WIPM Lectures on Models in Statistical Mechanics

Lecture 2: More Techniques and 1D Ising Model

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Last lecture was technical at times, but let me first summarize what the theorems are that we should remember of the technical part, leaving out the details of the proofs. First some general remarks:

* We want to discuss both classical 2-dimensional models and 1-dimensional quantum chain models in parallel. Therefore, we shall use operator methods.
* For the Ising-type models we must use the Jordan–Wigner transformation to change from mixed commutation rules to fermion operators.
* To deal with the fermion operators we have to use Wick theorems and Pfaffians. (Pfaffians appear also in most non-operator approaches.)
* We also need to introduce transfer matrices and that is most easily done treating the 1-dimensional Ising model first.

Pfaffians of triangular arrays

$$\boxed{\mathsf{Pf\,A} \equiv \sideset{}{'}\sum_{\substack{\mathrm{P} \\ \mathrm{P}(2i-1)<\mathrm{P}(2i) \\ \mathrm{P}(2i-1)<\mathrm{P}(2i+1)}} (-1)^{\mathrm{P}} \prod_{i=1}^{s} A_{\mathrm{P}(2i-1),\mathrm{P}(2i)}}\,, \qquad \boxed{\begin{array}{c}\mathrm{Pf}(\{A_{\mathrm{P}i,\mathrm{P}j}\}) = (-1)^{\mathrm{P}}\,\mathrm{Pf}\,\mathsf{A} \\ \mathsf{A}\ \text{antisymmetrically extended}\end{array}}\,.$$

$$\boxed{\det\,\mathsf{A} = (\mathrm{Pf}\,\mathsf{A})^2 \quad \begin{array}{l}\text{for antisymmetric matrix } \mathsf{A} \\ \text{extending triangular array } \mathsf{A}\end{array}}\,,$$

$$\boxed{\mathrm{Pf}\,\mathsf{A} = \sum_{j=2}^{2s} (-1)^j A_{1j}\,\mathrm{Pf}\,\mathsf{A}[1,j]}\,.$$

$$\boxed{\mathrm{Pf}\,\mathsf{A} = \frac{1}{s} \sum_{1\leqslant l<m\leqslant 2s}\sum (-1)^{l+m-1} A_{lm}\,\mathrm{Pf}\,\mathsf{A}[l,m]}\,,$$

$\mathsf{A}[l,m]$ obtained by deleting rows and columns l and m from triangular array A.

Example of Evaluating Pfaffian by First Row

If you evaluate a determinant by rows, then you take a sum of $\pm$ products of an element times the determinant with the corresponding row and column deleted. Now you have to strike out two columns and rows each time:

$$\mathrm{Pf}\,\mathsf{A} = \left| \begin{array}{ccc} A_{12} & A_{13} & A_{14} \\ & A_{23} & A_{24} \\ & & A_{34} \end{array} \right|$$

$$= A_{12} \left| \begin{array}{ccc} A_{12} & A_{13} & A_{14} \\ & A_{23} & A_{24} \\ & & A_{34} \end{array} \right| - A_{13} \left| \begin{array}{ccc} A_{12} & A_{13} & A_{14} \\ & A_{23} & A_{24} \\ & & A_{34} \end{array} \right| + A_{14} \left| \begin{array}{ccc} A_{12} & A_{13} & A_{14} \\ & A_{23} & A_{24} \\ & & A_{34} \end{array} \right|$$

$$= A_{12}A_{34} - A_{13}A_{24} + A_{14}A_{23}.$$

General Fermionic Wick Theorem

Case $s = 2$:

$$\begin{aligned}
&\mathrm{Tr}(Q_1Q_2Q_3Q_4)\,\mathrm{Tr}(\Gamma_1Q_1\Gamma_2Q_2\Gamma_3Q_3\Gamma_4Q_4)\\
&\quad= \mathrm{Tr}(\Gamma_1Q_1\Gamma_2Q_2Q_3Q_4)\,\mathrm{Tr}(Q_1Q_2\Gamma_3Q_3\Gamma_4Q_4)\\
&\qquad - \mathrm{Tr}(\Gamma_1Q_1Q_2\Gamma_3Q_3Q_4)\,\mathrm{Tr}(Q_1\Gamma_2Q_2Q_3\Gamma_4Q_4)\\
&\qquad + \mathrm{Tr}(\Gamma_1Q_1Q_2Q_3\Gamma_4Q_4)\,\mathrm{Tr}(Q_1\Gamma_2Q_2\Gamma_3Q_3Q_4).
\end{aligned}$$

Each Q_j is a product of factors that are either exponentials of quadratic forms or linear expressions in fermion operators. The Γ_j are fermion operators.

General case $s \geqslant 2$:

$$\left(\mathrm{Tr}\prod_{k=1}^{2s} Q_k\right)^{s-1} \mathrm{Tr}\prod_{k=1}^{2s}\Gamma_{p_k}Q_k = \operatorname*{Pf}_{1\leqslant k<l\leqslant 2s}\left\{\mathrm{Tr}\left(\prod_{i<k}Q_i\right)\Gamma_{p_k}Q_k\left(\prod_{k<i<l}Q_i\right)\Gamma_{p_l}Q_l\left(\prod_{i>l}Q_i\right)\right\}.$$

Remark: Compound Pfaffians

If we introduce the notation

$$\mathrm{Pf}(\mathrm{S}) \equiv \underset{\substack{\{i,j\}\subset \mathrm{S}\\ i<j}}{\mathrm{Pf}} (\{A_{ij}\}),$$

with S an index set of even size and A a triangular array, then the general Wick theorem can be seen to be equivalent to

$$\boxed{\frac{\mathrm{Pf}(\mathrm{S}_1 \cup \mathrm{S}_2)}{\mathrm{Pf}(\mathrm{S}_2)} = \underset{\{i,j\}\subset \mathrm{S}_1}{\mathrm{Pf}} \left(\left\{ \frac{\mathrm{Pf}(\{i,j\} \cup \mathrm{S}_2)}{\mathrm{Pf}(\mathrm{S}_2)} \right\} \right)}.$$

This is a compound Pfaffian theorem : A Pfaffian of Pfaffians is a Pfaffian.

Though not widely known, this version is particularly useful in approaches to Ising-class models when one does not use operator techniques. It can be shown to be equivalent to the general Wick theorem. The smallest nontrivial example has S_1 having size 4 and S_2 size 2.

Example of Compound Pfaffian Identity

Take $\mathrm{S}_1 = \{1, 2, 3, 4\}$ and $\mathrm{S}_2 = \{5, 6\}$, then the compound Pfaffian theorem says

$$\begin{aligned}&\mathrm{Pf}\, A[1,2,3,4]\, \mathrm{Pf}\, A \\ &\qquad = \mathrm{Pf}\, A[3,4]\, \mathrm{Pf}\, A[1,2] - \mathrm{Pf}\, A[2,4]\, \mathrm{Pf}\, A[1,3] + \mathrm{Pf}\, A[2,3]\, \mathrm{Pf}\, A[1,4],\end{aligned}$$

which is a Pfaffian of Pfaffians. Indeed, we have (exercise):

$$\begin{aligned}A_{5,6}\Big(&A_{1,2}A_{3,4}A_{5,6} - A_{1,2}A_{3,5}A_{4,6} + A_{1,2}A_{3,6}A_{4,5} - A_{1,3}A_{2,4}A_{5,6} \\ &+ A_{1,3}A_{2,5}A_{4,6} - A_{1,3}A_{2,6}A_{4,5} + A_{1,4}A_{2,3}A_{5,6} - A_{1,4}A_{2,5}A_{3,6} \\ &+ A_{1,4}A_{2,6}A_{3,5} - A_{1,5}A_{2,3}A_{4,6} + A_{1,5}A_{2,4}A_{3,6} - A_{1,5}A_{2,6}A_{3,4} \\ &+ A_{1,6}A_{2,3}A_{4,5} - A_{1,6}A_{2,4}A_{3,5} + A_{1,6}A_{2,5}A_{3,4}\Big) \\ = &\left(A_{3,4}A_{5,6} - A_{3,5}A_{4,6} + A_{3,6}A_{4,5}\right)\left(A_{1,2}A_{5,6} - A_{1,5}A_{2,6} + A_{1,6}A_{2,5}\right) \\ &- \left(A_{2,4}A_{5,6} - A_{2,5}A_{4,6} + A_{2,6}A_{4,5}\right)\left(A_{1,3}A_{5,6} - A_{1,5}A_{3,6} + A_{1,6}A_{3,5}\right) \\ &+ \left(A_{2,3}A_{5,6} - A_{2,5}A_{3,6} + A_{2,6}A_{3,5}\right)\left(A_{1,4}A_{5,6} - A_{1,5}A_{4,6} + A_{1,6}A_{4,5}\right).\end{aligned}$$

One-Dimensional Ising Model

Open Ising Chain in Zero Field

We have N spins $\sigma_j = \pm 1$ on sites $j = 1, \cdots N$. Nearest neighbors are coupled with energy $-J$ if they are parallel and $-J$ otherwise. Thus the interaction energy is

$$\mathcal{H} = -J \sum_{j=1}^{N-1} \sigma_j \sigma_{j+1}.$$

The partition function is

$$Z = \sum_{\{\sigma\}} \mathrm{e}^{-\beta\mathcal{H}} = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \cdots \sum_{\sigma_N=\pm 1} \mathrm{e}^{-\beta\mathcal{H}},$$

with the sum over all allowed spin configurations and $\beta = 1/(k_{\mathrm{B}}T)$. Commonly one uses the dimensionless inverse temperature

$$K = \beta J = \frac{J}{k_{\mathrm{B}}T},$$

so that

$$Z = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \cdots \sum_{\sigma_N=\pm 1} \mathrm{e}^{K\sigma_1\sigma_2 + K\sigma_1\sigma_2 + \cdots + K\sigma_{N-1}\sigma_N}.$$

We can next go to the new spin variables

$$\tau_j = \sigma_j \sigma_{j+1}, \quad \text{for } j = 1, \cdots, N-1, \quad \text{and} \quad \tau_N = \sigma_N,$$

with the inverse transformation

$$\sigma_j = \prod_{k=j}^{N} \tau_k,$$

making

$$\mathcal{H} = -J \sum_{j=1}^{N-1} \tau_j,$$

and

$$Z = \sum_{\tau_1=\pm 1} \mathrm{e}^{K\tau_1} \sum_{\tau_2=\pm 1} \mathrm{e}^{K\tau_2} \cdots \sum_{\tau_{N-1}=\pm 1} \mathrm{e}^{K\tau_{N-1}} \sum_{\tau_N=\pm 1} 1$$

$$= 2 \left(\sum_{\tau=\pm 1} \mathrm{e}^{K\tau} \right)^{N-1} = 2\,(2\cosh K)^{N-1} = \mathrm{e}^{-\beta F},$$

with F the total free energy. The free energy per site $f = F/N$ is given by

$$-\beta f = \log(2\cosh K) - N^{-1}\log(\cosh K) \to \log(2\cosh K), \quad \text{as } N \to \infty.$$

The $\mathrm{O}(N^{-1})$ term vanishes in the thermodynamic limit. The pair correlation function can also easily be obtained:

$$\langle \sigma_j \sigma_{j+p} \rangle \equiv \frac{\sum\limits_{\{\sigma\}} \mathrm{e}^{-\beta\mathcal{H}} \sigma_j \sigma_{j+p}}{\sum\limits_{\{\sigma\}} \mathrm{e}^{-\beta\mathcal{H}}} = \frac{\sum\limits_{\{\tau\}} \mathrm{e}^{-\beta\mathcal{H}} \prod\limits_{k=j}^{j+p-1} \tau_k}{\sum\limits_{\{\tau\}} \mathrm{e}^{-\beta\mathcal{H}}}$$

$$= \frac{\left(\sum\limits_{\tau=\pm1} \tau\, \mathrm{e}^{K\tau}\right)^p \left(\sum\limits_{\tau=\pm1} \mathrm{e}^{K\tau}\right)^{N-p-1} \sum\limits_{\tau=\pm1} 1}{\left(\sum\limits_{\tau=\pm1} \mathrm{e}^{K\tau}\right)^{N-1} \sum\limits_{\tau=\pm1} 1} = \left(\frac{2\sinh K}{2\cosh K}\right)^p = \left(\tanh K\right)^p.$$

The results are very simple, as the interaction is ‘pure gauge’ ($\sigma_j \sigma_{j+1} = \sigma_j \sigma_{j+1}^{-1}$).

Periodic Ising Chain in Nonzero Field

The interaction energy with scaled magnetic field B is

$$\mathcal{H} = -J\sum_{j=1}^{N}\sigma_j\sigma_{j+1} - B\sum_{j=1}^{N}\sigma_j, \quad \text{with} \quad \sigma_{N+1}\equiv\sigma_1.$$

Writing $H = \beta B$ and symmetrizing the magnetic field term (convenient but not needed), we have

$$-\beta\mathcal{H} = \sum_{j=1}^{N}\left(K\sigma_j\sigma_{j+1} + \frac{1}{2}H(\sigma_j+\sigma_{j+1})\right),$$

so

$$Z = \sum_{\{\sigma\}} \mathrm{e}^{-\beta\mathcal{H}} = \sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1}\cdots\sum_{\sigma_N=\pm1} T(\sigma_1,\sigma_2)T(\sigma_2,\sigma_3)\cdots T(\sigma_{N-1},\sigma_N)T(\sigma_N,\sigma_1),$$

with

$$\boxed{T(\sigma_j,\sigma_{j+1}) \equiv \exp\left(K\sigma_j\sigma_{j+1} + \frac{1}{2}H(\sigma_j+\sigma_{j+1})\right)}.$$

Thus we have defined the transfer matrix T:

$$T(\sigma,\sigma') = \mathrm{e}^{K\sigma\sigma' + \frac{1}{2}H(\sigma+\sigma')}, \qquad \boxed{\mathsf{T} = \begin{array}{c} \\ \sigma=+1 \\ \sigma=-1 \end{array} \begin{array}{c} \begin{array}{cc} \sigma'=+1 & \sigma'=-1 \end{array} \\ \begin{pmatrix} \mathrm{e}^{K+H} & \mathrm{e}^{-K} \\ \mathrm{e}^{-K} & \mathrm{e}^{K-H} \end{pmatrix} \end{array}},$$

and

$$\begin{aligned} Z &= \sum_{\sigma_1=\pm1} \sum_{\sigma_2=\pm1} \cdots \sum_{\sigma_N=\pm1} T(\sigma_1,\sigma_2)T(\sigma_2,\sigma_3)\cdots T(\sigma_{N-1},\sigma_N)T(\sigma_N,\sigma_1) \\ &= \sum_{\sigma_1=\pm1} T^N(\sigma_1,\sigma_1) = \mathrm{Tr}\,\mathsf{T}^N = \lambda_1^N + \lambda_2^N. \end{aligned}$$

The eigenvalues λ_1 and λ_2 of T satisfy

$$\det\begin{pmatrix} \mathrm{e}^{K+H} - \lambda & \mathrm{e}^{-K} \\ \mathrm{e}^{-K} & \mathrm{e}^{K-H} - \lambda \end{pmatrix} = 0,$$

so that

$$\lambda_{1,2} = \mathrm{e}^{K}\cosh H \pm \sqrt{\mathrm{e}^{2K}\sinh^2 H + \mathrm{e}^{-2K}}.$$

Using the Pauli matrices

$$\sigma^x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y \equiv \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma^z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma^0 \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

we can also rewrite T as

$$\mathsf{T} = \begin{pmatrix} \mathrm{e}^{K+H} & \mathrm{e}^{-K} \\ \mathrm{e}^{-K} & \mathrm{e}^{K-H} \end{pmatrix} = (\mathrm{e}^K \cosh H)\,\sigma^0 + \mathrm{e}^{-K}\sigma^x + (\mathrm{e}^K \sinh H)\,\sigma^z,$$

and use the well-known fact that the eigenvalues of $a_0\,\sigma^0 + \vec{a}\cdot\vec{\sigma}$ are $a_o \pm |\vec{a}|$.

Clearly, $\lambda_1 > 0$ and $|\lambda_2| < \lambda_1$, so that

$$-\beta f = \frac{1}{N}\log(\lambda_1^N + \lambda_2^N) = \log\lambda_1 + \frac{1}{N}\log\left(1 + \left(\frac{\lambda_2}{\lambda_1}\right)^N\right) \to \log\lambda_1, \quad \text{as } N \to \infty.$$

Thus

$$\lim_{N\to\infty}(-\beta f) = \log\left(\mathrm{e}^K \cosh H + \sqrt{\mathrm{e}^{2K}\sinh^2 H + \mathrm{e}^{-2K}}\right).$$

If one also calculates the eigenvectors of T, then one can also obtain the pair-correlation function $\langle \sigma_j \sigma_k \rangle$ and solve the open-chain problem with fixed or free boundary conditions.

For the open chain

$$\mathcal{H} = -J \sum_{j=1}^{N-1} \sigma_j \sigma_{j+1} - B \sum_{j=1}^{N} \sigma_j .$$

Then with

$$\mathsf{T} = \begin{pmatrix} \mathrm{e}^{K+H} & \mathrm{e}^{-K} \\ \mathrm{e}^{-K} & \mathrm{e}^{K-H} \end{pmatrix}, \qquad \mathsf{T}_H = \begin{pmatrix} \mathrm{e}^{\frac{1}{2}H} & 0 \\ 0 & \mathrm{e}^{-\frac{1}{2}H} \end{pmatrix},$$

we have

$$Z = \langle \phi_1 | \mathsf{T}_H \mathsf{T}^{N-1} \mathsf{T}_H | \phi_2 \rangle, \qquad \text{with} \quad \langle \phi_1 | = | \phi_1 \rangle^\dagger,$$

and $|\phi_{1,2}\rangle = \binom{1}{1}$ for a free boundary and $\binom{1}{0}$ or $\binom{0}{1}$ for a fixed boundary. This is easily worked out and extended to the pair correlation function. We leave the further details as an exercise.

It may be good to mention two important theorems now:

The Theorem of Perron–Frobenius: *A square matrix with only positive elements has a unique eigenvalue with largest absolute value λ_0, which is positive and its corresponding eigenvector suitably normalized has only positive elements.*

Here we shall only give a simple proof assuming that T is symmetric and positive, i.e., $T_{kl} = T_{lk} > 0$ for all k and l. Then all eigenvalues are real and we have a complete orthonormal set of real eigenvectors $\mathbf{v}^{(j)}$ satisfying

$$\mathsf{T}\mathbf{v}^{(j)} = \lambda_j \mathbf{v}^{(j)} \quad \text{or} \quad \sum_l T_{kl} v_l^{(j)} = \lambda_j v_k^{(j)} \quad \text{and} \quad \mathbf{v}^{(j)} \cdot \mathbf{v}^{(j')} = \delta_{j,j'}.$$

Reality follows, since with $\mathbf{v}^{(j)}$ also $\operatorname{Re}\mathbf{v}^{(j)}$ and $\operatorname{Im}\mathbf{v}^{(j)}$ are eigenvectors. From orthonormality we can have only one eigenvector with only positive elements. It cannot be positive or zero, as application of T then produces a strictly positive vector. From an eigenvector $\mathbf{v}^{(j)}$ with negative components and with $|\lambda_j| = \lambda_0$ maximal, one could show a contradiction for $\mathbf{v}'$, with components $v'_k = |v_k^{(j)}|$:

$$|\mathsf{T}\mathbf{v}'|^2 = \sum_k \Big(\sum_l T_{kl} |v_l^{(j)}| \Big)^2 > \sum_k \Big(\sum_i T_{kl} v_l^{(j)} \Big)^2 = \lambda_0^2 \sum_k \big(v_l^{(j)} \big)^2 = \lambda_0^2 |\mathbf{v}'|^2,$$

while we must have $|\mathsf{T}\mathbf{v}'| \leqslant \lambda_0 |\mathbf{v}'|$.

Remarks:

* The Perron–Frobenius theorem can be proved for more general cases with T not symmetric and even (under specific conditions) with several zero elements. (See, for example, the Wikipedia article on the Perron–Frobenius theorem for more discussion and references.)

* The eigenvalues of transfer matrix T are solutions of a polynomial equation. They are analytic, if T is analytic, except at branchpoints, where two of more eigenvalues coincide. In classical one-dimensional models with short-range interactions there are generally no phase transitions at finite temperature, as degeneracy is forbidden by Perron–Frobenius.

* Perron–Frobenius does not apply when T has too many zero elements or becomes infinite, which typically happens at zero temperature.

* Perron–Frobenius often fails, when the dimension of the space on which T acts becomes infinite. This failure happens with mean-field models in one dimensions with infinite-range interactions and the two-dimensional Ising model in the thermodynamic limit.

The Bogolyubov Inequality:

Given two interaction energies or Hermitian Hamiltonians $\mathcal{H}$ and $\mathcal{H}_0$, then

$$\boxed{F[\mathcal{H}] - F[\mathcal{H}_0] \leqslant \langle \mathcal{H} - \mathcal{H}_0 \rangle_{\mathcal{H}_0}},$$

where we used the notations for any $\mathcal{H}$ and O:

$$F[\mathcal{H}] \equiv -\beta^{-1} \log \mathrm{Tr}\, \mathrm{e}^{-\beta\mathcal{H}}, \qquad \langle O \rangle_{\mathcal{H}} \equiv \frac{\mathrm{Tr}\, O\, \mathrm{e}^{-\beta\mathcal{H}}}{\mathrm{Tr}\, \mathrm{e}^{-\beta\mathcal{H}}}.$$

Remarks:

* Here Tr stands for trace in the quantum case and for the sum over all configurations in the classical case.
* This inequality is useful to show convergence and independence of boundary conditions in the thermodynamic limit. If $\mathcal{H} - \mathcal{H}_0$ is bounded and growing slower than the system size, then the free energies per site $f[\mathcal{H}]$ and $f[\mathcal{H}_0]$ become equal in the large system limit.

Proof: We first introduce

$$\mathcal{H}(\lambda) \equiv \mathcal{H}_0 + \lambda(\mathcal{H} - \mathcal{H}_0), \qquad \mathcal{H}(0) = \mathcal{H}_0, \quad \mathcal{H}(1) = \mathcal{H},$$

and derive

$$\boxed{\frac{\partial}{\partial\lambda} \mathrm{e}^{-\beta\mathcal{H}(\lambda)} = -\int_0^\beta \mathrm{d}\tau \, \mathrm{e}^{-\tau\mathcal{H}(\lambda)} (\mathcal{H} - \mathcal{H}_0) \mathrm{e}^{-(\beta-\tau)\mathcal{H}(\lambda)}},$$

which is needed when $\mathcal{H}$ and $\mathcal{H}_0$ do not commute. In the commuting case it simplifies to $-\beta(\mathcal{H} - \mathcal{H}_0)\mathrm{e}^{-\beta\mathcal{H}(\lambda)}$, as it should.

The simplest way to see this is to write

$$\begin{aligned} \frac{\partial}{\partial\lambda} \mathrm{e}^{-\beta\mathcal{H}(\lambda)} &= \frac{\partial}{\partial\lambda} \lim_{n\to\infty} \prod_{j=1}^{n} \mathrm{e}^{-\frac{1}{n}\beta\mathcal{H}(\lambda)} \\ &= \lim_{n\to\infty} \sum_{k=0}^{n} \left[\prod_{j=1}^{k} \mathrm{e}^{-\frac{1}{n}\beta\mathcal{H}(\lambda)} \right] \frac{\partial}{\partial\lambda} \Big(-\frac{1}{n}\beta\mathcal{H}(\lambda) \Big) \left[\prod_{j=k+1}^{n} \mathrm{e}^{-\frac{1}{n}\beta\mathcal{H}(\lambda)} \right] \end{aligned}$$

and then replace the sum by an integral setting $\tau = \frac{k}{n}\beta$.

Use this and the cyclic property of trace, $\mathrm{Tr}\, ABC = \mathrm{Tr}\, CAB$, to find

$$\frac{\partial}{\partial\lambda} F[\mathcal{H}(\lambda)] = -\beta^{-1} \frac{\partial}{\partial\lambda} \log \mathrm{Tr}\, \mathrm{e}^{-\beta\mathcal{H}(\lambda)} = \frac{\int_0^\beta \mathrm{d}\tau\, \mathrm{Tr}\, \mathrm{e}^{-\tau\mathcal{H}(\lambda)} (\mathcal{H} - \mathcal{H}_0) \mathrm{e}^{-(\beta-\tau)\mathcal{H}(\lambda)}}{\beta\, \mathrm{Tr}\, \mathrm{e}^{-\beta\mathcal{H}(\lambda)}}$$

$$= \frac{\int_0^\beta \mathrm{d}\tau\, \mathrm{Tr}\, (\mathcal{H} - \mathcal{H}_0) \mathrm{e}^{-\beta\mathcal{H}(\lambda)}}{\beta\, \mathrm{Tr}\, \mathrm{e}^{-\beta\mathcal{H}(\lambda)}} = \frac{\mathrm{Tr}\, (\mathcal{H} - \mathcal{H}_0) \mathrm{e}^{-\beta\mathcal{H}(\lambda)}}{\mathrm{Tr}\, \mathrm{e}^{-\beta\mathcal{H}(\lambda)}} = \langle \mathcal{H} - \mathcal{H}_0 \rangle_{\mathcal{H}(\lambda)}.$$

Taking another derivative,

$$\frac{\partial^2}{\partial\lambda^2} F[\mathcal{H}(\lambda)] = -\int_0^\beta \mathrm{d}\tau \left[\frac{\mathrm{Tr}\, (\mathcal{H} - \mathcal{H}_0) \mathrm{e}^{-\tau\mathcal{H}(\lambda)} (\mathcal{H} - \mathcal{H}_0) \mathrm{e}^{-(\beta-\tau)\mathcal{H}(\lambda)}}{\mathrm{Tr}\, \mathrm{e}^{-\beta\mathcal{H}(\lambda)}} - \frac{\left(\mathrm{Tr}\, (\mathcal{H} - \mathcal{H}_0) \mathrm{e}^{-\beta\mathcal{H}(\lambda)} \right)^2}{\left(\mathrm{Tr}\, \mathrm{e}^{-\beta\mathcal{H}(\lambda)} \right)^2} \right]$$

$$= -\int_0^\beta \mathrm{d}\tau \left\langle \left(\mathcal{H} - \mathcal{H}_0 - \langle \mathcal{H} - \mathcal{H}_0 \rangle_{\mathcal{H}(\lambda)} \right) \mathrm{e}^{-\tau\mathcal{H}(\lambda)} \left(\mathcal{H} - \mathcal{H}_0 - \langle \mathcal{H} - \mathcal{H}_0 \rangle_{\mathcal{H}(\lambda)} \right) \mathrm{e}^{\tau\mathcal{H}(\lambda)} \right\rangle_{\mathcal{H}(\lambda)}.$$

If we write $\mathsf{A} \equiv \mathrm{e}^{-\frac{1}{2}\tau\mathcal{H}(\lambda)}\big(\mathcal{H}-\mathcal{H}_0-\langle\mathcal{H}-\mathcal{H}_0\rangle_{\mathcal{H}(\lambda)}\big)\mathrm{e}^{\frac{1}{2}\tau\mathcal{H}(\lambda)}$, then we get

$$\frac{\partial^2}{\partial\lambda^2}F[\mathcal{H}(\lambda)] = -\int_0^\beta \mathrm{d}\tau \, \langle \mathsf{A}^\dagger \mathsf{A} \rangle \leqslant 0, \quad \text{or} \quad F[\mathcal{H}(\lambda)] \text{ is concave.}$$

This means that any tangent to the curve $F[\mathcal{H}(\lambda)]$ lies above the curve, or

$$F[\mathcal{H}(\lambda)] \leqslant F[\mathcal{H}(0)] + \lambda \left(\frac{\partial}{\partial\lambda} F[\mathcal{H}(\lambda)] \Big|_{\lambda=0} \right).$$

Setting $\lambda = 1$, we get

$$F[\mathcal{H}] \leqslant F[\mathcal{H}_0] + \langle \mathcal{H} - \mathcal{H}_0 \rangle_{\mathcal{H}_0},$$

which is the Bogolyubov inequality.

<u>Remark</u>: This implies also

$$\boxed{\big|F[\mathcal{H}] - F[\mathcal{H}_0]\big| \leqslant \|\mathcal{H} - \mathcal{H}_0\|},$$

with $\|O\|$ the norm of O.

One More Setup for Periodic Ising Chain in Nonzero Field

As a finger exercise to prepare for the two-dimensional case, we revisit the one-dimensional periodic case with

$$-\beta\mathcal{H} = K\sum_{j=1}^{N}\sigma_j\sigma_{j+1} + H\sum_{j=1}^{N}\sigma_j, \quad \text{with} \quad \sigma_{N+1}\equiv\sigma_1, \quad K\equiv\beta J, \quad H\equiv\beta B.$$

The partition function is

$$\begin{aligned} Z = \sum_{\{\sigma\}} \mathrm{e}^{-\beta\mathcal{H}} = &\sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1}\cdots\sum_{\sigma_N=\pm1} T_1(\sigma_1,\sigma_2)T_2(\sigma_2,\sigma_2)T_1(\sigma_2,\sigma_3) \\ &\times T_2(\sigma_3,\sigma_3)\cdots T_1(\sigma_{N-1},\sigma_N)T_2(\sigma_N,\sigma_N)T_1(\sigma_N,\sigma_1)T_2(\sigma_1,\sigma_1) \\ &= \mathrm{Tr}\left(\mathsf{T}_1\mathsf{T}_2\right)^N, \end{aligned}$$

with

$$\boxed{T_1(\sigma,\sigma')\equiv\exp\left(K\sigma\sigma'\right), \quad T_2(\sigma,\sigma')\equiv\exp\left(H\sigma\right)\delta_{\sigma,\sigma'}},$$

or

$$\mathsf{T}_1 = \begin{pmatrix} e^{K} & e^{-K} \\ e^{-K} & e^{K} \end{pmatrix} = \sqrt{2\sinh(2K)}\, e^{K^*\sigma^x}, \qquad \mathsf{T}_2 = \begin{pmatrix} e^{H} & 0 \\ 0 & e^{-H} \end{pmatrix} = e^{H\sigma^z},$$

where

$$K^* \equiv \operatorname{artanh} e^{-2K}, \quad \tanh K^* = e^{-2K}.$$

Indeed, we can write T_1 in terms of Pauli matrices:

$$\begin{aligned}\mathsf{T}_1 &= e^{K}\mathbf{1} + e^{-K}\sigma^x = e^{K}\left(\mathbf{1} + e^{-2K}\sigma^x\right) = e^{K}\left(\mathbf{1} + \sigma^x \tanh K^*\right) \\ &= \frac{e^{K}}{\cosh K^*}\left(\mathbf{1}\cosh K^* + \sigma^x \sinh K^*\right) = \sqrt{2\sinh(2K)}\, e^{K^*\sigma^x}.\end{aligned}$$

One can easily check the equivalence of (exercise)

$$\boxed{\begin{aligned}&\tanh K^* = e^{-2K}, \quad \tanh K = e^{-2K^*}, \quad \sinh(2K)\sinh(2K^*) = 1, \\ &\cosh(2K^*) = \coth(2K), \quad \cosh(2K) = \coth(2K^*).\end{aligned}}$$

Also,

$$\left(\frac{e^{K}}{\cosh K^*}\right)^2 = \frac{1}{\tanh K^* \cosh^2 K^*} = \frac{2}{\sinh(2K^*)} = 2\sinh(2K).$$

Next: Two-Dimensional Ising Model in Zero Field