1} = \begin{pmatrix} \frac{1}{4} & 0 & 0 & \frac{1}{2} \\ 0 & -\frac{1}{4} & 0 & 0 \\ 0 & 0 & -\frac{1}{4} & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{4} \end{pmatrix}.$$

Note that T is Hermitian and block-diagonal (with two 2×2 blocks). It is straightforward to find out the four eigenvectors $|a\rangle$ ($a = 1, 2, 3, 4$) and their corresponding eigenvalues λ_a

$$T|a\rangle = \lambda_a |a\rangle,$$

where

$$\lambda_1 = \frac{3}{4}, \quad \lambda_2 = \lambda_3 = \lambda_4 = -\frac{1}{4},$$

and

$$|1\rangle = \begin{pmatrix} \frac{\sqrt{2}}{2} \\ 0 \\ 0 \\ \frac{\sqrt{2}}{2} \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} \frac{\sqrt{2}}{2} \\ 0 \\ 0 \\ -\frac{\sqrt{2}}{2} \end{pmatrix}, \quad |3\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |4\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}.$$

It is also worth noting that T has a *unique* largest eigenvalue.

(b) By using the tensor product form, the transfer matrices for $\hat{S}_z$ and $e^{i\pi\hat{S}^z}$ are given by

$$\begin{aligned} T^{\hat{S}_z} &= \sum_{s_l, s_l'} [A^{s_l} \otimes (A^{s_l'})^*] \langle s_l | \hat{S}_z | s_l' \rangle \quad \Leftarrow \text{use } \langle +1|\hat{S}_z| + 1\rangle = -\langle -1|\hat{S}_z| - 1\rangle = 1 \\ &= A^{+1} \otimes A^{+1} - A^{-1} \otimes A^{-1} \\ &= \begin{pmatrix} 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \end{pmatrix}, \end{aligned}$$

and

$$\begin{aligned} T^{e^{i\pi\hat{S}^z}} &= \sum_{s_l, s_l'} [A^{s_l} \otimes (A^{s_l'})^*] \langle s_l | \hat{S}_z | s_l' \rangle \quad \Leftarrow \text{use } \langle +1|e^{i\pi\hat{S}^z}| + 1\rangle = \langle -1|e^{i\pi\hat{S}^z}| - 1\rangle = -\langle 0|e^{i\pi\hat{S}^z}|0\rangle = -1 \\ &= -A^{+1} \otimes A^{+1} + A^0 \otimes A^0 - A^{-1} \otimes A^{-1} \\ &= \begin{pmatrix} \frac{1}{4} & 0 & 0 & -\frac{1}{2} \\ 0 & -\frac{1}{4} & 0 & 0 \\ 0 & 0 & -\frac{1}{4} & 0 \\ -\frac{1}{2} & 0 & 0 & \frac{1}{4} \end{pmatrix}. \end{aligned}$$

(c) By using the transfer matrix approach (see pages 8-9 in the lecture note 1d-2.pdf), the spin-spin correlation function is given by

$$\begin{aligned} C_{ij}^{zz} &\equiv \frac{\langle \Psi | \hat{S}_i^z \hat{S}_j^z | \Psi \rangle}{\langle \Psi | \Psi \rangle} \\ &= \frac{\text{tr}(T^{i-1} T^{\hat{S}_z} T^{j-i-1} T^{\hat{S}_z} T^{N-j})}{\text{tr}(T^N)} \\ &= \frac{\text{tr}(T^{\hat{S}_z} T^{j-i-1} T^{\hat{S}_z} T^{N-j+i-1})}{\text{tr}(T^N)} \\ &= \frac{\sum_{a=1}^4 \langle a | T^{\hat{S}_z} T^{j-i-1} T^{\hat{S}_z} T^{N-j+i-1} | a \rangle}{\sum_{a=1}^4 \langle a | T^N | a \rangle} \quad \Leftarrow \text{use } T|a\rangle = \lambda_a|a\rangle \text{ and insert } \sum_{b=1}^4 |b\rangle\langle b| = I \\ &= \frac{\sum_{a,b=1}^4 \langle a | T^{\hat{S}_z} | b \rangle \langle b | T^{\hat{S}_z} | a \rangle \lambda_a^{N-j+i-1} \lambda_b^{j-i-1}}{\sum_{a=1}^4 \lambda_a^N}. \end{aligned}$$

In the thermodynamic limit $N \to \infty$, only $a = 1$ term (corresponding to the largest eigenvalue $\lambda_{a=1} = \frac{3}{4}$ of the transfer matrix T) survives, other terms with $a = 2, 3, 4$ decay exponentially with respect to N. In this limit, the spin-spin correlation function is simplified as

$$\begin{aligned} C_{ij}^{zz} &\to \lambda_1^{-j+i-1} \sum_{b=1}^{4} \langle 1|T^{\hat{S}_z}|b\rangle\langle b|T^{\hat{S}_z}|1\rangle \lambda_b^{j-i-1} \quad \Leftarrow T^{\hat{S}_z}|1\rangle = \frac{1}{2}|2\rangle,\ \langle 1|T^{\hat{S}_z} = -\frac{1}{2}\langle 2| \text{ (i.e., } b = 2 \text{ survives)} \\ &= \lambda_1^{-j+i-1} \frac{1}{2} \cdot \left(-\frac{1}{2}\right) \lambda_2^{j-i-1} \quad \Leftarrow \text{substitute } \lambda_1 = \frac{3}{4} \text{ and } \lambda_2 = -\frac{1}{4} \\ &= \frac{4}{3}\left(-\frac{1}{3}\right)^{j-i}. \end{aligned}$$

Thus, the spin-spin correlation function decays exponentially, $C_{ij}^{zz} \sim e^{-|j-i|/\xi}$ with correlation length $\xi = 1/\ln 3$.

For general MPS, the procedure of calculating the two-point correlation functions is exactly the same. It is worth nothing that, if the largest eigenvalue of the transfer matrix T is unique (largest in the sense of their absolute values), the two-point correlation functions *always* decay exponentially at large distance $|j - i| \to \infty$. If the transfer matrix T has degenerate largest eigenvalues, some of two-point correlation functions are long-ranged (i.e., nonzero when $|j - i| \to \infty$), corresponding to certain kind of symmetry breaking. Therefore, the MPS *cannot* have *powerlaw* decaying two-point correlation functions, indicating its deficiency for describing critical systems.

For the string correlation function, the transfer matrix approach also applies

$$\begin{aligned} C_{ij}^{\text{string}} &\equiv -\frac{\langle\Psi|\hat{S}_i^z \prod_{l=i+1}^{j-1} e^{i\pi \hat{S}_l^z} \hat{S}_j^z|\Psi\rangle}{\langle\Psi|\Psi\rangle} \\ &= -\frac{\text{tr}[T^{\hat{S}_z}(T^{e^{i\pi\hat{S}^z}})^{j-i-1} T^{\hat{S}_z} T^{N-j+i-1}]}{\text{tr}(T^N)} \\ &= -\frac{\sum_{a=1}^{4} \langle a|T^{\hat{S}_z}(T^{e^{i\pi\hat{S}^z}})^{j-i-1} T^{\hat{S}_z}|a\rangle \lambda_a^{N-j+i-1}}{\sum_{a=1}^{4} \lambda_a^N} \quad \Leftarrow \text{for } N \to \infty, \text{ only } \lambda_{a=1} = \frac{3}{4} \text{ contributes} \\ &\to -\lambda_1^{-j+i-1} \langle 1|T^{\hat{S}_z}(T^{e^{i\pi\hat{S}^z}})^{j-i-1} T^{\hat{S}_z}|1\rangle \quad \Leftarrow \text{use } T^{\hat{S}_z}|1\rangle = \frac{1}{2}|2\rangle \text{ and } \langle 1|T^{\hat{S}_z} = -\frac{1}{2}\langle 2| \\ &= -\lambda_1^{-j+i-1}\left(-\frac{1}{4}\right) \langle 2|(T^{e^{i\pi\hat{S}^z}})^{j-i-1}|2\rangle \quad \Leftarrow \text{use } T^{e^{i\pi\hat{S}^z}}|2\rangle = \frac{3}{4}|2\rangle = \lambda_1|2\rangle \\ &= -\lambda_1^{-j+i-1}\left(-\frac{1}{4}\right) \lambda_1^{j-i-1} \quad \Leftarrow \text{substitute } \lambda_1 = \frac{3}{4} \\ &= \frac{4}{9}. \end{aligned}$$

Thus, the string correlation function is nonvanishing at large distance $|j - i| \to \infty$.

In the above derivation, you may see that the crucial point for having a nonvanishing string correlation function is $T^{e^{i\pi\hat{S}^z}}|2\rangle = \frac{3}{4}|2\rangle = \lambda_1|2\rangle$, i.e., the transfer matrix for the string operator, $T^{e^{i\pi\hat{S}^z}}$, has an eigenvalue (in fact, this must be its largest eigenvalue) which is the same as the largest eigenvalue λ_1 for T. If this were not the case, the string correlation function would decay exponentially when $|j - i| \to \infty$.

2. **Correlation function in the spin-1/2 XY chain** (3+1 points)

Consider a spin-1/2 XY chain with periodic boundary condition

$$\hat{H}_{\text{PBC}} = -J \sum_{j=1}^{N} (\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y),$$

where N is even and $J > 0$.

(a) Follow the exact solution of $\hat{H}_{\text{PBC}}$ via Jordan-Wigner transformation. Calculate the longitudinal spin-spin correlation function

$$C_{ij}^{zz} \equiv \langle\Psi|\hat{S}_i^z \hat{S}_j^z|\Psi\rangle,$$

where $|\Psi\rangle$ is the (normalized) ground state of $\hat{H}_{\text{PBC}}$, written in terms of Jordan-Wigner fermions as $|\Psi\rangle = \prod_{|k|<\frac{\pi}{2}} \hat{d}_k^\dagger|0\rangle$. When $N/2$ is even (odd), the ground state $|\Psi\rangle$ appears in the Neveu-Schwarz (Ramond) sector with allowed momenta $k = \pm\frac{\pi}{N}, \pm\frac{3\pi}{N}, \ldots, \pm\frac{(N-1)\pi}{N}$ ($k = 0, \pm\frac{2\pi}{N}, \pm\frac{4\pi}{N}, \ldots, \pm\frac{(N-2)\pi}{N}, \pi$). How does C_{ij}^{zz} decay asymptotically ($\lim_{|j-i|\to\infty}\lim_{N\to\infty}$)?

(b) The transverse spin-spin correlation function $C_{ij}^{xx} \equiv \langle\Psi|\hat{S}_i^x\hat{S}_j^x|\Psi\rangle$ is not easy to calculate by using the above approach. Why?

Solution: (a) The exact solution of the Hamiltonian $\hat{H}_{\text{PBC}}$ via Jordan-Wigner (JW) transformation has been extensively discussed in the lecture note 1d-4.pdf, where the case with *even* $N/2$ is considered. We will start with this case and comment on the odd $N/2$ case later.

For even $N/2$, the ground state is a half-filled Fermi sea

$$|\Psi\rangle = \prod_{|k|<\frac{\pi}{2}, k\in\text{APBC}} \hat{d}_k^\dagger|0\rangle,$$

where APBC means that fermions have antiperiodic boundary condition with allowed momenta $k = \pm\frac{\pi}{N}, \pm\frac{3\pi}{N}, \ldots, \pm\frac{(N-1)\pi}{N}$. We note that the occupied single-particle momenta in $|\Psi\rangle$ are

$$k = -\frac{\pi}{2} + \frac{\pi}{N},\ -\frac{\pi}{2} + \frac{3\pi}{N},\ \ldots, -\frac{\pi}{N},\ \frac{\pi}{N},\ \ldots, \frac{\pi}{2} - \frac{3\pi}{N},\ \frac{\pi}{2} - \frac{\pi}{N},$$

so $k = \pm\frac{\pi}{2}$ are *not* allowed in the APBC sector when $N/2$ is even.

By using the JW transformation, the longitudinal spin-spin correlation function becomes the density-density correlation function of fermions

$$\begin{aligned}
C_{jl}^{zz} &\equiv \langle\Psi|\hat{S}_j^z\hat{S}_l^z|\Psi\rangle \quad \Leftarrow \text{use JW transformation } \hat{S}_j^z = \hat{c}_j^\dagger\hat{c}_j - \frac{1}{2} \\
&= \langle\Psi|(\hat{c}_j^\dagger\hat{c}_j - \frac{1}{2})(\hat{c}_l^\dagger\hat{c}_l - \frac{1}{2})|\Psi\rangle \quad \Leftarrow \text{consider } j \neq l \\
&= \langle\Psi|\hat{c}_j^\dagger\hat{c}_l^\dagger\hat{c}_l\hat{c}_j|\Psi\rangle + \frac{1}{4} - \frac{1}{2}\langle\Psi|\hat{c}_j^\dagger\hat{c}_j|\Psi\rangle - \frac{1}{2}\langle\Psi|\hat{c}_l^\dagger\hat{c}_l|\Psi\rangle \\
&= \langle\Psi|\hat{c}_j^\dagger\hat{c}_l^\dagger\hat{c}_l\hat{c}_j|\Psi\rangle + \frac{1}{4} - \frac{1}{2}\times\frac{1}{2} - \frac{1}{2}\times\frac{1}{2} \\
&= \langle\Psi|\hat{c}_j^\dagger\hat{c}_l^\dagger\hat{c}_l\hat{c}_j|\Psi\rangle - \frac{1}{4},
\end{aligned}$$

where from the third line to the fourth line we have used $\langle\Psi|\hat{c}_j^\dagger\hat{c}_j|\Psi\rangle = \langle\Psi|\hat{c}_l^\dagger\hat{c}_l|\Psi\rangle = \frac{1}{2}$ ($|\Psi\rangle$ is half-filled and translation invariant). To proceed, we calculate $\langle\Psi|\hat{c}_j^\dagger\hat{c}_l^\dagger\hat{c}_l\hat{c}_j|\Psi\rangle$ by switching to momentum space

$$\begin{aligned}
&\langle\Psi|\hat{c}_j^\dagger\hat{c}_l^\dagger\hat{c}_l\hat{c}_j|\Psi\rangle \\
=\ & \frac{1}{N^2}\sum_{k_1,k_2,k_3,k_4\in\text{APBC}} \langle\Psi|\hat{d}_{k_1}^\dagger\hat{d}_{k_2}^\dagger\hat{d}_{k_3}\hat{d}_{k_4}|\Psi\rangle e^{-ik_1j-ik_2l+ik_3l+ik_4j} \quad \Leftarrow \hat{d}_k\text{-mode occupied in } |\Psi\rangle \text{ if } |k| < \frac{\pi}{2} \\
=\ & \frac{1}{N^2}\sum_{k_1,k_2,k_3,k_4\in\text{APBC},|k_{1\to4}|<\frac{\pi}{2},k_1\neq k_2,k_3\neq k_4} (-\delta_{k_1,k_3}\delta_{k_2,k_4} + \delta_{k_1,k_4}\delta_{k_2,k_3})e^{-ik_1j-ik_2l+ik_3l+ik_4j} \\
=\ & -\frac{1}{N^2}\sum_{k_1,k_2\in\text{APBC},|k_{1,2}|<\frac{\pi}{2},k_1\neq k_2} e^{ik_1(l-j)-ik_2(l-j)} + \frac{1}{N^2}\sum_{k_1,k_2\in\text{APBC},|k_{1,2}|<\frac{\pi}{2},k_1\neq k_2} \\
=\ & -\frac{1}{N^2}\left[\sum_{k_1\in\text{APBC},|k_1|<\frac{\pi}{2}} e^{ik_1(l-j)} \sum_{k_2\in\text{APBC},|k_2|<\frac{\pi}{2}} e^{-ik_2(l-j)} - \sum_{k_1\in\text{APBC},|k_1|<\frac{\pi}{2}}\right] + \frac{1}{N^2}\cdot\frac{N}{2}\left(\frac{N}{2}-1\right) \\
=\ & -\frac{1}{N^2}\left|\sum_{k_1\in\text{APBC},|k_1|<\frac{\pi}{2}} e^{ik_1(l-j)}\right|^2 + \frac{1}{N^2}\cdot\frac{N}{2} + \frac{1}{N^2}\cdot\frac{N}{2}\left(\frac{N}{2}-1\right) \\
=\ & -\frac{1}{N^2}\left|\sum_{k_1\in\text{APBC},|k_1|<\frac{\pi}{2}} e^{ik_1(l-j)}\right|^2 + \frac{1}{4},
\end{aligned}$$

where the discrete sum corresponds to a sum of geometric series

$$\begin{aligned}
\sum_{k_1\in\text{APBC},|k_1|<\frac{\pi}{2}} e^{ik_1(l-j)} &= \frac{e^{i(-\frac{\pi}{2}+\frac{\pi}{N})(l-j)}\left[1-\left(e^{i\frac{2\pi}{N}(l-j)}\right)^{\frac{N}{2}}\right]}{1-e^{i\frac{2\pi}{N}(l-j)}} \\
&= \frac{e^{i(-\frac{\pi}{2}+\frac{\pi}{N})(l-j)}\left[1-e^{i\pi(l-j)}\right]}{1-e^{i\frac{2\pi}{N}(l-j)}} \\
&= \frac{e^{-i\frac{\pi}{2}(l-j)}\left[1-(-1)^{l-j}\right]}{e^{-i\frac{\pi}{N}(l-j)}-e^{i\frac{\pi}{N}(l-j)}} \\
&= \frac{e^{-i\frac{\pi}{2}(l-j)}\left[1-(-1)^{l-j}\right]}{-2i\sin\frac{\pi(l-j)}{N}} \\
&= \begin{cases} \frac{e^{-i\frac{\pi}{2}(l-j)}}{-i\sin\frac{\pi(l-j)}{N}} & \text{for odd } l-j \\ 0 & \text{for even } l-j \end{cases}.
\end{aligned}$$

By using the above results, the longitudinal spin-spin correlation function is given by

$$\begin{aligned}
C^{zz}_{jl} &= \langle\Psi|\hat{c}^\dagger_j\hat{c}^\dagger_l\hat{c}_l\hat{c}_j|\Psi\rangle - \frac{1}{4} \\
&= -\frac{1}{N^2}\left|\sum_{k_1\in\text{APBC},|k_1|<\pi/2} e^{ik_1(l-j)}\right|^2 + \frac{1}{4} - \frac{1}{4} \\
&= \begin{cases} -\frac{1}{N^2\sin^2\frac{\pi(l-j)}{N}} & \text{for odd } l-j \\ 0 & \text{for even } l-j \end{cases}.
\end{aligned}$$

In the thermodynamic limit ($N\to\infty$), $C^{zz}_{jl}\sim -\frac{1}{\pi^2(l-j)^2}$ for odd $l-j \ll N$, which decays algebraically with a critical exponent $\nu = 2$. This is a sharp signature of a critical system.

Now we briefly comment on the case with *odd* $N/2$, which was not addressed during the lecture (but the analysis is rather similar). In this case, the ground state is again a half-filled Fermi sea

$$|\Psi\rangle = \prod_{|k|<\frac{\pi}{2},k\in\text{PBC}} \hat{d}^\dagger_k|0\rangle,$$

where the fermions have allowed momenta $k = 0, \pm\frac{2\pi}{N}, \pm\frac{4\pi}{N}, \ldots, \pm\frac{(N-2)\pi}{N}, \pi$ and the occupied single-particle momenta in $|\Psi\rangle$ are

$$k = -\frac{\pi}{2}+\frac{\pi}{N},\ -\frac{\pi}{2}+\frac{3\pi}{N},\ \ldots,-\frac{2\pi}{N},\ \frac{2\pi}{N},\ \ldots,\frac{\pi}{2}-\frac{3\pi}{N},\ \frac{\pi}{2}-\frac{\pi}{N},$$

so $k=\pm\frac{\pi}{2}$ are *not* allowed in the PBC sector when $N/2$ is odd. The rest of the calculations for C^{zz}_{jl} is essentially the same as above (except for all "$k\in$ APBC" being replaced by "$k\in$ PBC"), and the analytical expression for C^{zz}_{jl} is unchanged.

(b) After the JW transformation, the transverse spin-spin correlation function $C^{xx}_{jl}\equiv\langle\Psi|\hat{S}^x_j\hat{S}^x_l|\Psi\rangle$ is written as

$$\begin{aligned}
C^{xx}_{jl} &\equiv \langle\Psi|\hat{S}^x_j\hat{S}^x_l|\Psi\rangle \quad \Leftarrow \text{use } \hat{S}^x_j = \frac{1}{2}(\hat{c}^\dagger_j+\hat{c}_j)e^{i\pi\sum_{m<j}\hat{c}^\dagger_m\hat{c}_m} \text{ and consider } j\neq l \\
&= \frac{1}{4}\langle\Psi|(\hat{c}^\dagger_j+\hat{c}_j)e^{i\pi\sum_{m=j}^{l-1}\hat{c}^\dagger_m\hat{c}_m}(\hat{c}^\dagger_l+\hat{c}_l)|\Psi\rangle \\
&= \frac{1}{4}\langle\Psi|(\hat{c}^\dagger_j-\hat{c}_j)e^{i\pi\sum_{m=j+1}^{l-1}\hat{c}^\dagger_m\hat{c}_m}(\hat{c}^\dagger_l+\hat{c}_l)|\Psi\rangle \\
&= \frac{1}{4}\langle\Psi|(\hat{c}^\dagger_j-\hat{c}_j)\prod_{m=j+1}^{l-1}(1-2\hat{c}^\dagger_m\hat{c}_m)(\hat{c}^\dagger_l+\hat{c}_l)|\Psi\rangle,
\end{aligned}$$

which is a nonlocal string string correlation function of fermions. If one uses the Wick's theorem, a large number of terms would be generated. The question whether there is a simple closed form for C_{jl}^{xx} remains open.

Nevertheless, we note that alternative approaches are available – the asymptotic behavior of C_{jl}^{xx} can be obtained by using the bosonization method ($C_{jl}^{xx} \sim |l-j|^{-1/2}$ when $N \to \infty$ and $|l-j|$ is large) and the numerical values of C_{jl}^{xx} can be accurately calculated by using Monte Carlo simulations (based on the Jastrow form of the ground-state wave function; see page 9 in the lecture note 1d-4.pdf).

3. **Spin-1/2 XY chain with open boundaries** (3+2+2 points)

Consider a spin-1/2 XY chain with open boundary condition, defined by the Hamiltonian

$$\hat{H}_{\mathrm{OBC}} = -J \sum_{j=1}^{N-1} (\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y),$$

where N is even and $J > 0$.

(a) Map $\hat{H}_{\mathrm{OBC}}$ to a quadratic Hamiltonian of fermions by using the Jordan-Wigner transformation. Diagonalize the fermionic Hamiltonian.

(b) Determine the ground-state energy E_0 and the eigenenergy E_1 of the first excited state. How does the energy difference $E_1 - E_0$ scale with the system size N?

(c) How does the ground-state wave function look like in the original spin basis?

Solution: (a) After the Jordan-Wigner (JW) transformation, $\hat{H}_{\mathrm{OBC}}$ becomes a tight-binding chain of fermions

$$\begin{aligned}
\hat{H}_{\mathrm{OBC}} &= -J \sum_{j=1}^{N-1} (\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y) \\
&= -\frac{J}{2} \sum_{j=1}^{N-1} (\hat{\sigma}_j^+ \hat{\sigma}_{j+1}^- + \hat{\sigma}_j^- \hat{\sigma}_{j+1}^+) \quad \Leftarrow \text{use JW transformation} \\
&= -\frac{J}{2} \sum_{j=1}^{N-1} (\hat{c}_j^\dagger e^{i\pi \hat{c}_j^\dagger \hat{c}_j} \hat{c}_{j+1} + \hat{c}_j e^{i\pi \hat{c}_j^\dagger \hat{c}_j} \hat{c}_{j+1}^\dagger) \\
&= -\frac{J}{2} \sum_{j=1}^{N-1} (\hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j).
\end{aligned}$$

In order to diagonalize $\hat{H}_{\mathrm{OBC}}$, it is convenient to write it into a matrix form

$$\hat{H}_{\mathrm{OBC}} = \hat{c}^\dagger h \hat{c},$$

where $\hat{c} = \begin{pmatrix} \hat{c}_1 & \hat{c}_2 & \dots & \hat{c}_N \end{pmatrix}^T$ and h is a tridiagonal Hermitian matrix

$$h = -\frac{J}{2} \begin{pmatrix} 0 & 1 & & & & \\ 1 & 0 & 1 & & & \\ & 1 & 0 & 1 & & \\ & & 1 & 0 & \ddots & \\ & & & \ddots & \ddots & 1 \\ & & & & 1 & 0 \end{pmatrix}.$$

The next step is to find the unitary matrix U which diagonalizes h, so that

$$\begin{aligned}
\hat{H}_{\mathrm{OBC}} &= \hat{c}^\dagger h \hat{c} \qquad \Leftarrow U^\dagger U = I \\
&= \hat{c}^\dagger U^\dagger U h U^\dagger U \hat{c} \qquad \Leftarrow \text{define new fermionic modes } \hat{d} = U\hat{c} \\
&= \hat{d}^\dagger (U h U^\dagger) \hat{d}.
\end{aligned}$$

Thus, the columns of $U^\dagger$ must be the eigenvectors of h.

Actually, the eigenvectors of h take the form of standing waves

$$
\begin{aligned}
h\begin{pmatrix}\sin\frac{m\pi}{N+1}\\ \sin\frac{2m\pi}{N+1}\\ \sin\frac{3m\pi}{N+1}\\ \sin\frac{4m\pi}{N+1}\\ \vdots\\ \sin\frac{Nm\pi}{N+1}\end{pmatrix}
&= -\frac{J}{2}\begin{pmatrix}0&1&&&&\\1&0&1&&&\\&1&0&1&&\\&&1&0&\ddots&\\&&&\ddots&\ddots&1\\&&&&1&0\end{pmatrix}\begin{pmatrix}\sin\frac{m\pi}{N+1}\\ \sin\frac{2m\pi}{N+1}\\ \sin\frac{3m\pi}{N+1}\\ \sin\frac{4m\pi}{N+1}\\ \vdots\\ \sin\frac{Nm\pi}{N+1}\end{pmatrix} = -\frac{J}{2}\begin{pmatrix}\sin\frac{2m\pi}{N+1}\\ \sin\frac{m\pi}{N+1}+\sin\frac{3m\pi}{N+1}\\ \sin\frac{2m\pi}{N+1}+\sin\frac{4m\pi}{N+1}\\ \vdots\\ \sin\frac{(N-2)m\pi}{N+1}+\sin\frac{Nm\pi}{N+1}\\ \sin\frac{(N-1)m\pi}{N+1}\end{pmatrix}\\
&= -\frac{J}{2}\begin{pmatrix}2\sin\frac{m\pi}{N+1}\cos\frac{m\pi}{N+1}\\ 2\sin\frac{2m\pi}{N+1}\cos\frac{m\pi}{N+1}\\ 2\sin\frac{3m\pi}{N+1}\cos\frac{m\pi}{N+1}\\ \vdots\\ 2\sin\frac{(N-1)m\pi}{N+1}\cos\frac{m\pi}{N+1}\\ 2\sin\frac{Nm\pi}{N+1}\cos\frac{m\pi}{N+1}\end{pmatrix} = -J\cos\frac{m\pi}{N+1}\begin{pmatrix}\sin\frac{m\pi}{N+1}\\ \sin\frac{2m\pi}{N+1}\\ \sin\frac{3m\pi}{N+1}\\ \sin\frac{4m\pi}{N+1}\\ \vdots\\ \sin\frac{Nm\pi}{N+1}\end{pmatrix},
\end{aligned}
$$

from which we also read out the corresponding eigenvalue

$$\varepsilon_m = -J\cos\frac{m\pi}{N+1}, \qquad (m = 1,\ldots,N).$$

From the eigenvectors of h, the unitary matrix U is obtained

$$U^*_{jm} = U_{mj} = \sqrt{\frac{2}{N+1}}\sin\frac{\pi m j}{N+1},$$

where the prefactor $\sqrt{\frac{2}{N+1}}$ ensures normalization. Note that $U = U^\dagger$. The unitarity of U is proved as follows:

$$
\begin{aligned}
(UU^\dagger)_{mm'} &= \sum_{j=1}^{N} U_{mj}U^*_{jm'}\\
&= \frac{2}{N+1}\sum_{j=1}^{N}\sin\frac{\pi m j}{N+1}\sin\frac{\pi m' j}{N+1}\\
&= \frac{1}{N+1}\sum_{j=1}^{N}\left[\cos\frac{\pi(m-m')j}{N+1} - \cos\frac{\pi(m+m')j}{N+1}\right]\\
&= \begin{cases}\frac{1}{N+1}\left[-\frac{1+(-1)^{m-m'}}{2} + \frac{1+(-1)^{m+m'}}{2}\right] & \text{for } m\neq m'\\[2ex] \frac{1}{N+1}\left[N + \frac{1+(-1)^{2m}}{2}\right] & \text{for } m = m'\end{cases}\\
&= \begin{cases}0 & \text{for } m\neq m'\\ 1 & \text{for } m = m'\end{cases}\\
&= \delta_{mm'},
\end{aligned}
$$

where in the third line we used an identity

$$
\begin{aligned}
\sum_{j=1}^{N}\cos\frac{\pi\alpha j}{N+1} &= \frac{1}{2}\sum_{j=1}^{N}\left(e^{\frac{i\pi\alpha j}{N+1}} + e^{-\frac{i\pi\alpha j}{N+1}}\right)\\
&= \frac{1}{2}\frac{e^{\frac{i\pi\alpha}{N+1}}\left[1-\left(e^{\frac{i\pi\alpha}{N+1}}\right)^N\right]}{1-e^{\frac{i\pi\alpha}{N+1}}} + \text{c.c.}\\
&= \frac{1}{2}\left[\frac{e^{\frac{i\pi\alpha}{N+1}}-(-1)^\alpha}{1-e^{\frac{i\pi\alpha}{N+1}}} + \frac{e^{-\frac{i\pi\alpha}{N+1}}-(-1)^\alpha}{1-e^{-\frac{i\pi\alpha}{N+1}}}\right]\\
&= -\frac{1+(-1)^\alpha}{2},
\end{aligned}
$$

which is valid for $\alpha = 1, \ldots, 2N+1$. We note that, for $\alpha = N+1$, the above sum is no longer a sum of geometric series, but the identity is still valid and can be easily verified.

Now $\hat{H}_{\rm OBC}$ can be brought into a diagonal form

$$\begin{aligned} \hat{H}_{\rm OBC} &= \hat{d}^\dagger (UhU^\dagger)\hat{d} \\ &= \hat{d}^\dagger \begin{pmatrix} \varepsilon_1 & & & & \\ & \varepsilon_2 & & & \\ & & \varepsilon_3 & & \\ & & & \ddots & \\ & & & & \varepsilon_N \end{pmatrix} \hat{d} \\ &= \sum_{m=1}^{N} \varepsilon_m \hat{d}_m^\dagger \hat{d}_m, \end{aligned}$$

where $\hat{d}_m = \sum_{j=1}^N U_{mj}\hat{c}_j$. The fact that $\hat{d}_m$-modes satisfy standard fermionic commutation relations $\{\hat{d}_m, \hat{d}_{m'}^\dagger\} = \delta_{mm'}$ is ensured by the unitarity of U.

(b) When $J > 0$ and N is even, the single-particle spectrum $\varepsilon_m = -J\cos\frac{m\pi}{N+1} < 0$ ($\varepsilon_m > 0$) for $1 \le m \le N/2$ ($N/2+1 \le m \le N$). Therefore, the ground state of $\hat{H}_{\rm OBC}$ is a half-filled Fermi sea

$$|\Psi\rangle = \prod_{m=1}^{N/2} \hat{d}_m^\dagger |0\rangle$$

with ground-state energy

$$\begin{aligned} E_0 &= \sum_{m=1}^{N/2} \varepsilon_m \\ &= -\frac{J}{2}\sum_{m=1}^{N/2} e^{\frac{im\pi}{N+1}} + \text{c.c.} \\ &= \frac{J}{2}\left[1 - \frac{1}{\sin\frac{\pi}{2(N+1)}}\right]. \end{aligned}$$

The first excited states are two-fold degenerate – one may create a hole at $m = N/2$ (wave function written as $\hat{d}_{m=N/2}|\Psi\rangle$) or create an electron at $m = N/2+1$ (wave function written as $\hat{d}^\dagger_{m=N/2+1}|\Psi\rangle$), with the same eigenenergy

$$\begin{aligned} E_1 &= E_0 + \varepsilon_{m=N/2+1} \\ &= E_0 - J\cos\frac{(\frac{N}{2}+1)\pi}{N+1} \\ &= E_0 + J\sin\frac{\pi}{2(N+1)}. \end{aligned}$$

Therefore, the energy gap vanishes in the thermodynamic limit, $E_1 - E_0 = J\sin\frac{\pi}{2(N+1)} \sim \frac{\pi J}{2}\frac{1}{N}$.

(c) To derive the real-space form of the ground state, we start from its Fermi sea form

$$\begin{aligned} |\Psi\rangle &= \hat{d}^\dagger_{m=1}\hat{d}^\dagger_{m=2}\ldots\hat{d}^\dagger_{m=N/2}|0\rangle \\ &= \sum_{x_1,x_2,\ldots,x_{N/2}=1}^{N} U^*_{x_1,m=1}U^*_{x_2,m=2}\cdots U^*_{x_{N/2},m=N/2}\hat{c}^\dagger_{x_1}\hat{c}^\dagger_{x_2}\ldots\hat{c}^\dagger_{x_{N/2}}|0\rangle \quad \Leftarrow U = U^\dagger \\ &= \sum_{x_1,x_2,\ldots,x_{N/2}=1}^{N} U_{m=1,x_1}U_{m=2,x_2}\cdots U_{m=N/2,x_{N/2}}\hat{c}^\dagger_{x_1}\hat{c}^\dagger_{x_2}\ldots\hat{c}^\dagger_{x_{N/2}}|0\rangle \\ &= \sum_{1\le x_1<x_2<\ldots<x_{N/2}\le N}\ \sum_{p\in S_{N/2}} \text{sgn}(p)U_{m=1,x_{p_1}}U_{m=2,x_{p_2}}\cdots U_{m=N/2,x_{p_{N/2}}}\hat{c}^\dagger_{x_1}\hat{c}^\dagger_{x_2}\ldots\hat{c}^\dagger_{x_{N/2}}|0\rangle \\ &= \sum_{1\le x_1<x_2<\ldots<x_{N/2}\le N} \det(U_{1\le m\le N/2, x_1\to x_{N/2}})\hat{c}^\dagger_{x_1}\hat{c}^\dagger_{x_2}\ldots\hat{c}^\dagger_{x_{N/2}}|0\rangle, \end{aligned}$$

where the Slater determinant is written as

$$
\begin{aligned}
&\det(U_{1\le m\le N/2, x_1\to x_{N/2}}) \\
=&\left(\sqrt{\frac{2}{N+1}}\right)^{N/2}\det\begin{pmatrix}
\sin\frac{\pi x_1}{N+1} & \sin\frac{\pi x_2}{N+1} & \sin\frac{\pi x_3}{N+1} & \cdots & \sin\frac{\pi x_{N/2}}{N+1}\\
\sin\frac{2\pi x_1}{N+1} & \sin\frac{2\pi x_2}{N+1} & \sin\frac{2\pi x_3}{N+1} & \cdots & \sin\frac{2\pi x_{N/2}}{N+1}\\
\sin\frac{3\pi x_1}{N+1} & \sin\frac{3\pi x_2}{N+1} & \sin\frac{3\pi x_3}{N+1} & \cdots & \sin\frac{3\pi x_{N/2}}{N+1}\\
\vdots & \vdots & \vdots & \ddots & \vdots\\
\sin\frac{\frac{N}{2}\pi x_1}{N+1} & \sin\frac{\frac{N}{2}\pi x_2}{N+1} & \sin\frac{\frac{N}{2}\pi x_3}{N+1} & \cdots & \sin\frac{\frac{N}{2}\pi x_{N/2}}{N+1}
\end{pmatrix}_{N/2\times N/2}\\
\propto&\ \det\begin{pmatrix}
\sin\frac{\pi x_1}{N+1} & \sin\frac{\pi x_2}{N+1} & \sin\frac{\pi x_3}{N+1} & \cdots\\
\sin\frac{\pi x_1}{N+1}(2\cos\frac{\pi x_1}{N+1}) & \sin\frac{\pi x_2}{N+1}(2\cos\frac{\pi x_2}{N+1}) & \sin\frac{\pi x_3}{N+1}(2\cos\frac{\pi x_3}{N+1}) & \cdots\\
\sin\frac{\pi x_1}{N+1}(4\cos^2\frac{\pi x_1}{N+1}-1) & \sin\frac{\pi x_2}{N+1}(4\cos^2\frac{\pi x_2}{N+1}-1) & \sin\frac{\pi x_3}{N+1}(4\cos^2\frac{\pi x_3}{N+1}-1) & \cdots\\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}_{N/2\times N/2}\\
=&\prod_{i=1}^{N/2}\sin\frac{\pi x_i}{N+1}\det\begin{pmatrix}
1 & 1 & 1 & \cdots\\
2\cos\frac{\pi x_1}{N+1} & 2\cos\frac{\pi x_2}{N+1} & 2\cos\frac{\pi x_3}{N+1} & \cdots\\
4\cos^2\frac{\pi x_1}{N+1}-1 & 4\cos^2\frac{\pi x_2}{N+1}-1 & 4\cos^2\frac{\pi x_3}{N+1}-1 & \cdots\\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}_{N/2\times N/2}.
\end{aligned}
$$

In the above derivation, we have used that $\sin\frac{m\pi x_p}{N+1}=\sin\frac{\pi x_p}{N+1}U_m(\cos\frac{\pi x_p}{N+1})$, where $U_m(\cos\frac{\pi x_p}{N+1})$ is a polynomial of $\cos\frac{\pi x_p}{N+1}$ up to degree $m-1$ [$U_m(\cos\frac{\pi x_p}{N+1})$ are actually the Chebyshev polynomials of the second kind; see wikipedia page for the Chebyshev polynomials]. The fact that $\sin\frac{m\pi x_p}{N+1}/\sin\frac{\pi x_p}{N+1}$ yields a polynomial of $\cos\frac{\pi x_p}{N+1}$ allows us to simplify the above determinant by adding its rows (which does not change the determinant). Then, we obtain

$$
\begin{aligned}
\det(U_{1\le m\le N/2, x_1\to x_{N/2}}) &\propto \prod_{i=1}^{N/2}\sin\frac{\pi x_i}{N+1}\det\begin{pmatrix}
1 & 1 & 1 & \cdots\\
2\cos\frac{\pi x_1}{N+1} & 2\cos\frac{\pi x_2}{N+1} & 2\cos\frac{\pi x_3}{N+1} & \cdots\\
4\cos^2\frac{\pi x_1}{N+1} & 4\cos^2\frac{\pi x_2}{N+1} & 4\cos^2\frac{\pi x_3}{N+1} & \cdots\\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}_{N/2\times N/2}\\
&\propto \prod_{i=1}^{N/2}\sin\frac{\pi x_i}{N+1}\det\begin{pmatrix}
1 & 1 & 1 & \cdots\\
\cos\frac{\pi x_1}{N+1} & \cos\frac{\pi x_2}{N+1} & \cos\frac{\pi x_3}{N+1} & \cdots\\
\cos^2\frac{\pi x_1}{N+1} & \cos^2\frac{\pi x_2}{N+1} & \cos^2\frac{\pi x_3}{N+1} & \cdots\\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}_{N/2\times N/2}\\
&\propto \prod_{i=1}^{N/2}\sin\frac{\pi x_i}{N+1}\prod_{1\le j<l\le N/2}\left(\cos\frac{\pi x_j}{N+1}-\cos\frac{\pi x_l}{N+1}\right),
\end{aligned}
$$

where to arrive at the last line we used the Vandermonde determinant

$$
\det\begin{pmatrix}
1 & 1 & 1 & \cdots & 1\\
z_1 & z_2 & z_3 & \cdots & z_M\\
z_1^2 & z_2^2 & z_3^2 & \cdots & z_M^2\\
\vdots & \vdots & \vdots & \ddots & \vdots\\
z_1^{M-1} & z_2^{M-1} & z_3^{M-1} & \cdots & z_M^{M-1}
\end{pmatrix} = (-1)^{\frac{1}{2}M(M-1)}\prod_{1\le j<l\le M}(z_j-z_l).
$$

According to how JW transformation is defined, the fermionic state $\hat{c}^\dagger_{x_1}\hat{c}^\dagger_{x_2}\ldots\hat{c}^\dagger_{x_{N/2}}|0\rangle$ (with $x_1<x_2<\cdots<x_{N/2}$) corresponds to the spin state $\hat{\sigma}^+_{x_1}\hat{\sigma}^+_{x_2}\cdots\hat{\sigma}^+_{x_{N/2}}|\downarrow,\downarrow\ldots,\downarrow\rangle$.

By combining the above results, we arrive at the real-space form of the ground-state wave function

$$
|\Psi\rangle = \sum_{1\le x_1<x_2<\cdots<x_{N/2}\le N}\Psi(x_1,x_2,\ldots,x_{N/2})\hat{\sigma}^+_{x_1}\hat{\sigma}^+_{x_2}\cdots\hat{\sigma}^+_{x_{N/2}}|\downarrow,\downarrow\ldots,\downarrow\rangle,
$$

where

$$
\Psi(x_1,x_2,\ldots,x_{N/2}) \propto \prod_{i=1}^{N/2}\sin\frac{\pi x_i}{N+1}\prod_{1\le j<l\le N/2}\left(\cos\frac{\pi x_j}{N+1}-\cos\frac{\pi x_l}{N+1}\right).
$$