Problem Set 2: Solution

1. **Majorana edge mode** (2+2+2 points)

Consider a 1D chain with L sites and open boundary condition with the Hamiltonian

$$\hat{H} = i\Delta \sum_{j=1}^{L-1} \hat{c}_{2j}\hat{c}_{2j+1} + i\mu \sum_{j=1}^{L} \hat{c}_{2j-1}\hat{c}_{2j},$$

where $\hat{c}_j$ are Majorana fermions satisfying $\{\hat{c}_j, \hat{c}_l\} = 2\delta_{jl}$ and Δ, μ are real parameters. This model is a special case of the Kitaev's Majorana chain (see cond-mat/0010440), which describes a topological (trivial) superconductor with (without) Majorana edge modes for $|\mu/\Delta| < 1$ ($|\mu/\Delta| > 1$).

(a) For $\mu = 2$ and $\Delta = 1$, diagonalize $\hat{H}$ numerically for $L = 6, 10, 16, 20, 50$. Plot the single-particle excitation energies of $\hat{H}$. Verify that the Hamiltonian has a gap and does not support Majorana edge modes.

(b) For $\mu = 1$ and $\Delta = 2$, plot the single-particle excitation energies of $\hat{H}$ for $L = 6, 10, 16, 20, 50$. Verify that the Hamiltonian has a gap and two Majorana edge modes.

(c) In the topological phase with $|\mu/\Delta| < 1$, show that the exponentially localized zero-energy Majorana edge modes $\hat{b}_\mathrm{L}$ and $\hat{b}_\mathrm{R}$ take the form $\hat{b}_\mathrm{L} \propto \sum_{j=1}^{L} (\mu/\Delta)^{j-1}\hat{c}_{2j-1}$ and $\hat{b}_\mathrm{R} \propto \sum_{j=1}^{L} (\mu/\Delta)^{L-j}\hat{c}_{2j}$ in the thermodynamic limit $L \to \infty$.

Solution: In order to diagonalize $\hat{H}$, we write it as

$$\hat{H} = \frac{i}{4}\hat{c}^T A \hat{c},$$

where $\hat{c} = (\hat{c}_1, \hat{c}_2, \ldots, \hat{c}_{2L})$ and A is a tridiagonal antisymmetric real matrix

$$A = \begin{pmatrix} 0 & 2\mu & & & & & & & \\ -2\mu & 0 & 2\Delta & & & & & & \\ & -2\Delta & 0 & 2\mu & & & & & \\ & & -2\mu & 0 & 2\Delta & & & & \\ & & & -2\Delta & 0 & 2\mu & & & \\ & & & & -2\mu & \ddots & \ddots & & \\ & & & & & \ddots & 0 & 2\Delta & \\ & & & & & & -2\Delta & 0 & 2\mu \\ & & & & & & & -2\mu & 0 \end{pmatrix}_{2L\times 2L}. \quad (1)$$

By using the orthogonal matrix O which brings A into the following diagonal form,

$$OAO^T = \begin{pmatrix} 0 & \varepsilon_1 & & & & & \\ -\varepsilon_1 & 0 & & & & & \\ & & 0 & \varepsilon_2 & & & \\ & & -\varepsilon_2 & 0 & & & \\ & & & & \ddots & & \\ & & & & & 0 & \varepsilon_L \\ & & & & & -\varepsilon_L & 0 \end{pmatrix} = \bigoplus_{m=1}^{L} \begin{pmatrix} 0 & \varepsilon_m \\ -\varepsilon_m & 0 \end{pmatrix} \quad \text{(without loss of generality, } \varepsilon_m \geq 0\text{)},$$

one immediately obtains the unitary matrix U which diagonalizes A,

$$UAU^\dagger = \bigoplus_{m=1}^{L} \begin{pmatrix} i\varepsilon_m & 0 \\ 0 & -i\varepsilon_m \end{pmatrix},$$

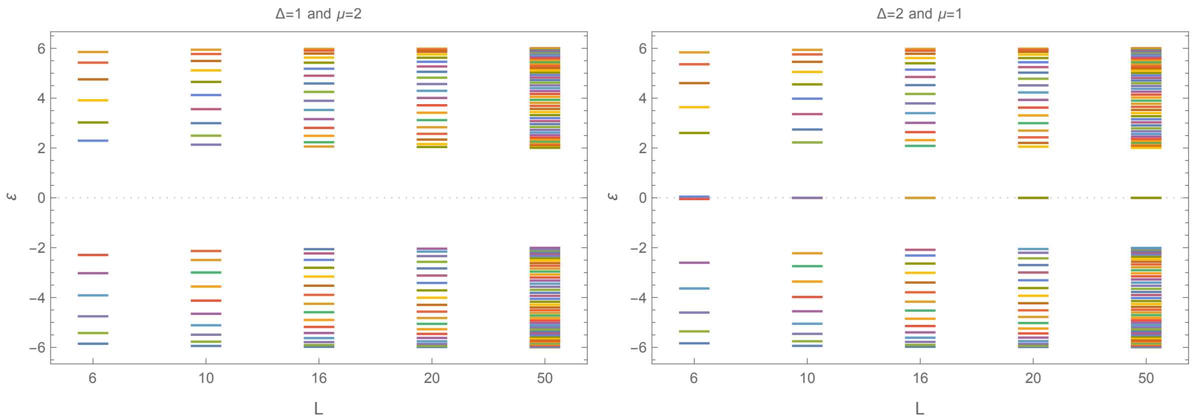

Figure 1: Eigenvalues of the matrix iA for $\mu = 2$, $\Delta = 1$ (left panel) and $\mu = 1$, $\Delta = 2$ (right panel) with $L = 6, 10, 16, 20, 50$, where the non-negative eigenvalues correspond to the single-particle energies of $\hat{H}$. Note that the vanishing eigenvalues in the right panel correspond to two Majorana zero-energy edge modes.

where $\pm i\varepsilon_m$ $(m = 1, \ldots, L)$ are eigenvalues of the matrix A in (1) and $U = \left[\bigoplus_{m=1}^{L} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix}\right] O$.

To show that ε_m are single-particle excitation energies, we have

$$\begin{aligned}
\hat{H} &= \frac{i}{4}\hat{c}^T A \hat{c} \\
&= \frac{i}{4}\hat{c}^T O^T (OAO^T) O\hat{c} \qquad \Leftarrow \text{new Majorana operators } \hat{b} = O\hat{c} \\
&= \frac{i}{4}\hat{b}^T \bigoplus_{m=1}^{L} \begin{pmatrix} 0 & \varepsilon_m \\ -\varepsilon_m & 0 \end{pmatrix} \hat{b} \\
&= \frac{i}{2}\sum_{m=1}^{L} \varepsilon_m \hat{b}_{2m-1}\hat{b}_{2m} \qquad \Leftarrow \text{new fermionic operators } \hat{d}_m = \frac{1}{2}(\hat{b}_{2m-1} + i\hat{b}_{2m}) \\
&= \sum_{m=1}^{L} \varepsilon_m (\hat{d}_m^\dagger \hat{d}_m - \frac{1}{2}),
\end{aligned} \tag{2}$$

which proves that ε_m are indeed single-particle excitation energies.

(a) The single-particle energies of $\hat{H}$ for $\mu = 2$ and $\Delta = 1$ with $L = 6, 10, 16, 20, 50$ are plotted in Fig. 1 (left panel). Note that the single-particle energies are gapped (i.e., above a threshold $\varepsilon \geq 2$ which does not vanish when increasing L).

(b) The single-particle energies of $\hat{H}$ for $\mu = 1$ and $\Delta = 2$ with $L = 6, 10, 16, 20, 50$ are plotted in Fig. 1 (right panel). Note that the smallest single-particle energy ε_m is vanishing when L is increasing, indicating one zero-energy fermionic modes (two zero-energy Majorana modes). Except for the zero mode, all other single-particle excitations are gapped with $\varepsilon \geq 2$.

(c) According to (2), the zero mode with vanishing single-particle energy $\varepsilon_1 \to 0$ implies that

$$[\hat{H}, \hat{d}_1] = [\hat{H}, \hat{d}_1^\dagger] = 0,$$

or equivalently,

$$[\hat{H}, \hat{b}_1] = [\hat{H}, \hat{b}_2] = 0,$$

where $\hat{b}_1$ and $\hat{b}_2$ are Majorana operators forming the fermionic mode $\hat{d}_1, \hat{d}_1^\dagger$.

Let us consider a general expansion of $\hat{b}_1$ in terms of the original Majorana operators $\hat{c}_j$,

$$\hat{b}_1 = \sum_{j=1}^{2L} \alpha_j \hat{c}_j, \qquad \Leftarrow \alpha_j \text{ real and } \sum_{j=1}^{2L} \alpha_j^2 = 1.$$

If $\hat{b}_1$ commutes with $\hat{H}$, the column vector $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_{2L})^T$ must be the eigenvector of the matrix A with zero eigenvalue; see proof as follows:

$$\begin{aligned}
[\hat{H}, \hat{b}_1] &= [\frac{i}{4}\hat{c}^T A \hat{c}, \alpha^T \hat{c}] \\
&= \sum_{j,l,p=1}^{2L} [\frac{i}{4}\hat{c}_j A_{jl} \hat{c}_l, \alpha_p \hat{c}_p] \\
&= \sum_{j,l,p=1}^{2L} \frac{i}{4} A_{jl}\alpha_p [\hat{c}_j \hat{c}_l, \hat{c}_p] \qquad \Leftarrow \text{use } [\hat{A}\hat{B}, \hat{C}] = \hat{A}\{\hat{B}, \hat{C}\} - \{\hat{A}, \hat{C}\}\hat{B} \text{ and } \{\hat{c}_j, \hat{c}_p\} = 2\delta_{jp} \\
&= \sum_{j,l,p=1}^{2L} \frac{i}{4} A_{jl}\alpha_p (2\hat{c}_j \delta_{pl} - 2\hat{c}_l \delta_{jp}) \\
&= \frac{i}{2}\left(\sum_{j,l=1}^{2L} A_{jl}\alpha_l \hat{c}_j - \sum_{l,p=1}^{2L} A_{pl}\alpha_p \hat{c}_l \right) \qquad \Leftarrow A \text{ antisymmetric, so } A_{jl} = -A_{lj} \\
&= i \sum_{j=1}^{2L} (A\alpha)_j \hat{c}_j,
\end{aligned}$$

which means that $[\hat{H}, \hat{b}_1] = 0$ if and only if $A\alpha = 0$.

In the topological phase with $|\mu/\Delta| < 1$, the eigenvectors of the tridiagonal matrix A with zero eigenvalue can be obtained by inspection, e.g.,

$$\begin{pmatrix}
0 & 2\mu & & & & & & & \\
-2\mu & 0 & 2\Delta & & & & & & \\
 & -2\Delta & 0 & 2\mu & & & & & \\
 & & -2\mu & 0 & 2\Delta & & & & \\
 & & & -2\Delta & 0 & 2\mu & & & \\
 & & & & -2\mu & \ddots & \ddots & & \\
 & & & & & \ddots & 0 & 2\Delta & \\
 & & & & & & -2\Delta & 0 & 2\mu \\
 & & & & & & & -2\mu & 0
\end{pmatrix}
\begin{pmatrix} 1 \\ 0 \\ \frac{\mu}{\Delta} \\ 0 \\ (\frac{\mu}{\Delta})^2 \\ 0 \\ \vdots \\ (\frac{\mu}{\Delta})^{L-1} \\ 0 \end{pmatrix}
=
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ -2\mu(\frac{\Delta}{\mu})^{L-1} \end{pmatrix} \to 0$$

for $|\mu/\Delta| < 1$ and $L \to \infty$. Similarly, the other eigenvector corresponding to a vanishing eigenvalue is $(0, (\frac{\mu}{\Delta})^{L-1}, 0, (\frac{\mu}{\Delta})^{L-2}, \ldots, 0, \frac{\mu}{\Delta}, 0, 1)^T$. Obviously, these two vectors are orthogonal to each other. Accordingly, the two Majorana zero modes, up to a normalization factor, are written as

$$\hat{b}_{\rm L} \equiv \hat{b}_1 \propto \sum_{j=1}^{L} (\mu/\Delta)^{j-1} \hat{c}_{2j-1}, \qquad \hat{b}_{\rm R} \equiv \hat{b}_2 \propto \sum_{j=1}^{L} (\mu/\Delta)^{L-j} \hat{c}_{2j},$$

which are exponentially localized at the left and right boundaries, respectively.

2. **SU(2) spin coherent state** (2+2+3 points)

For a single spin-S, the SU(2) spin coherent state is defined by $|\vec{\Omega}\rangle = \frac{1}{\sqrt{(2S)!}}(z_1 \hat{a}^\dagger + z_2 \hat{b}^\dagger)^{2S}|0\rangle$, where $\hat{a}^\dagger$, $\hat{b}^\dagger$ are Schwinger bosons, $(z_1, z_2) = (\cos\frac{\theta}{2}, \sin\frac{\theta}{2}e^{i\phi})$, and the O(3) unit vector $\vec{\Omega} = (\Omega^x, \Omega^y, \Omega^z) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. The spin operators are represented by Schwinger boson operators, $\hat{S}^x = \frac{1}{2}(\hat{a}^\dagger\hat{b} + \hat{b}^\dagger\hat{a})$, $\hat{S}^y = \frac{1}{2i}(\hat{a}^\dagger\hat{b} - \hat{b}^\dagger\hat{a})$, and $\hat{S}^z = \frac{1}{2}(\hat{a}^\dagger\hat{a} - \hat{b}^\dagger\hat{b})$, with the constraint $\hat{a}^\dagger\hat{a} + \hat{b}^\dagger\hat{b} = 2S$. The physical spin states $|S, m\rangle$ are related to the Schwinger boson occupation basis via $|S, m\rangle = \frac{(\hat{a}^\dagger)^{S+m}(\hat{b}^\dagger)^{S-m}}{\sqrt{(S+m)!(S-m)!}}|0\rangle$ $(m = -S, -S+1, \ldots, S)$.

(a) Prove that the spin coherent state satisfies the overcompleteness relation

$$\frac{2S+1}{4\pi}\int d\vec{\Omega}\ |\vec{\Omega}\rangle\langle\vec{\Omega}| = \sum_{m=-S}^{S} |S, m\rangle\langle S, m| = 1, \tag{3}$$

where $\int d\vec{\Omega} = \int_0^\pi \sin\theta \; d\theta \int_0^{2\pi} d\phi$.

(b) Show that the expectation value of the spin operators in the spin coherent state is given by

$$\langle \vec{\Omega} | \hat{S}^a | \vec{\Omega} \rangle = S\Omega^a, \qquad (a = x, y, z). \tag{4}$$

(c) The quantum spin-S Heisenberg model on a lattice is defined by $\hat{H} = J \sum_{\langle i,j \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j$. By discretizing the imaginary-time evolution into small time-slices and inserting the overcompleteness relation of spin coherent states, show that the partition function $Z = \mathrm{Tr} e^{-\beta \hat{H}}$ has the following path integral formulation:

$$Z = \int_{\vec{\Omega}(0)=\vec{\Omega}(\beta)} \mathcal{D}\vec{\Omega}(\tau) \; e^{-S[\vec{\Omega}]}, \tag{5}$$

where

$$S[\vec{\Omega}] = \int_0^\beta d\tau \; \left[iS \sum_j (1 - \cos\theta_j)\dot{\phi}_j + JS^2 \sum_{\langle j,l \rangle} \vec{\Omega}_j \cdot \vec{\Omega}_l \right]. \tag{6}$$

Solution: (a) The spin coherent state is expanded in the S^z-basis as

$$\begin{aligned}
|\vec{\Omega}\rangle &= \frac{1}{\sqrt{(2S)!}} (z_1 \hat{a}^\dagger + z_2 \hat{b}^\dagger)^{2S} |0\rangle \\
&= \frac{1}{\sqrt{(2S)!}} \sum_{m=-S}^{S} \binom{2S}{S+m} z_1^{S+m} z_2^{S-m} (\hat{a}^\dagger)^{S+m} (\hat{b}^\dagger)^{S-m} |0\rangle \quad \Leftarrow \text{use } |S,m\rangle = \frac{(\hat{a}^\dagger)^{S+m}(\hat{b}^\dagger)^{S-m}}{\sqrt{(S+m)!(S-m)!}} |0\rangle \\
&= \sum_{m=-S}^{S} \sqrt{\binom{2S}{S+m}} z_1^{S+m} z_2^{S-m} |S,m\rangle.
\end{aligned}$$

By using $(z_1, z_2) = (\cos\frac{\theta}{2}, \sin\frac{\theta}{2} e^{i\phi})$, the left hand side of (3) is simplified as

$$\begin{aligned}
& \frac{2S+1}{4\pi} \int d\vec{\Omega} \; |\vec{\Omega}\rangle\langle\vec{\Omega}| \\
= \; & \frac{2S+1}{4\pi} \int d\vec{\Omega} \sum_{m,m'=-S}^{S} \sqrt{\binom{2S}{S+m}\binom{2S}{S+m'}} z_1^{S+m} z_2^{S-m} (z_1^*)^{S+m'} (z_2^*)^{S-m'} |S,m\rangle\langle S,m'| \\
= \; & \frac{2S+1}{4\pi} \sum_{m,m'=-S}^{S} \sqrt{\binom{2S}{S+m}\binom{2S}{S+m'}} \int_0^\pi d\theta \sin\theta (\cos\frac{\theta}{2})^{2S+m+m'} (\sin\frac{\theta}{2})^{2S-m-m'} \\
& \times \int_0^{2\pi} d\phi e^{i(m'-m)\phi} |S,m\rangle\langle S,m'| \\
= \; & \frac{2S+1}{2} \sum_{m=-S}^{S} \binom{2S}{S+m} \int_0^\pi d\theta \sin\theta (\cos\frac{\theta}{2})^{2(S+m)} (\sin\frac{\theta}{2})^{2(S-m)} |S,m\rangle\langle S,m| \\
= \; & (2S+1) \sum_{m=-S}^{S} \binom{2S}{S+m} \frac{1}{2} \int_{-1}^{1} d\cos\theta \left(\frac{1+\cos\theta}{2}\right)^{S+m} \left(\frac{1-\cos\theta}{2}\right)^{S-m} |S,m\rangle\langle S,m|,
\end{aligned} \tag{7}$$

where the remaining integral can be written as

$$\begin{aligned}
I_{S,m} &= \frac{1}{2} \int_{-1}^{1} d\cos\theta \left(\frac{1+\cos\theta}{2}\right)^{S+m} \left(\frac{1-\cos\theta}{2}\right)^{S-m} \qquad \Leftarrow \text{define } x = \frac{1+\cos\theta}{2} \\
&= \int_0^1 dx \, x^{S+m} (1-x)^{S-m}.
\end{aligned}$$

To proceed, it is convenient to introduce an auxiliary function

$$f_S(w) = \sum_{m=-S}^{S} \binom{2S}{S+m} I_{S,m} \, w^{S+m}, \tag{8}$$

which is a polynomial of w (up to degree $2S$).

$$
\begin{aligned}
f_S(w) &= \sum_{m=-S}^{S} \binom{2S}{S+m} w^{S+m} \int_0^1 dx\, x^{S+m}(1-x)^{S-m} \\
&= \int_0^1 dx \sum_{m=-S}^{S} \binom{2S}{S+m} (wx)^{S+m}(1-x)^{S-m} \\
&= \int_0^1 dx\, (wx+1-x)^{2S} \\
&= \int_0^1 dx\, [(w-1)x+1]^{2S} \qquad \Leftarrow y=(w-1)x+1 \\
&= \frac{1}{w-1}\int_1^w dy\, y^{2S} \\
&= \frac{1}{2S+1}\frac{w^{2S+1}-1}{w-1} \\
&= \frac{1}{2S+1}(1+w+\cdots+w^{2S}). \qquad (9)
\end{aligned}
$$

Comparing the coefficients of the polynomial in (8) and (9), one obtains $I_{S,m} = \frac{1}{2S+1}\frac{1}{\binom{2S}{S+m}}$, the substitution of which into (7) proves the overcompleteness relation.

(b) By using $\langle S, m'|\hat{S}^+|S,m\rangle = \sqrt{(S-m)(S+m+1)}\delta_{m',m+1}$, the expectation value of $\hat{S}^+$ in the spin coherent state is given by

$$
\begin{aligned}
\langle\vec{\Omega}|\hat{S}^+|\vec{\Omega}\rangle &= \sum_{m,m'=-S}^{S} \sqrt{\binom{2S}{S+m}\binom{2S}{S+m'}} z_1^{S+m} z_2^{S-m} (z_1^*)^{S+m'} (z_2^*)^{S-m'} \langle S,m'|\hat{S}^+|S,m\rangle \\
&= \sum_{m,m'=-S}^{S} \sqrt{\binom{2S}{S+m}\binom{2S}{S+m'}} z_1^{S+m} z_2^{S-m} (z_1^*)^{S+m'} (z_2^*)^{S-m'} \sqrt{(S-m)(S+m+1)}\delta_{m',m+1} \\
&= \sum_{m=-S}^{S} \sqrt{\binom{2S}{S+m}\binom{2S}{S+m+1}} z_1^{S+m} z_2^{S-m} (z_1^*)^{S+m+1} (z_2^*)^{S-m-1} \sqrt{(S-m)(S+m+1)} \\
&= \sum_{m=-S}^{S} \frac{(2S)!}{(S+m)!(S-m-1)!} (|z_1|^2)^{S+m}(|z_2|^2)^{S-m-1} z_1^* z_2 \\
&= 2S(|z_1|^2+|z_2|^2)^{2S-1} z_1^* z_2 \qquad \Leftarrow \text{use } |z_1|^2+|z_2|^2=1 \\
&= 2S z_1^* z_2 \\
&= 2S\cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{i\phi} \\
&= S\sin\theta e^{i\phi}.
\end{aligned}
$$

Since $\hat{S}^-$ is the Hermitian conjugate of $\hat{S}^+$, we have $\langle\vec{\Omega}|\hat{S}^-|\vec{\Omega}\rangle = (\langle\vec{\Omega}|\hat{S}^+|\vec{\Omega}\rangle)^* = S\sin\theta e^{-i\phi}$. Thus, we obtain

$$
\begin{aligned}
\langle\vec{\Omega}|\hat{S}^x|\vec{\Omega}\rangle &= \langle\vec{\Omega}|\frac{1}{2}(\hat{S}^+ + \hat{S}^-)|\vec{\Omega}\rangle = S\sin\theta\cos\phi, \\
\langle\vec{\Omega}|\hat{S}^y|\vec{\Omega}\rangle &= \langle\vec{\Omega}|\frac{1}{2i}(\hat{S}^+ - \hat{S}^-)|\vec{\Omega}\rangle = S\sin\theta\sin\phi.
\end{aligned}
$$

By using $\langle S, m'|\hat{S}^z|S, m\rangle = m\delta_{m',m}$, the expectation value of $\hat{S}^z$ in $|\vec{\Omega}\rangle$ is given by

$$
\begin{aligned}
\langle\vec{\Omega}|\hat{S}^z|\vec{\Omega}\rangle &= \sum_{m,m'=-S}^{S} \sqrt{\binom{2S}{S+m}\binom{2S}{S+m'}} z_1^{S+m} z_2^{S-m} (z_1^*)^{S+m'} (z_2^*)^{S-m'} \langle S, m'|\hat{S}^z|S, m\rangle \\
&= \sum_{m,m'=-S}^{S} \sqrt{\binom{2S}{S+m}\binom{2S}{S+m'}} z_1^{S+m} z_2^{S-m} (z_1^*)^{S+m'} (z_2^*)^{S-m'} m\delta_{m',m} \\
&= \sum_{m=-S}^{S} \binom{2S}{S+m} (|z_1|^2)^{S+m} (|z_2|^2)^{S-m} m \\
&= \sum_{m=-S}^{S} \binom{2S}{S+m} (|z_1|^2)^{S+m} (|z_2|^2)^{S-m} \frac{1}{2}[(S+m)-(S-m)] \\
&= \frac{1}{2}\sum_{m=-S}^{S} \frac{(2S)!}{(S+m-1)!(S-m)!} (|z_1|^2)^{S+m-1} (|z_2|^2)^{S-m} |z_1|^2 \\
&\quad -\frac{1}{2}\sum_{m=-S}^{S} \frac{(2S)!}{(S+m)!(S-m-1)!} (|z_1|^2)^{S+m-1} (|z_2|^2)^{S-m} |z_2|^2 \\
&= S(|z_1|^2 + |z_2|^2)^{2S-1}(|z_1|^2 - |z_2|^2) \\
&= S(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}) \\
&= S\cos\theta.
\end{aligned}
$$

(c) For formulating the path integral, it is sufficient to consider a single spin, which simplifies the notation. The trace in the partition function is first replaced by an average in the spin coherent state,

$$
\begin{aligned}
Z &= \mathrm{Tr} e^{-\beta\hat{H}} \\
&= \sum_{m=-S}^{S} \langle S, m|e^{-\beta\hat{H}}|S, m\rangle \qquad \Leftarrow \text{insert overcompleteness relation (3)} \\
&= \frac{2S+1}{4\pi}\int d\vec{\Omega}_0 \sum_{m=-S}^{S} \langle S, m|\vec{\Omega}_0\rangle\langle\vec{\Omega}_0|e^{-\beta\hat{H}}|S, m\rangle \\
&= \frac{2S+1}{4\pi}\int d\vec{\Omega}_0 \sum_{m=-S}^{S} \langle\vec{\Omega}_0|e^{-\beta\hat{H}}|S, m\rangle\langle S, m|\vec{\Omega}_0\rangle \qquad \Leftarrow \text{use} \sum_{m=-S}^{S} |S, m\rangle\langle S, m| = 1 \\
&= \frac{2S+1}{4\pi}\int d\vec{\Omega}_0 \, \langle\vec{\Omega}_0|e^{-\beta\hat{H}}|\vec{\Omega}_0\rangle,
\end{aligned}
$$

which is followed by dividing imaginary-time evolution into small time-slices and inserting $N-1$ overcompleteness relation,

$$
Z = \left(\frac{2S+1}{4\pi}\right)^N \int \prod_{k=0}^{N-1} d\vec{\Omega}_k \, \langle\vec{\Omega}_0|e^{-\Delta\tau\hat{H}}|\vec{\Omega}_{N-1}\rangle \cdots \langle\vec{\Omega}_1|e^{-\Delta\tau\hat{H}}|\vec{\Omega}_0\rangle,
$$

where the evolution in a small time-slice is given by

$$\begin{aligned}
& \langle\vec{\Omega}_{k+1}|e^{-\Delta\tau\hat{H}}|\vec{\Omega}_k\rangle \\
\simeq\ & \langle\vec{\Omega}_{k+1}|(1-\Delta\tau\hat{H})|\vec{\Omega}_k\rangle \\
=\ & \langle\vec{\Omega}_{k+1}|\vec{\Omega}_k\rangle - \Delta\tau\langle\vec{\Omega}_{k+1}|\hat{H}|\vec{\Omega}_k\rangle \quad \Leftarrow \text{use } \langle\vec{\Omega}_{k+1}| = \langle\vec{\Omega}_k| + \Delta\tau\langle\frac{d\vec{\Omega}_k}{d\tau}| \text{ and } \langle\frac{d\vec{\Omega}_k}{d\tau}| \text{ to be determined below} \\
=\ & \langle\vec{\Omega}_k|\vec{\Omega}_k\rangle + \Delta\tau\langle\frac{d\vec{\Omega}_k}{d\tau}|\vec{\Omega}_k\rangle - \Delta\tau\langle\vec{\Omega}_k|\hat{H}|\vec{\Omega}_k\rangle + O(\Delta\tau^2) \quad \Leftarrow \text{use } \langle\vec{\Omega}_k|\vec{\Omega}_k\rangle = 1 \\
\simeq\ & 1 + \Delta\tau\langle\frac{d\vec{\Omega}_k}{d\tau}|\vec{\Omega}_k\rangle - \Delta\tau\langle\vec{\Omega}_k|\hat{H}|\vec{\Omega}_k\rangle \quad \Leftarrow \text{use Eq. (4), spin operators in } \hat{H} \text{ replaced by } S\vec{\Omega}_k \\
=\ & 1 + \Delta\tau\langle\frac{d\vec{\Omega}_k}{d\tau}|\vec{\Omega}_k\rangle - \Delta\tau H(S\vec{\Omega}_k) \\
\simeq\ & e^{\Delta\tau[\langle\frac{d\vec{\Omega}_k}{d\tau}|\vec{\Omega}_k\rangle - H(S\vec{\Omega}_k)]}. \qquad (10)
\end{aligned}$$

Now we determine $\langle\frac{d\vec{\Omega}_k}{d\tau}|$ and its overlap with $|\vec{\Omega}_k\rangle$,

$$\begin{aligned}
\langle\frac{d\vec{\Omega}_k}{d\tau}| &= \frac{d}{d\tau}\left[\sum_{m=-S}^{S}\sqrt{\binom{2S}{S+m}}[(z_1^*)^{S+m}(z_2^*)^{S-m}]\langle S,m|\right]|_{\tau=\tau_k} \\
&= \sum_{m=-S}^{S}\sqrt{\binom{2S}{S+m}}[(S+m)(z_{k,1}^*)^{S+m-1}\dot{z}_{k,1}^*(z_{k,2}^*)^{S-m} + (S-m)(z_{k,1}^*)^{S+m}(z_{k,2}^*)^{S-m-1}\dot{z}_{k,2}^*]\langle S,m|,
\end{aligned}$$

and

$$\begin{aligned}
& \langle\frac{d\vec{\Omega}_k}{d\tau}|\vec{\Omega}_k\rangle \\
=\ & \sum_{m=-S}^{S}\binom{2S}{S+m}[(S+m)(z_{k,1}^*)^{S+m-1}\dot{z}_{k,1}^*(z_{k,2}^*)^{S-m} + (S-m)(z_{k,1}^*)^{S+m}(z_{k,2}^*)^{S-m-1}\dot{z}_{k,2}^*]z_{k,1}^{S+m}z_{k,2}^{S-m} \\
=\ & \sum_{m=-S}^{S}\binom{2S}{S+m}[(S+m)(|z_{k,1}|^2)^{S+m-1}(|z_{k,2}|^2)^{S-m}\dot{z}_{k,1}^*z_{k,1} + (S-m)(|z_{k,1}|^2)^{S+m}(|z_{k,2}|^2)^{S-m-1}\dot{z}_{k,2}^*z_{k,2}] \\
=\ & 2S(|z_{k,1}|^2+|z_{k,2}|^2)^{2S-1}(\dot{z}_{k,1}^*z_{k,1}+\dot{z}_{k,2}^*z_{k,2}) \quad \Leftarrow \text{use } |z_{k,1}|^2+|z_{k,2}|^2 = 1 \\
=\ & 2S(\dot{z}_{k,1}^*z_{k,1}+\dot{z}_{k,2}^*z_{k,2}) \\
=\ & 2S\left[-\frac{1}{2}\sin\frac{\theta_k}{2}\ \dot{\theta}_k\ \cos\frac{\theta_k}{2} + \left(\frac{1}{2}\cos\frac{\theta_k}{2}\ \dot{\theta}_k\ e^{-i\phi_k} + \sin\frac{\theta_k}{2}e^{-i\phi_k}(-i\dot{\phi}_k)\right)\sin\frac{\theta_k}{2}e^{i\phi_k}\right] \\
=\ & -2iS\sin^2\frac{\theta_k}{2}\ \dot{\phi}_k \\
=\ & -iS(1-\cos\theta_k)\dot{\phi}_k,
\end{aligned}$$

where the last expression is just the Berry connection. Then, the propagator in (10) is given by

$$\langle\vec{\Omega}_{k+1}|e^{-\Delta\tau\hat{H}}|\vec{\Omega}_k\rangle \simeq e^{\Delta\tau[-iS(1-\cos\theta_k)\dot{\phi}_k - H(S\vec{\Omega}_k)]}.$$

After collecting the propagators for all small time-slices and taking the limit $\Delta\tau \to 0$ ($N \to \infty$ and $N\Delta\tau = \beta$), we arrive at

$$\begin{aligned}
Z &= \left(\frac{2S+1}{4\pi}\right)^N \int \prod_{k=0}^{N-1} d\vec{\Omega}_k\ \langle\vec{\Omega}_0|e^{-\Delta\tau\hat{H}}|\vec{\Omega}_{N-1}\rangle \cdots \langle\vec{\Omega}_1|e^{-\Delta\tau\hat{H}}|\vec{\Omega}_0\rangle \\
&\to \left(\frac{2S+1}{4\pi}\right)^N \int \prod_{k=0}^{N-1} d\vec{\Omega}_k\ e^{\Delta\tau\sum_{k=0}^{N-1}[-iS(1-\cos\theta_k)\dot{\phi}_k - H(S\vec{\Omega}_k)]} \\
&= \int_{\vec{\Omega}(0)=\vec{\Omega}(\beta)} \mathcal{D}\vec{\Omega}(\tau)\ e^{-\int_0^\beta d\tau[iS(1-\cos\theta)\dot{\phi} + H(S\vec{\Omega})]},
\end{aligned}$$

which indeed agrees with the "shortcut" derivation based on Schwinger bosons (see page 7 in the lecture note QM-7.pdf).

For the spin-S Heisenberg model, the derivation is essentially the same, expect that one needs to consider a product of spin coherent states for each site, $|\{\vec{\Omega}\}\rangle = \prod_j |\vec{\Omega}_j\rangle$. In the path integral, the Hamiltonian $\hat{H} = J\sum_{\langle i,j\rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j$ is replaced by $H(S\vec{\Omega}) = \langle\{\vec{\Omega}\}|\hat{H}|\{\vec{\Omega}\}\rangle = JS^2 \sum_{\langle i,j\rangle} \vec{\Omega}_i \cdot \vec{\Omega}_j$, and the Berry's phase is now a sum of individual Berry phases in each site, thus confirming the correctness of (5) and (6).

3. **1D classical XY model** (2+3 points)

Consider the partition function of the 1D classical XY model

$$Z = \int_0^{2\pi} \prod_{i=1}^{L} \frac{d\theta_i}{2\pi} e^{-\beta H},$$

where $\beta = 1/T$ and $H = -J\sum_{i=1}^{L} \mathbf{I}_i \cdot \mathbf{I}_{i+1}$ with $\mathbf{I}_i = I(\cos\theta_i, \sin\theta_i)$ and periodic boundary condition ($\theta_1 = \theta_{L+1}$). The partition function can be represented as

$$Z = \int_0^{2\pi} \prod_{i=1}^{L} \frac{d\theta_i}{2\pi} \mathrm{T}(\theta_1,\theta_2)\mathrm{T}(\theta_2,\theta_3)\cdots\mathrm{T}(\theta_L,\theta_1),$$

where $\mathrm{T}(\theta_i,\theta_{i+1}) = e^{\beta J I^2 \cos(\theta_i - \theta_{i+1})}$ is the so-called transfer matrix.

(a) Calculate the partition function Z.

(b) Calculate the correlation function

$$\langle \mathbf{I}_j \cdot \mathbf{I}_l\rangle = \frac{1}{Z}\int_0^{2\pi} \prod_{i=1}^{L} \frac{d\theta_i}{2\pi} (\mathbf{I}_j \cdot \mathbf{I}_l) e^{-\beta H}$$

by using the transfer matrix approach. Show that the correlation function $\langle \mathbf{I}_j \cdot \mathbf{I}_l\rangle$ decays exponentially at large distance $|j-l| \gg 1$,

$$\lim_{L\to\infty} \langle \mathbf{I}_j \cdot \mathbf{I}_l\rangle \sim e^{-|j-l|/\xi}$$

for any finite temperature $T > 0$. Determine the correlation length ξ.

Solution: (a) The most straightforward approach would be an expansion of the transfer matrix as

$$
\begin{aligned}
& \mathrm{T}(\theta,\theta') \\
= \;& e^{\beta J I^2 \cos(\theta-\theta')} \\
= \;& \sum_{n=0}^{\infty} \frac{1}{n!}[\beta J I^2 \cos(\theta-\theta')]^n \\
= \;& \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{\beta J I^2}{2}\right)^n [e^{i(\theta-\theta')} + e^{-i(\theta-\theta')}]^n \qquad \Leftarrow \text{consider } n \text{ even and } n \text{ odd separately} \\
= \;& \sum_{n=0}^{\infty} \frac{1}{(2n)!}\left(\frac{\beta J I^2}{2}\right)^{2n} \sum_{m=-n}^{n} \binom{2n}{n+m} e^{i(n+m)(\theta-\theta')} e^{-i(n-m)(\theta-\theta')} \\
& + \sum_{n=1}^{\infty} \frac{1}{(2n-1)!}\left(\frac{\beta J I^2}{2}\right)^{2n-1} \sum_{m=-n+1}^{n} \binom{2n-1}{n+m-1} e^{i(n+m-1)(\theta-\theta')} e^{-i(n-m)(\theta-\theta')} \\
= \;& \sum_{n=0}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n} \sum_{m=-n}^{n} \frac{1}{(n+m)!(n-m)!} e^{i2m(\theta-\theta')} \qquad \Leftarrow \text{consider } n=0 \text{ and } n \geq 2 \text{ separately} \\
& + \sum_{n=1}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n-1} \sum_{m=-n+1}^{n} \frac{1}{(n+m-1)!(n-m)!} e^{i(2m-1)(\theta-\theta')} \\
= \;& \sum_{n=0}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n} \frac{1}{(n!)^2} + 2\sum_{n=1}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n} \sum_{m=1}^{n} \frac{1}{(n+m)!(n-m)!} \cos[2m(\theta-\theta')] \\
& + 2\sum_{n=1}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n-1} \sum_{m=1}^{n} \frac{1}{(n+m-1)!(n-m)!} \cos[(2m-1)(\theta-\theta')] \quad \Leftarrow \text{use } \sum_{n=1}^{\infty}\sum_{m=1}^{n} = \sum_{m=1}^{\infty}\sum_{n=m}^{\infty} \\
= \;& \sum_{n=0}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n} \frac{1}{(n!)^2} + 2\sum_{m=1}^{\infty}\sum_{n=m}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n} \frac{1}{(n+m)!(n-m)!} \cos[2m(\theta-\theta')] \\
& + 2\sum_{m=1}^{\infty}\sum_{n=m}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n-1} \frac{1}{(n+m-1)!(n-m)!} \cos[(2m-1)(\theta-\theta')] \quad \Leftarrow \text{define } n' = n-m \\
= \;& \sum_{n=0}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n} \frac{1}{(n!)^2} + 2\sum_{m=1}^{\infty}\sum_{n'=0}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n'+2m} \frac{1}{(n'+2m)!n'!} \cos[2m(\theta-\theta')] \\
& + 2\sum_{m=1}^{\infty}\sum_{n'=0}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n'+2m-1} \frac{1}{(n'+2m-1)!n'!} \cos[(2m-1)(\theta-\theta')] \quad \Leftarrow \text{combine even/odd terms} \\
= \;& \sum_{n=0}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n} \frac{1}{(n!)^2} + 2\sum_{m=1}^{\infty}\sum_{n=0}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n+m} \frac{1}{(n+m)!n!} \cos[m(\theta-\theta')] \\
= \;& A_{m=0} + 2\sum_{m=1}^{\infty} A_m \cos[m(\theta-\theta')], \qquad (11)
\end{aligned}
$$

where

$$A_m = \sum_{n=0}^{\infty} \left(\frac{\beta J I^2}{2}\right)^{2n+m} \frac{1}{(n+m)!n!}, \qquad (m \geq 0). \qquad (12)$$

Actually, the above expansion generates the modified Bessel function of the first kind, $e^{z\cos\theta} = I_0(z) + 2\sum_{m=1}^{\infty} I_m(z)\cos(m\theta)$, where $I_m(z) = \sum_{n=0}^{\infty} \frac{1}{(n+m)!n!}(\frac{z}{2})^{2n+m}$; see wikipedia page for the Bessel functions.

The expansion in (11) diagonalizes the transfer matrix,

$$\mathrm{T}(\theta,\theta') = \sum_{m=-\infty}^{\infty} A_m e^{im(\theta-\theta')} \qquad \Leftarrow A_m = A_{-m} \text{ assumed}$$

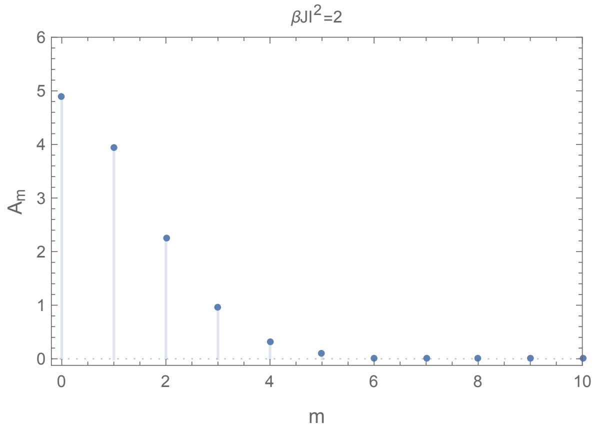

Figure 2: Eigenvalues of the transfer matrix: A_m for $\beta JI^2 = 2$. Note that the largest eigenvalue $A_{m=0}$ is unique and only $A_{m\geq 0}$ is plotted since $A_m = A_{-m}$.

and

$$\begin{aligned}\int_0^{2\pi} \frac{d\theta'}{2\pi} \mathrm{T}(\theta,\theta') e^{im\theta'} &= \int_0^{2\pi} \frac{d\theta'}{2\pi} \sum_{m'=-\infty}^{\infty} A_{m'} e^{im'(\theta-\theta')} e^{im\theta'} \Leftarrow \int_0^{2\pi} \frac{d\theta'}{2\pi} e^{i(m'-m)\theta'} = \delta_{m'm} \\ &= A_m e^{im\theta}, \qquad (m = 0, \pm 1, \pm 2, \ldots).\end{aligned}$$

With the eigenvalues of the transfer matrix, the partition function can be immediately evaluated,

$$\begin{aligned}Z &= \int_0^{2\pi} \prod_{i=1}^{L} \frac{d\theta_i}{2\pi} \mathrm{T}(\theta_1,\theta_2)\mathrm{T}(\theta_2,\theta_3)\cdots\mathrm{T}(\theta_L,\theta_1) \\ &= \sum_{m=-\infty}^{\infty} A_m^L. \end{aligned} \tag{13}$$

Note that the largest eigenvalue of the transfer matrix is always *unique* and appears at $m = 0$ (see Fig. 2 for an example), so the partition function converges to $A_{m=0}^L$ in the thermodynamic limit.

(b) By using the transfer matrix approach, the correlation function $\langle \mathbf{I}_j \cdot \mathbf{I}_l \rangle$ can be written as

$$\begin{aligned}\langle \mathbf{I}_j \cdot \mathbf{I}_l \rangle &= \frac{1}{Z} \int_0^{2\pi} \prod_{i=1}^{L} \frac{d\theta_i}{2\pi} (\mathbf{I}_j \cdot \mathbf{I}_l) e^{-\beta H} \\ &= \frac{I^2}{Z} \int_0^{2\pi} \prod_{i=1}^{L} \frac{d\theta_i}{2\pi} \cos(\theta_j - \theta_l) \mathrm{T}(\theta_1,\theta_2)\mathrm{T}(\theta_2,\theta_3)\cdots\mathrm{T}(\theta_L,\theta_1) \\ &= \frac{I^2}{2Z} \int_0^{2\pi} \prod_{i=1}^{L} \frac{d\theta_i}{2\pi} [e^{i(\theta_j-\theta_l)} + e^{-i(\theta_j-\theta_l)}] \mathrm{T}(\theta_1,\theta_2)\mathrm{T}(\theta_2,\theta_3)\cdots\mathrm{T}(\theta_L,\theta_1),\end{aligned}$$

where the integration over θ_j (similarly, over θ_l) can be done using the expansion of the transfer matrix, e.g.,

$$\begin{aligned}\int_0^{2\pi} \frac{d\theta_j}{2\pi} e^{i\theta_j} \mathrm{T}(\theta_{j-1},\theta_j)\mathrm{T}(\theta_j,\theta_{j+1}) &= \int_0^{2\pi} \frac{d\theta_j}{2\pi} e^{i\theta_j} \sum_{m=-\infty}^{\infty} \sum_{m'=-\infty}^{\infty} A_m A_{m'} e^{im(\theta_{j-1}-\theta_j)} e^{im'(\theta_j-\theta_{j+1})} \\ &= \int_0^{2\pi} \frac{d\theta_j}{2\pi} \sum_{m=-\infty}^{\infty} \sum_{m'=-\infty}^{\infty} A_m A_{m'} e^{im\theta_{j-1} - im'\theta_{j+1}} e^{i(m'-m+1)\theta_j} \\ &= \sum_{m=-\infty}^{\infty} \sum_{m'=-\infty}^{\infty} A_m A_{m'} e^{im\theta_{j-1} - im'\theta_{j+1}} \delta_{m',m-1} \\ &= \sum_{m=-\infty}^{\infty} A_m A_{m-1} e^{im(\theta_{j-1}-\theta_{j+1})} e^{i\theta_{j+1}}.\end{aligned}$$

The above expression is quite useful for evaluating the correlation function

$$\begin{aligned}
\langle \mathbf{I}_j \cdot \mathbf{I}_l \rangle &= \frac{I^2}{2Z} \int_0^{2\pi} \prod_{i=1}^{L} \frac{d\theta_i}{2\pi} [e^{i(\theta_j - \theta_l)} + e^{-i(\theta_j - \theta_l)}] \mathrm{T}(\theta_1, \theta_2) \mathrm{T}(\theta_2, \theta_3) \cdots \mathrm{T}(\theta_L, \theta_1) \quad \Leftarrow \text{assume } j < l \\
&= \frac{I^2}{2Z} \sum_{m=-\infty}^{\infty} A_m^{j-1} [(A_{m-1})^{l-j} + (A_{m+1})^{l-j}] A_m^{L-l+1} \\
&= \frac{I^2}{2Z} \sum_{m=-\infty}^{\infty} [(A_{m-1})^{l-j} + (A_{m+1})^{l-j}] A_m^{L-(l-j)} \quad \Leftarrow \text{substitute } Z \text{ in Eq. (13)} \\
&= \frac{I^2}{2} \frac{\sum_{m=-\infty}^{\infty} [(A_{m-1})^{l-j} + (A_{m+1})^{l-j}] A_m^{L-(l-j)}}{\sum_{m=-\infty}^{\infty} A_m^L}.
\end{aligned}$$

In the limit $L \to \infty$, the unique largest eigenvalue corresponding to $m = 0$ dominates the above sums

$$\begin{aligned}
\lim_{L \to \infty} \langle \mathbf{I}_j \cdot \mathbf{I}_l \rangle &= \frac{I^2}{2} \left[\left(\frac{A_{-1}}{A_0} \right)^{l-j} + \left(\frac{A_1}{A_0} \right)^{l-j} \right] \qquad \Leftarrow \text{use } A_1 = A_{-1} \\
&= I^2 e^{-(l-j)/\xi},
\end{aligned}$$

where the correlation length $\xi = \ln(A_0/A_1)$.

At the high temperature limit ($\beta J I^2$ small), the analytical expression (12) suggests that $A_0 \to 1$ and $A_1 \to \frac{\beta J I^2}{2}$, so the correlation length $\xi \to \ln(\frac{2}{\beta J I^2}) = \ln(\frac{2T}{J I^2})$, which recovers the high-temperature expansion result discussed during the lecture (see page 5 in the lecture note PT-1.pdf).