WIPM Lectures on Models in Statistical Mechanics

Lecture 3: 2D Ising Model and 1D Quantum Ising Model

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Last lecture we introduced the transfer matrix method to solve the 1-dimensional Ising model. We also proved the Perron–Frobenius theorem and the Bogolyubov variational inequality. Today:

* We shall first set up the transfer matrix for the 2-dimensional zero-field Ising model.
* We next shall see that the model is closely related to the Ising chain in a transverse field.
* Then we need to apply the Jordan–Wigner transformation to translate the model into a fermionic Gaussian problem.
* We shall also show that the 2-dimensional Ising model in a field and the 3-dimensional Ising model can not be solved by fermionic Gaussian methods.

Review of Last Lecture on Periodic Ising Chain

The one-dimensional periodic Ising chain is defined by the Hamiltonian

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

Its partition function is

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

with

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

or

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

where

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

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

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

The following identities are also important for the 2-dimensional case:

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

Also,

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

Two-Dimensional Ising Model in Zero Field

We start with a periodic rectangular lattice with sites (m, n), with horizontal component $m = 1, 2, \cdots, M$ and vertical component $n = 1, 2, \cdots, N$. Spins $\sigma_{mn} = \pm 1$ live on these sites and the interaction energy $\mathcal{H}$ is given by

$$-\beta\mathcal{H} = \sum_{m=1}^{M}\sum_{n=1}^{N}\big(K_{m,n}\sigma_{m,n}\sigma_{m+1,n} + K'_{m,n}\sigma_{m,n}\sigma_{m,n+1}\big).$$

This defines an Ising model with non-uniform (inhomogeneous) interactions on a torus, i.e., with periodic boundary conditions in both directions. If we set either $K_{M,n} \equiv 0$ or $K_{m,N} \equiv 0$, we have an Ising model on a cylinder, namely with periodic boundary conditions in one direction and free boundary conditions in the other direction. If $K_{M,n} \equiv K_{m,N} \equiv 0$, we have an Ising model with free boundary conditions in both directions.

The Ising model on other planar lattices (no crossing bonds/pair interactions) are included in this general setup as special limiting cases, setting certain K's equal to 0 (removing an interaction) or ∞ (identifying spins).

Onsager's original 1944 solution has all $K_{m,n} \equiv K$ and $K'_{m,n} \equiv K'$.

Row-to-Row Transfer Matrices

Let us introduce a notation for the collection of all spin values in row n,

$$\sigma^{(n)} \equiv \{\sigma_{1,n}, \sigma_{2,n}, \cdots, \sigma_{M,n}\}.$$

Then the total Boltzmann factor for all interactions within that row n is

$$W_n = W_2\big(\sigma^{(n)}\big) = \exp\left(\sum_{m=1}^{M} K_{m,n}\sigma_{m,n}\sigma_{m+1,n}\right),$$

whereas the Boltzmann factor for the interaction between rows n and $n+1$ is

$$W_{n+\frac{1}{2}} = W_1\big(\sigma^{(n)}, \sigma^{(n+1)}\big) = \exp\left(\sum_{m=1}^{M} K'_{m,n}\sigma_{m,n}\sigma_{m,n+1}\right).$$

Now compare with what we did for the Ising chain in magnetic field, if we orient it vertically:

$$
\begin{array}{llll}
\sigma_{N+1} = \sigma_1 & \cdots\cdots\cdots\cdots & \mathsf{T}_1 & \mathsf{T}_2 \\
 & & \mathsf{T}_{\frac{1}{2}} & \mathsf{T}_1 \\
\sigma_N & \cdots\cdots\cdots\cdots & \mathsf{T}_N & \mathsf{T}_2 \\
 & & \mathsf{T}_{N-\frac{1}{2}} & \mathsf{T}_1 \\
\sigma_{N-1} & \cdots\cdots\cdots\cdots & \mathsf{T}_{N-1} & \mathsf{T}_2 \\
 & & \mathsf{T}_{N-\frac{3}{2}} & \mathsf{T}_1 \\
\vdots & \vdots & \vdots & \vdots \\
 & & \mathsf{T}_{\frac{7}{2}} & \mathsf{T}_1 \\
\sigma_3 & \cdots\cdots\cdots\cdots & \mathsf{T}_3 & \mathsf{T}_2 \\
 & & \mathsf{T}_{\frac{5}{2}} & \mathsf{T}_1 \\
\sigma_2 & \cdots\cdots\cdots\cdots & \mathsf{T}_2 & \mathsf{T}_2 \\
 & & \mathsf{T}_{\frac{3}{2}} & \mathsf{T}_1 \\
\sigma_1 & \cdots\cdots\cdots\cdots & \mathsf{T}_1 & \mathsf{T}_2 \\
 & & \mathsf{T}_{\frac{1}{2}} & \mathsf{T}_1
\end{array}
$$

For the Ising chain in a field we have the corresponding weights and transfer matrices (now going in the vertical direction):

$$W_{n+\frac{1}{2}} = W_1\big(\sigma_n, \sigma_{n+1}\big) = \exp\big(K\sigma_n\sigma_{n+1}\big)\,, \quad W_n = W_2\big(\sigma_n\big) = \exp\big(H\sigma_n\big).$$

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

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

Similarly, for the two-dimensional Ising model, W_n for row n corresponds to a diagonal transfer matrix, just replacing $\sigma_{m,n} \to \sigma^z_m$,

$$\boxed{\mathsf{T}_n = \exp\left(\sum_{m=1}^{M} K_{m,n}\sigma^z_m\sigma^z_{m+1}\right)},$$

whereas now

$$\mathsf{T}_{n+\frac{1}{2}} = \begin{pmatrix} \mathrm{e}^{K_{1,n}} & \mathrm{e}^{-K_{1,n}} \\ \mathrm{e}^{-K_{1,n}} & \mathrm{e}^{K_{1,n}} \end{pmatrix} \otimes \begin{pmatrix} \mathrm{e}^{K_{2,n}} & \mathrm{e}^{-K_{2,n}} \\ \mathrm{e}^{-K_{2,n}} & \mathrm{e}^{K_{2,n}} \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} \mathrm{e}^{K_{M,n}} & \mathrm{e}^{-K_{M,n}} \\ \mathrm{e}^{-K_{M,n}} & \mathrm{e}^{K_{M,n}} \end{pmatrix},$$

or

$$\boxed{\mathsf{T}_{n+\frac{1}{2}} = \left(\prod_{m=1}^{M} 2\sinh(2K'_{m,n}) \right)^{1/2} \exp\left(\sum_{m=1}^{M} K'^{*}_{m,n} \sigma_m^x \right)},$$

$$\boxed{\mathsf{T}_n = \exp\left(\sum_{m=1}^{M} K_{m,n} \sigma_m^z \sigma_{m+1}^z \right)},$$

and

$$\boxed{Z = \mathrm{Tr} \prod_{n=1}^{N} \left(\mathsf{T}_n \mathsf{T}_{n+\frac{1}{2}} \right)}.$$

At this point it is now tradition to make the rotation in spin matrix space,

$$\left(\sigma_m^x, \sigma_m^y, \sigma_m^z \right) \to \left(\sigma_m^z, -\sigma_m^y, \sigma_m^x \right).$$

This can be done by the unitary similarity transform $\mathsf{U} = \exp(\frac{1}{4}\pi \mathrm{i} \sigma^y) \exp(\frac{1}{2}\pi \mathrm{i} \sigma^x)$. Then we can use the identical Jordan–Wigner transform as in the XY model.

Also, let us choose the fully homogeneous case $K_{m,n} = K$, $K'_{m,n} = K'$

$$\boxed{\mathsf{T}_{n+\frac{1}{2}} = \mathsf{T}_1 = \big(2\sinh(2K')\big)^{M/2} \exp\left(K'^{*} \sum_{m=1}^{M} \sigma_m^z \right)},$$

$$\boxed{\mathsf{T}_n = \mathsf{T}_2 = \exp\left(K \sum_{m=1}^{M} \sigma_m^x \sigma_{m+1}^x \right)},$$

$$\boxed{Z = \mathrm{Tr} \left(\mathsf{T}_1 \mathsf{T}_2 \right)^N}.$$

This is clearly related to the Ising chain in transverse field with Hamiltonian

$$\mathcal{H} = -J \sum_{m=1}^{M} \sigma_m^x \sigma_{m+1}^x - B \sum_{m=1}^{M} \sigma_m^z,$$

in the "time-continuum" limit $K \propto K'^{*} \to 0$.

Indeed setting $K = \lambda J/n$ and $K'^{*} = \lambda B/n$ and dropping all front factors $\big(2\sinh(2K')\big)^{M/2}$, we can use the Trotter identity

$$\boxed{\lim_{n\to\infty}\left(\mathrm{e}^{A/n}\mathrm{e}^{B/n}\right)^n = \mathrm{e}^{A+B}}$$

to obtain

$$\lim_{n\to\infty}\left(\frac{\mathsf{T}_1\mathsf{T}_2}{\big(2\sinh(2K')\big)^{M/2}}\right)^n = \mathrm{e}^{-\lambda\mathcal{H}}.$$

By taking a suitable anisotropic limit of the 2-dimensional Ising model with $K \to 0$ and $K' \to \infty$, while taking a the number of transfer matrix steps also infinitely large, we can reproduce properties of the Ising chain in a field in the transverse direction. This process changes the discrete coordinate in the vertical direction into a continuous variable, the so-called imaginary time, related to the inverse temperature variable β.

Therefore, one calls this process the time-continuum limit, or also sometimes the Suzuki limit. Masuo Suzuki wrote about this in the 1970s relating d-dimensional quantum systems with $(d+1)$-dimensional classical systems. His works also became the basis for the quantum Monte Carlo method.

Remark: For the two-dimensional Ising model in a field,

$$-\beta\mathcal{H} = \sum_{m=1}^{M}\sum_{n=1}^{N}\left(K\sigma_{m,n}\sigma_{m+1,n} + K'\sigma_{m,n}\sigma_{m,n+1} + H\sigma_{m,n}\right),$$

the two transfer matrices are

$$\mathsf{T}_1 = \big(2\sinh(2K')\big)^{M/2}\exp\left(K'^{*}\sum_{m=1}^{M}\sigma_m^z\right),$$

$$\mathsf{T}_2 = \exp\left(K\sum_{m=1}^{M}\sigma_m^x\sigma_{m+1}^x + \sum_{m=1}^{M}H\sigma_m^x\right),$$

with T_1 giving again the Boltzmann weight contributions between two successive rows and T_2 all contributions from interactions within one row. Again we have,

$$Z = \mathrm{Tr}\left(\mathsf{T}_1\mathsf{T}_2\right)^N.$$

We leave this all as an exercise.

Remark: For the three-dimensional Ising model in zero field,

$$-\beta\mathcal{H} = \sum_{l=1}^{L}\sum_{m=1}^{M}\sum_{n=1}^{N} \big(K_1\sigma_{l,m,n}\sigma_{l+1,m,n} + K_2\sigma_{l,m,n}\sigma_{l,m+1,n} + K_3\sigma_{l,m,n}\sigma_{l,m,n+1}\big),$$

the two transfer matrices are

$$\mathsf{T}_1 = \big(2\sinh(2K_3)\big)^{LM/2}\exp\left(K_3^*\sum_{l=1}^{L}\sum_{m=1}^{M}\sigma^z_{l,m}\right),$$

$$\mathsf{T}_2 = \exp\left(K_1\sum_{l=1}^{L}\sum_{m=1}^{M}\sigma^x_{l,m}\sigma^x_{l+1,m} + K_2\sum_{l=1}^{L}\sum_{m=1}^{M}\sigma^x_{l,m}\sigma^x_{l,m+1}\right),$$

with T_1 now giving the Boltzmann weight contributions between two successive horizontal planes and T_2 all contributions from interactions within one horizontal plane. Of course,

$$Z = \mathrm{Tr}\,\big(\mathsf{T}_1\mathsf{T}_2\big)^N.$$

We leave this also as an exercise.

Now we need to use the Jordan–Wigner transform of lecture 1:

$$\Gamma_{2j-1} = \left[\prod_{k=1}^{j-1}(-\sigma^z_k)\right]\sigma^x_j, \qquad \Gamma_{2j} = \left[\prod_{k=1}^{j-1}(-\sigma^z_k)\right]\sigma^y_j, \qquad \{\Gamma_p,\Gamma_q\} = 2\delta_{pq}\mathbf{1}.$$

Its inverse is given by

$$\sigma^x_j = \left[\prod_{k=1}^{j-1}(\mathrm{i}\,\Gamma_{2k-1}\Gamma_{2k})\right]\Gamma_{2j-1}, \quad \sigma^y_j = \left[\prod_{k=1}^{j-1}(\mathrm{i}\,\Gamma_{2k-1}\Gamma_{2k})\right]\Gamma_{2j}, \quad \sigma^z_j = -\mathrm{i}\,\Gamma_{2j-1}\Gamma_{2j}.$$

As now σ^z_m is already quadratic in Γ's, we now first work out $\sigma^x_m\sigma^x_{m+1}$ for $1\leqslant m < M$:

$$\sigma^x_m\sigma^x_{m+1} = \left[\prod_{k=1}^{m-1}(\mathrm{i}\,\Gamma_{2k-1}\Gamma_{2k})\right]\Gamma_{2m-1}\left[\prod_{k=1}^{m}(\mathrm{i}\,\Gamma_{2k-1}\Gamma_{2k})\right]\Gamma_{2m+1}$$

$$= \left[\prod_{k=1}^{m-1}(\mathrm{i}\,\Gamma_{2k-1}\Gamma_{2k})\right]^2\Gamma_{2m-1}\big(\mathrm{i}\,\Gamma_{2m-1}\Gamma_{2m}\big)\Gamma_{2m+1} = \mathrm{i}\,\Gamma_{2m}\Gamma_{2m+1}.$$

The case $m = M$ has to be treated separately:

$$
\begin{aligned}
\sigma^x_M\sigma^x_1 &= \left[\prod_{k=1}^{M-1}(\mathrm{i}\,\Gamma_{2k-1}\Gamma_{2k})\right]\Gamma_{2M-1}\Gamma_1 \\
&= \left[\prod_{k=1}^{M}(\mathrm{i}\,\Gamma_{2k-1}\Gamma_{2k})\right]\big(\mathrm{i}\,\Gamma_{2M-1}\Gamma_{2M}\big)\Gamma_{2M-1}\Gamma_1 \\
&= -\left[\prod_{k=1}^{M}(\mathrm{i}\,\Gamma_{2k-1}\Gamma_{2k})\right]\mathrm{i}\,\Gamma_{2M}\Gamma_1 = -\mathrm{i}\,\Gamma_{2M}\Gamma_1\mathsf{P}.
\end{aligned}
$$

with

$$
\boxed{\mathsf{P} \equiv \prod_{k=1}^{M}\big(\mathrm{i}\,\Gamma_{2k-1}\Gamma_{2k}\big) = \prod_{k=1}^{M}\big(-\sigma^z_k\big)}
$$

being the product of all M Jordan–Wigner sign factors. It involves the product of all $2M$ Γ's and thus it commutes with any even product of Γ operators and anticommutes with any odd product,

$$
\boxed{[\mathsf{P},\Gamma_i\Gamma_j]=0,\quad \{\mathsf{P},\Gamma_i\}=0,\quad \mathsf{P}^2=1}.
$$

Because of these special properties, the presence of this P can be handled as shown by Bruria Kaufman in 1949. Since the first round of superstring theory about 1970 one talks about Ramond and Neveu–Schwarz sectors.

If P is present, one has to introduce two sectors (or subspaces) on one of which the P acts as $+1$ and on the other as -1. This causing either periodic or antiperiodic boundary conditions for the fermion operators, i.e.,

$$
\Gamma_{m+2M} = +\Gamma_m \quad \text{(periodic)} \quad \text{or} \quad \Gamma_{m+2M} = -\Gamma_m \quad \text{(antiperiodic)}.
$$

We have derived the Bogolyubov variational inequality and this shows that the free energy is independent of boundary conditions in the thermodynamic limit. Thus, for the free energy may ignore the P complication and impose cyclic (periodic) boundary conditions from now on.

However, for spin-spin correlations in the 2-dimensional Ising model and for time-dependent correlations in the transverse Ising chain, one cannot ignore the effects of the P, even in the thermodynamic limit.

For the 2-dimensional Ising model in a field and the related (in Suzuki's time-continuum limit) Ising chain in parallel and transverse field,

$$\mathcal{H} = -J \sum_{m=1}^{M} \sigma_m^x \sigma_{m+1}^x - B_\perp \sum_{m=1}^{M} \sigma_m^z - B_\parallel \sum_{m=1}^{M} \sigma_m^x,$$

it is not possible to find a Jordan-Wigner transformation to make this quadratic in fermion operators, except for the very special case of Yang and Lee with B an integer multiple of $\frac{1}{2}\pi \mathrm{i} k_\mathrm{B} T$ in the 2D case.*

Indeed, if one could find a working Jordan-Wigner transformation, one has to make all σ_m^x and σ_m^z quadratic in Γ's and thus also all $\sigma_m^y = \mathrm{i}[\sigma_m^z, \sigma_m^x]$, as the commutator of two quadratic expressions is again quadratic.

There are also indications that there is no Yang–Baxter method available, so that there may not be an exact solution. Still one can get very accurate approximations using series, Monte Carlo, corner transfer matrices, etc.

* This special case can be mapped into the product of two zero-field Ising models.

For the 3-dimensional Ising model in zero field and the related (in Suzuki's time-continuum limit) 2-dimensional Ising model in transverse field,

$$\mathcal{H} = -\sum_{l=1}^{L} \sum_{m=1}^{M} (J\sigma_{l,m}^x \sigma_{l+1,m}^x + J'\sigma_{l,m}^x \sigma_{l,m+1}^x + B_\perp \sigma_{l,m}^z),$$

it is also not possible to find a Jordan-Wigner transformation to make this quadratic in fermion operators.

Indeed, we have to order all sites linearly, $(l, m) \to (m-1)M + l$, for example. Then,

$$\sigma_{l,m}^z = -\mathrm{i}\Gamma_{2(m-1)M+2l-1}\Gamma_{2(m-1)M+2l}, \quad \sigma_{l,m}^x \sigma_{l+1,m}^x = \mathrm{i}\Gamma_{2(m-1)M+2l}\Gamma_{2(m-1)M+2l+1},$$

but

$$\sigma_{l,m}^x \sigma_{l,m+1}^x = \prod_{k=(m-1)M+l}^{mM+l-1} \left(\mathrm{i}\Gamma_{2k}\Gamma_{2k+1}\right) \neq \mathrm{i}\Gamma_{2(m-1)M+2l}\Gamma_{2mM+2l-1},$$

with the last member being an error often made, most recently by Z.-D. Zhang.

Remarks:

- Some of the best approximate results for the scaling function of the two-dimensional Ising model in a field have been obtained by the ANU group in Canberra using Baxter's variational corner-transfer-matrix method, see the thesis https://digitalcollections.anu.edu.au/handle/1885/9860 by Dudalev and Phys. Rev. E **81**, 060103(R) (2010) [arXiv:1002.4234].
- In 1991, for the 2-dimensional Ising model in the field theory limit near the critical point, Zamolodchikov has conjectured an exact result for the magnetic field dependence based on the Lie group E_8.
- For the 3-dimensional Ising model at the critical point, there are some very interesting approximate recent results obtained using conformal invariance arguments, see arXiv:1403.4545 by El-Showk et al., (to be published in J. Stat. Phys.).
- The susceptibility of the 2-dimensional Ising model is known to extremely high precision, see J. Stat. Phys. **145** (2011) 549–590 [arXiv:1012.5272], but complications (like a natural boundary) make it unlikely that a nice formula for the free energy in a field exists.

For the calculation of the free energy per site in the thermodynamic limit for the system with Hamiltonian

$$\mathcal{H} = -J \sum_{m=1}^{M} \sigma_m^x \sigma_{m+1}^x - B \sum_{m=1}^{M} \sigma_m^z,$$

we may use the cyclic (periodic) fermion Hamiltonian

$$\mathcal{H}_{\rm c} = -J \sum_{m=1}^{M} {\rm i}\Gamma_{2m}\Gamma_{2m+1} + B \sum_{m=1}^{M} {\rm i}\Gamma_{2m-1}\Gamma_{2m},$$

with $\Gamma_{2M+1} \equiv \Gamma_1$. This follows, as was said, from the Bogolyubov inequality. Then,

$$-\beta f = \lim_{M\to\infty} \frac{1}{M} \log {\rm Tr}\, {\rm e}^{-\beta\mathcal{H}_{\rm c}}.$$

The internal energy per site is

$$u(\beta) = \lim_{M\to\infty} \frac{1}{M} \langle \mathcal{H}_{\rm c} \rangle = \frac{\partial}{\partial\beta}(\beta f), \qquad \beta f = -\log 2 + \int_0^\beta u(\beta'){\rm d}\beta'.$$

To calculate the equal-time xx-correlation in the large-M limit, we rewrite it as

$$\left\langle \sigma_m^x \sigma_{m+p}^x \right\rangle_{\mathcal{H}} = \left\langle \prod_{k=m}^{m+p-1} \left(\mathrm{i}\Gamma_{2k}\Gamma_{2k+1} \right) \right\rangle_{\mathcal{H}_\mathrm{c}}.$$

This can be evaluated as a Pfaffian using the thermodynamic Wick theorem, as soon as we know all $\langle \Gamma_i \Gamma_j \rangle$.

We can calculate $\langle \Gamma_i \Gamma_j \rangle$ after first diagonalizing $\mathcal{H}_\mathrm{c}$. But there is an easier way using the KMS property, first stated by Kubo, Martin and Schwinger. In our case it is just the cyclic property of trace,

$$\begin{aligned} \left\langle \Gamma_j \Gamma_i \right\rangle_{\mathcal{H}_\mathrm{c}} &= \frac{\mathrm{Tr}\,\Gamma_j \Gamma_i \mathrm{e}^{-\beta\mathcal{H}_\mathrm{c}}}{\mathrm{Tr}\,\mathrm{e}^{-\beta\mathcal{H}_\mathrm{c}}} = \frac{\mathrm{Tr}\,\Gamma_i \mathrm{e}^{-\beta\mathcal{H}_\mathrm{c}} \Gamma_j}{\mathrm{Tr}\,\mathrm{e}^{-\beta\mathcal{H}_\mathrm{c}}} = \frac{\mathrm{Tr}\,\mathrm{e}^{\beta\mathcal{H}_\mathrm{c}} \Gamma_i \mathrm{e}^{-\beta\mathcal{H}_\mathrm{c}} \Gamma_j \mathrm{e}^{-\beta\mathcal{H}_\mathrm{c}}}{\mathrm{Tr}\,\mathrm{e}^{-\beta\mathcal{H}_\mathrm{c}}} \\ &= \frac{\mathrm{Tr}\,\Gamma_i(-\mathrm{i}\beta)\,\Gamma_j \mathrm{e}^{-\beta\mathcal{H}_\mathrm{c}}}{\mathrm{Tr}\,\mathrm{e}^{-\beta\mathcal{H}_\mathrm{c}}} = \left\langle \Gamma_i(-\mathrm{i}\beta)\,\Gamma_j \right\rangle_{\mathcal{H}_\mathrm{c}}, \end{aligned}$$

using the time evolution (in $\hbar = 1$ units)

$$O(t) = \mathrm{e}^{\mathrm{i}t\mathcal{H}_\mathrm{c}} O \mathrm{e}^{-\mathrm{i}t\mathcal{H}_\mathrm{c}}.$$

We can write

$$\mathcal{H}_\mathrm{c} = \mathrm{i} \sum_{k=1}^{2M} \sum_{l=1}^{2M} C_{k,l} \Gamma_k \Gamma_l = \mathrm{i}\, \boldsymbol{\Gamma} \cdot \mathsf{C} \cdot \boldsymbol{\Gamma},$$

with C the antisymmetric block-cyclic $2M$-by-$2M$ matrix. Its nonzero elements are given by

$$C_{2m,2m+1} = -C_{2m+1,2m} = -\tfrac{1}{2}J, \quad C_{2m-1,2m} = -C_{2m,2m-1} = \tfrac{1}{2}B, \quad (1 \leqslant m < M),$$
$$C_{2M,1} = -C_{1,2M} = -\tfrac{1}{2}J.$$

Now,

$$\frac{\mathrm{d}}{\mathrm{d}t}\Gamma_i(t) = \frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{-t\boldsymbol{\Gamma}\cdot\mathsf{C}\cdot\boldsymbol{\Gamma}}\,\Gamma_i\,\mathrm{e}^{t\boldsymbol{\Gamma}\cdot\mathsf{C}\cdot\boldsymbol{\Gamma}} = \mathrm{e}^{-t\boldsymbol{\Gamma}\cdot\mathsf{C}\cdot\boldsymbol{\Gamma}}\,[\Gamma_i, \boldsymbol{\Gamma}\cdot\mathsf{C}\cdot\boldsymbol{\Gamma}]\,\mathrm{e}^{t\boldsymbol{\Gamma}\cdot\mathsf{C}\cdot\boldsymbol{\Gamma}},$$

and

$$\begin{aligned} [\Gamma_i, \boldsymbol{\Gamma}\cdot\mathsf{C}\cdot\boldsymbol{\Gamma}] &= \sum_{k=1}^{2M}\sum_{l=1}^{2M} C_{k,l}\,[\Gamma_i, \Gamma_k\Gamma_l] \\ &= \sum_{l=1}^{2M} C_{i,l}\,(\Gamma_i\Gamma_i\Gamma_l - \Gamma_i\Gamma_l\Gamma_i) + \sum_{k=1}^{2M} C_{k,i}\,(\Gamma_i\Gamma_k\Gamma_i - \Gamma_k\Gamma_i\Gamma_i) = 4\sum_{k=1}^{2M} C_{i,k}\,\Gamma_k. \end{aligned}$$

Thus,

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\Gamma}(t) = 4\mathsf{C}\cdot\boldsymbol{\Gamma}(t), \qquad \boldsymbol{\Gamma}(t) = \mathrm{e}^{4t\mathsf{C}}\cdot\boldsymbol{\Gamma}.$$

Using the anticommutation relation and the KMS result derived earlier,

$$\{\Gamma_i, \Gamma_j\} = 2\delta_{i,j}, \qquad \text{or} \quad \langle\Gamma_i\Gamma_j\rangle + \langle\Gamma_j\Gamma_i\rangle = \langle\Gamma_i\Gamma_j\rangle + \langle\Gamma_i(-\mathrm{i}\beta)\,\Gamma_j\rangle = 2\delta_{i,j},$$

we find

$$(\mathbf{1} + \mathrm{e}^{-4\mathrm{i}\beta\mathsf{C}})\cdot\langle\boldsymbol{\Gamma}\,\boldsymbol{\Gamma}\rangle = 2\,\mathbf{1} \quad \text{or} \quad \boxed{\langle\boldsymbol{\Gamma}\,\boldsymbol{\Gamma}\rangle = 2(\mathbf{1} + \mathrm{e}^{-4\mathrm{i}\beta\mathsf{C}})^{-1}},$$

or

$$\langle\Gamma_i\Gamma_j\rangle = 2\big[(\mathbf{1} + \mathrm{e}^{-4\mathrm{i}\beta\mathsf{C}})^{-1}\big]_{i,j},$$

which is the (i, j) element of the inverse of a simple function of a block-cyclic matrix with 2-by-2 blocks. We shall see how this can be worked out using discrete Fourier transform.

Matrix A is an example of an n-by-n Toeplitz (or Töplitz) matrix:

$$\mathsf{A} = \begin{pmatrix} a & b & c & d \\ e & a & b & c \\ f & e & a & b \\ g & f & e & a \end{pmatrix}$$

It has the property $A_{i,j} = a(i - j)$, depending only on the difference of the two indices.

Matrix B is an example of an n-by-n cyclic matrix:

$$\mathsf{B} = \begin{pmatrix} a & b & c & d \\ d & a & b & c \\ c & d & a & b \\ b & c & d & a \end{pmatrix}$$

It has the property $B_{i,j} = b(i - j) = b(i - j \pm n)$. It depends only on the difference of the two indices and it is periodic modulo n.

Matrix C is block-cyclic. We give here the case $M = 6$ as an example:

$$2\mathsf{C} = \left(\begin{array}{cc|cc|cc|cc|cc|cc}
0 & B & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & J \\
-B & 0 & -J & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & J & 0 & B & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -B & 0 & -J & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & J & 0 & B & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -B & 0 & -J & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & J & 0 & B & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -B & 0 & -J & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & J & 0 & B & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -B & 0 & -J & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & J & 0 & B \\
-J & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -B & 0
\end{array}\right)$$