WIPM Lectures on Models in Statistical Mechanics

Lecture 4: 2D Ising Model and 1D Quantum Ising Model II

Jacques H. H. Perk, Oklahoma State University

Last lecture we set up the transfer matrix for the 2-dimensional Ising model. We also started calculations for the related quantum Ising chain in transverse field. Today:

- We first finish the set up for the 1D quantum Ising model, deriving the pair correlation of two Gamma operators in the thermodynamic limit.
- This then gives us immediately the internal energy per site and then the free energy per site by integration.
- Next we have an intermezzo, mentioning some problems of current interest related to a recent experiment related to finite-size scaling.
- After this we shall start similar calculations for the 2D Ising model, to find the pair correlation of two Gamma operators in the same row.

Review of Transverse-Field Ising Chain from Last Lecture

Because of the Bogolyubov inequality applied to the free energy per site in the thermodynamic limit,

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

we can replace the spin-cyclic Hamiltonian

$$\mathcal{H} = -J \sum_{m=1}^{M} \sigma_m^x \sigma_{m+1}^x - B \sum_{m=1}^{M} \sigma_m^z, \qquad \sigma_{M+1}^x \equiv \sigma_1^x,$$

with the cyclic (periodic) fermion Hamiltonian

$$\mathcal{H}_{\mathrm{c}} = -J \sum_{m=1}^{M} \mathrm{i}\Gamma_{2m}\Gamma_{2m+1} + B \sum_{m=1}^{M} \mathrm{i}\Gamma_{2m-1}\Gamma_{2m}, \qquad \Gamma_{2M+1} \equiv \Gamma_1.$$

This $\mathcal{H}_{\mathrm{c}}$ can be written more compactly as

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

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

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

Indeed, the nonzero elements of C are given by

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

From the free energy per site

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

we get the internal energy per site

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

where we used

$$-\beta f|_{\beta=0} = \lim_{M\to\infty} \frac{1}{M} \log \mathrm{Tr}\, \mathbf{1} = \lim_{M\to\infty} \frac{1}{M} \log 2^M = \log 2.$$

For the equal-time xx-correlation in the large-M limit, we have

$$\left\langle \sigma_m^x \sigma_{m+p}^x \right\rangle_{\mathcal{H}} = \left\langle \prod_{k=m}^{m+p-1} \left(\mathrm{i}\Gamma_{2k}\Gamma_{2k+1} \right) \right\rangle_{\mathcal{H}_\mathrm{c}} = \mathrm{i}^p \operatorname*{Pf}_{2m\leqslant i<j<2m+2p} \left\{ \left\langle \Gamma_i \Gamma_j \right\rangle_{\mathcal{H}_\mathrm{c}} \right\}.$$

We can calculate $\langle \Gamma_i \Gamma_j \rangle_{\mathcal{H}_\mathrm{c}}$ 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,

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

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

$$O(t) = \mathrm{e}^{\mathrm{i}t\mathcal{H}_\mathrm{c}} O \mathrm{e}^{-\mathrm{i}t\mathcal{H}_\mathrm{c}}, \qquad \mathcal{H}_\mathrm{c} = \mathrm{i}\, \mathbf{\Gamma}\cdot\mathsf{C}\cdot\mathbf{\Gamma}.$$

Now,

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

and

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

Thus,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{\Gamma}(t) = 4\mathsf{C}\cdot\mathbf{\Gamma}(t) \quad \text{with} \quad \mathbf{\Gamma}(0) = \mathbf{\Gamma} \qquad \Longrightarrow \qquad \boxed{\mathbf{\Gamma}(t) = \mathrm{e}^{4t\mathsf{C}}\cdot\mathbf{\Gamma}},$$

and

$$\mathbf{\Gamma}(-\mathrm{i}\beta) = \mathrm{e}^{-4\mathrm{i}\beta\mathsf{C}}\cdot\mathbf{\Gamma}.$$

Using the anticommutation relation and the KMS result just derived,*

$$\{\Gamma_i, \Gamma_j\} = 2\delta_{i,j}, \qquad \big\langle \Gamma_j \Gamma_i \big\rangle = \big\langle \Gamma_i(-\mathrm{i}\beta)\,\Gamma_j \big\rangle, \qquad \boldsymbol{\Gamma}(-\mathrm{i}\beta) = \mathrm{e}^{-4\mathrm{i}\beta\mathsf{C}} \cdot \boldsymbol{\Gamma},$$

we find

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

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

or

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

We can rewrite this as

$$\big\langle \boldsymbol{\Gamma}\,\boldsymbol{\Gamma} \big\rangle = \frac{\big(\mathbf{1} + \mathrm{e}^{-4\mathrm{i}\beta\mathsf{C}}\big) + \big(\mathbf{1} - \mathrm{e}^{-4\mathrm{i}\beta\mathsf{C}}\big)}{\mathbf{1} + \mathrm{e}^{-4\mathrm{i}\beta\mathsf{C}}} = \mathbf{1} + \tanh(2\mathrm{i}\beta\mathsf{C}),$$

$$\boxed{\big\langle \Gamma_i\,\Gamma_j \big\rangle = \delta_{i,j} + \big[\tanh(2\mathrm{i}\beta\mathsf{C})\big]_{i,j}}\,.$$

* From this point we write $\langle O \rangle$ as short hand for $\langle O \rangle_{\mathcal{H}_\mathrm{c}}$ until said differently.

Since C is a block-cyclic matrix with 2-by-2 blocks, the problem can be reduced immediately to 2-by-2 matrices using discrete Fourier transform.

Introducing the 2-by-2 matrices

$$\mathsf{c}_0 = \mathsf{c}_{\pm M} = \begin{pmatrix} 0 & B \\ -B & 0 \end{pmatrix}, \quad \mathsf{c}_1 = \mathsf{c}_{1-M} = \begin{pmatrix} 0 & J \\ 0 & 0 \end{pmatrix}, \quad \mathsf{c}_{-1} = \mathsf{c}_{M-1} = \begin{pmatrix} 0 & 0 \\ -J & 0 \end{pmatrix},$$

$$\mathsf{c}_k = \mathbf{0}_2 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \text{ for } 1-M<k<-1 \text{ and } 1<k<M-1, \quad \mathbf{1}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

we have, when $M = 6$ for example,

$$2\mathsf{C} = \begin{pmatrix} \mathsf{c}_0 & \mathsf{c}_{-1} & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \mathsf{c}_1 \\ \mathsf{c}_1 & \mathsf{c}_0 & \mathsf{c}_{-1} & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 \\ \mathbf{0}_2 & \mathsf{c}_1 & \mathsf{c}_0 & \mathsf{c}_{-1} & \mathbf{0}_2 & \mathbf{0}_2 \\ \mathbf{0}_2 & \mathbf{0}_2 & \mathsf{c}_1 & \mathsf{c}_0 & \mathsf{c}_{-1} & \mathbf{0}_2 \\ \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \mathsf{c}_1 & \mathsf{c}_0 & \mathsf{c}_{-1} \\ \mathsf{c}_{-1} & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \mathsf{c}_1 & \mathsf{c}_0 \end{pmatrix},$$

or

$$2C_{2(k-1)+p,2(l-1)+q} = (\mathsf{c}_{k-l})_{p,q}, \quad (k, l = 1, \cdots, M,\ p, q = 1, 2).$$

We apply discrete Fourier transform by the similarity transform

$$\hat{\mathsf{C}} = \mathsf{U}\mathsf{C}\mathsf{U}^{-1}, \qquad U_{2(k-1)+p,2(l-1)+q} = \frac{\mathrm{e}^{2\pi \mathrm{i} kl/M}}{\sqrt{M}}\delta_{p,q}.$$

Now

$$\sum_{l=1}^{M} \frac{\mathrm{e}^{2\pi \mathrm{i} kl/M}}{\sqrt{M}} \frac{\mathrm{e}^{-2\pi \mathrm{i} lk'/M}}{\sqrt{M}} = \sum_{l=1}^{M} \frac{1}{M}\mathrm{e}^{2\pi \mathrm{i}(k-k')l/M} = \delta_{k,k'}, \quad \text{or} \quad \mathsf{U}^{\dagger} = \mathsf{U}^{-1},$$

so U is unitary. Therefore,

$$\begin{aligned} 2\hat{\mathsf{C}}_{2(k-1)+p,2(k'-1)+q} &= \sum_{l=1}^{M}\sum_{l'=1}^{M} \frac{\mathrm{e}^{2\pi \mathrm{i} kl/M}}{\sqrt{M}} (\mathsf{c}_{l-l'})_{p,q} \frac{\mathrm{e}^{-2\pi \mathrm{i} l'k'/M}}{\sqrt{M}} \\ &= \frac{1}{M}\sum_{l'=1}^{M} \mathrm{e}^{2\pi \mathrm{i} l'(k-k')/M} \sum_{l=1}^{M} \mathrm{e}^{2\pi \mathrm{i} k(l-l')/M} (\mathsf{c}_{l-l'})_{p,q} \\ &= \delta_{k,k'} \sum_{l=1}^{M} \mathrm{e}^{2\pi \mathrm{i} kl/M} (\mathsf{c}_l)_{p,q} = \delta_{k,k'} \left(\hat{\mathsf{c}}(\phi_k)\right)_{p,q}, \quad \phi_k = \frac{2\pi k}{M}. \end{aligned}$$

We reduced the matrix size: $2^M \ \rightarrow \ 2M \ \rightarrow \ 2 \ \rightarrow$ essentially done!

We immediately get

$$\begin{aligned} \hat{\mathsf{c}}(\phi_k) &= \mathrm{e}^{\mathrm{i}\phi_k}\mathsf{c}_1 + \mathsf{c}_0 + \mathrm{e}^{-\mathrm{i}\phi_k}\mathsf{c}_{-1} = \begin{pmatrix} 0 & B + J\mathrm{e}^{\mathrm{i}\phi_k} \\ -B - J\mathrm{e}^{-\mathrm{i}\phi_k} & 0 \end{pmatrix} \\ &= \mathrm{i}(J\sin\phi_k)\sigma^x + \mathrm{i}(B + J\cos\phi_k)\sigma^y, \end{aligned}$$

and $\hat{\mathsf{C}} = \mathsf{U}\mathsf{C}\mathsf{U}^{-1}$ is block diagonal with the 2-by-2 blocks $\frac{1}{2}\hat{\mathsf{c}}(\phi_k)$ on the diagonal for $k = 1, \cdots, M$. For example, for $M = 6$,

$$2\hat{\mathsf{C}} = \begin{pmatrix} \hat{\mathsf{c}}(\phi_1) & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 \\ \mathbf{0}_2 & \hat{\mathsf{c}}(\phi_2) & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 \\ \mathbf{0}_2 & \mathbf{0}_2 & \hat{\mathsf{c}}(\phi_3) & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 \\ \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \hat{\mathsf{c}}(\phi_4) & \mathbf{0}_2 & \mathbf{0}_2 \\ \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \hat{\mathsf{c}}(\phi_5) & \mathbf{0}_2 \\ \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \hat{\mathsf{c}}(\phi_6) \end{pmatrix}.$$

Note that

$$\hat{\mathsf{c}}(\phi_M) = \hat{\mathsf{c}}(\phi_0) = \hat{\mathsf{c}}(0).$$

Similarly, from

$$\mathsf{G} = \left\langle \boldsymbol{\Gamma}\,\boldsymbol{\Gamma} \right\rangle = \mathbf{1} + \tanh(2\mathrm{i}\beta\mathsf{C})$$

we find that $\hat{\mathsf{G}} = \mathsf{U}\left\langle \boldsymbol{\Gamma}\,\boldsymbol{\Gamma} \right\rangle \mathsf{U}^{-1}$ is block diagonal with the M 2-by-2 blocks

$$\hat{\mathsf{g}}(\phi_k) = \mathbf{1}_2 + \tanh\bigl(\mathrm{i}\beta\hat{\mathsf{c}}(\phi_k)\bigr)$$

on the diagonal. Now tanh is an odd function. A function $f(x)$ is odd, if $f(-x) = -f(x)$. For such a function, using $(\mathbf{a}\cdot\boldsymbol{\sigma})^2 = |\mathbf{a}|^2$,

$$f(\mathbf{a}\cdot\boldsymbol{\sigma}) = \frac{\mathbf{a}\cdot\boldsymbol{\sigma}}{|\mathbf{a}|} f(|\mathbf{a}|),$$

as follows from Mclaurin expansion $f(x) = c_1 x + c_3 x^3 + \cdots$. Let

$$\Lambda(\phi_k) \equiv \sqrt{J^2 + 2BJ\cos\phi_k + B^2}, \qquad \bigl(\mathrm{i}\,\hat{\mathsf{c}}(\phi_k)\bigr)^2 = \Lambda(\phi_k)^2\mathbf{1}_2.$$

Then

$$\boxed{\hat{\mathsf{g}}(\phi_k) = \mathbf{1}_2 + \frac{\mathrm{i}\,\hat{\mathsf{c}}(\phi_k)}{\Lambda(\phi_k)}\tanh\bigl(\beta\Lambda(\phi_k)\bigr)},$$

and

$$\hat{\mathsf{G}}_{2(k-1)+p,2(k'-1)+q} = \delta_{k,k'}\left(\hat{\mathsf{g}}(\phi_k)\right)_{p,q}.$$

Having

$$\hat{\mathsf{G}}_{2(l-1)+p,2(l'-1)+q} = \delta_{l,l'}\left(\hat{\mathsf{g}}(\phi_l)\right)_{p,q}$$

explicitly, we can now apply the inverse block-Fourier transform

$$\mathsf{G} = \mathsf{U}^{-1}\hat{\mathsf{G}}\mathsf{U}$$

and obtain

$$\begin{aligned}
\mathsf{G}_{2(k-1)+p,2(k'-1)+q} &= \sum_{l=1}^{M}\sum_{l'=1}^{M} \frac{\mathrm{e}^{-2\pi\mathrm{i}kl/M}}{\sqrt{M}}\,\delta_{l,l'}\left(\hat{\mathsf{g}}(\phi_l)\right)_{p,q}\frac{\mathrm{e}^{2\pi\mathrm{i}l'k'/M}}{\sqrt{M}} \\
&= \frac{1}{M}\sum_{l=1}^{M} \mathrm{e}^{2\pi\mathrm{i}l(k'-k)/M}\left(\hat{\mathsf{g}}(\phi_l)\right)_{p,q} \\
&= \frac{1}{M}\sum_{l=1}^{M} \mathrm{e}^{\mathrm{i}(k'-k)\phi_l}\left(\hat{\mathsf{g}}(\phi_l)\right)_{p,q} \\
&= \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\,\mathrm{e}^{\mathrm{i}(k'-k)\phi}\left(\hat{\mathsf{g}}(\phi)\right)_{p,q}, \quad \text{as } M\to\infty.
\end{aligned}$$

We have $\phi = \frac{2\pi}{M}l$, so that $\Delta\phi = \frac{2\pi}{M}\Delta l = \frac{2\pi}{M}$ in the large-M limit.

Taking $p=1$ and $q=2$,

$$G_{2k-1,2k'} = \frac{\mathrm{i}}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\,\mathrm{e}^{\mathrm{i}(k'-k)\phi}\,\frac{B+J\mathrm{e}^{\mathrm{i}\phi}}{\Lambda(\phi)}\tanh(\beta\Lambda(\phi)),$$

while for $p=2$ and $q=1$,

$$G_{2k,2k'-1} = -\frac{\mathrm{i}}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\,\mathrm{e}^{\mathrm{i}(k'-k)\phi}\,\frac{B+J\mathrm{e}^{-\mathrm{i}\phi}}{\Lambda(\phi)}\tanh(\beta\Lambda(\phi)).$$

This is consistent with the anticommutation relation $\{\Gamma_{2k-1},\Gamma_{2k}\}=0$, as one can show that $G_{2k',2k-1}=G_{2k-1,2k'}$ holds by replacing $\phi\to-\phi$.

We can evaluate the internal energy per site

$$\begin{aligned}u(\beta) &= \lim_{M\to\infty}\frac{1}{M}\langle\mathcal{H}_\mathrm{c}\rangle = \lim_{M\to\infty}\frac{1}{M}\Big\langle -J\sum_{m=1}^{M}\mathrm{i}\Gamma_{2m}\Gamma_{2m+1} + B\sum_{m=1}^{M}\mathrm{i}\Gamma_{2m-1}\Gamma_{2m}\Big\rangle\\ &= -\mathrm{i}JG_{2k,2k+1}+\mathrm{i}BG_{2k-1,2k},\end{aligned}$$

independent of k. We find:

$$\begin{aligned}u(\beta) &= -\frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\,\frac{J(B\mathrm{e}^{\mathrm{i}\phi}+J)+B(B+J\mathrm{e}^{\mathrm{i}\phi})}{\Lambda(\phi)}\tanh(\beta\Lambda(\phi))\\ &= -\frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\,\frac{J^2+2JB\cos\phi+B^2}{\Lambda(\phi)}\tanh(\beta\Lambda(\phi)) \qquad ,\\ &= -\frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\,\Lambda(\phi)\tanh(\beta\Lambda(\phi))\end{aligned}$$

as the imaginary part vanishes. The free energy per site is given by

$$\beta f = -\log 2 + \int_0^{\beta} u(\beta')\mathrm{d}\beta' = -\log 2 - \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\,\log\cosh(\beta\Lambda(\phi)).$$

Remark: The same method can be used for the full one-dimensional XY model. Because we evaluated $\langle\Gamma_i\Gamma_j\rangle$, we also have the equal-time correlations explicitly as Pfaffians and determinants. However, for time-dependent correlations like $\langle\sigma_i^x(t)\sigma_j^x\rangle$ one cannot just replace $\mathcal{H}$ by $\mathcal{H}_\mathrm{c}$ as we have done.

Some problems to think about during your break

The scaling hypothesis:

Near the critical temperature T_{c}, we find that the specific heat c_v, spontaneous magnetization $M_0 = \langle\sigma\rangle$ (for $T < T_{\mathrm{c}}$), and the susceptibility χ behave as

$$\begin{aligned} c_v &\sim |t|^{-\alpha}, \\ M(T) &\sim |t|^{\beta}, \qquad \text{where} \quad t \equiv \frac{T}{T_{\mathrm{c}}} - 1. \\ \chi(T) &\sim |t|^{-\gamma}, \end{aligned}$$

For the 2-dimensional Ising model $\alpha = 0(\log)$, $\beta = 1/8$, $\gamma = 7/4$. More precisely, the specific heat diverges logarithmically, $c_v \sim \log|t|$, which diverges slower than any power of $1/|t|$.

In the absence of such a log, according to scaling theory, the leading singular part of the free energy behaves as

$$f_{\mathrm{s}}(t, B) = |t|^{2-\alpha}\Phi\Big(\frac{B}{|t|^{\beta+\gamma}}\Big), \qquad \text{as } t \text{ and } B \to 0,$$

so that $f_{\mathrm{s}}/|t|^{2-\alpha}$ is a function of the single variable $B/|t|^{\beta+\gamma}$. Also we are to have

$$\alpha + 2\beta + \gamma = 2.$$

Moreover, the spin-spin correlation decays exponentially as

$$\langle \sigma_0 \sigma_R \rangle \sim \frac{e^{-R/\xi}}{R^{(d-1)/2}}, \quad (T > T_c), \qquad \langle \sigma_0 \sigma_R \rangle \sim \frac{1}{R^{d-2+\eta}}, \quad (T = T_c),$$

where $\xi(T)$ is the correlation length, which diverges at the critical point, while at $T = T_c$, the correlation function decays algebraically.

$$\xi(T) \approx \xi_0/|t|^{\nu} \quad \text{with} \quad t = (T/T_c) - 1 \to 0,$$

where ν is a characteristic critical exponent. In 2d Ising $\nu = 1$, $\eta = 1/4$.

If $T < T$c we have to take the 'connected pair correlation', subtracting the square of the magnetization. In two dimensions this behaves anomalously:

$$\langle \sigma_0 \sigma_R \rangle_c \equiv \langle \sigma_0 \sigma_R \rangle - \langle \sigma \rangle^2 \sim \frac{e^{-2R/\xi}}{R^d}, \quad (T < T_c).$$

There is no 'one-particle band', so that the 'two-particle continuum' dominates.

Finite-size scaling

For a system limited in size by a finite length N, the scaling hypothesis asserts, in general terms, that when N and $\xi(T)$ are large enough, the critical point singularities are primarily controlled by the ratio $x = N/\xi(T)$, so that

$$C(N;T) \approx \frac{N^{\alpha/\nu}[Q(x) - Q_0]}{\alpha},$$

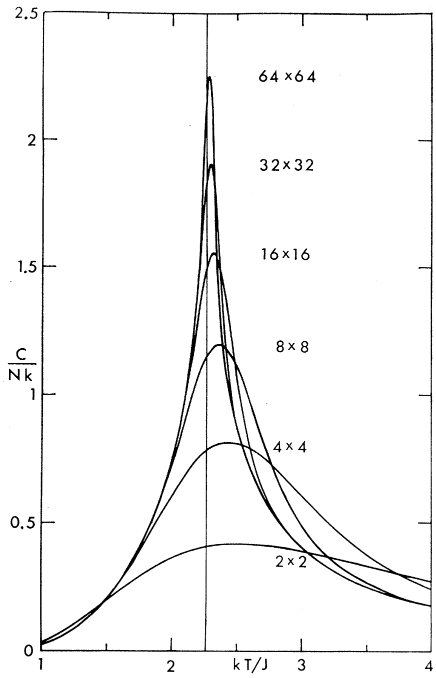
where $Q(x)$ is the scaling function while the scaled temperature is

$$N^{1/\nu} t \propto x^{1/\nu} = [N/\xi(T)]^{1/\nu}.$$

The exponent α in the denominator allows for the limit $\alpha \to 0$, which yields, with $Q(0) \to Q_0$, a logarithmic singularity as is appropriate for 2D Ising systems. More generally, to account for the finite-size behavior of the specific heat per site $c_v = C/N^d$, (which diverges in the bulk as $|t|^{-\alpha}$), when α is typically small (or even negative), the basic scaling hypothesis may be expressed as the above

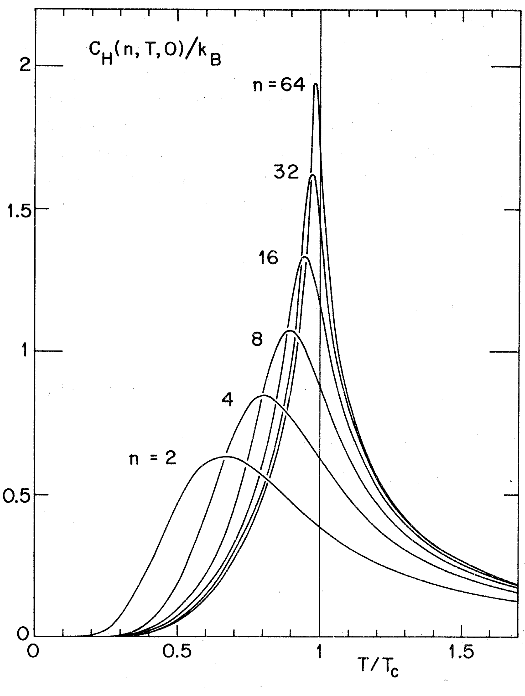
$$C(N;T) \approx N^{\alpha/\nu}[Q(x) - Q_0]/\alpha.$$

From Ferdinand and Fisher [Phys. Rev. **185**, 832–846 (1969)]: Specific heat of Ising model on an $N \times N$ torus.



The maximum is to the right of T_c, but as N increases the logarithmic singularity for $N = \infty$ becomes apparent.

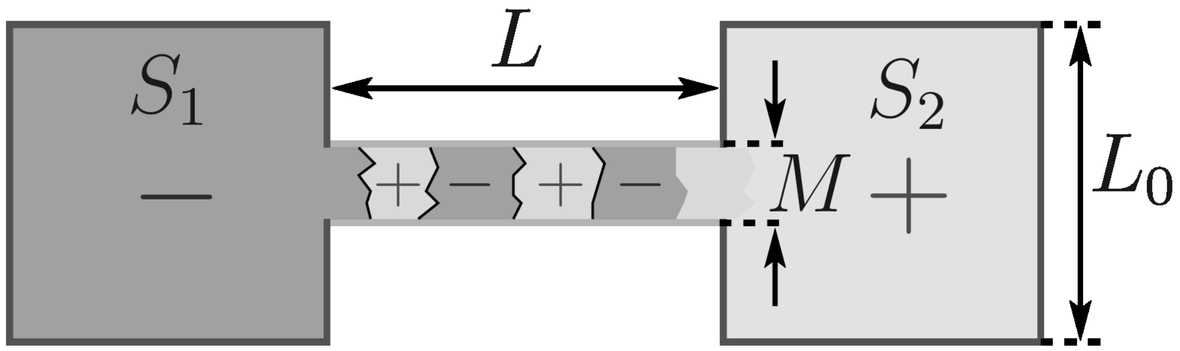
From Au-Yang and Fisher [Phys. Rev. **B 11**, 3469–3486 (1975)]: Specific heat of Ising model on an $n \times \infty$ strip.



The maximum is to the left of T_c, but as N increases the logarithmic singularity for $N = \infty$ becomes apparent.

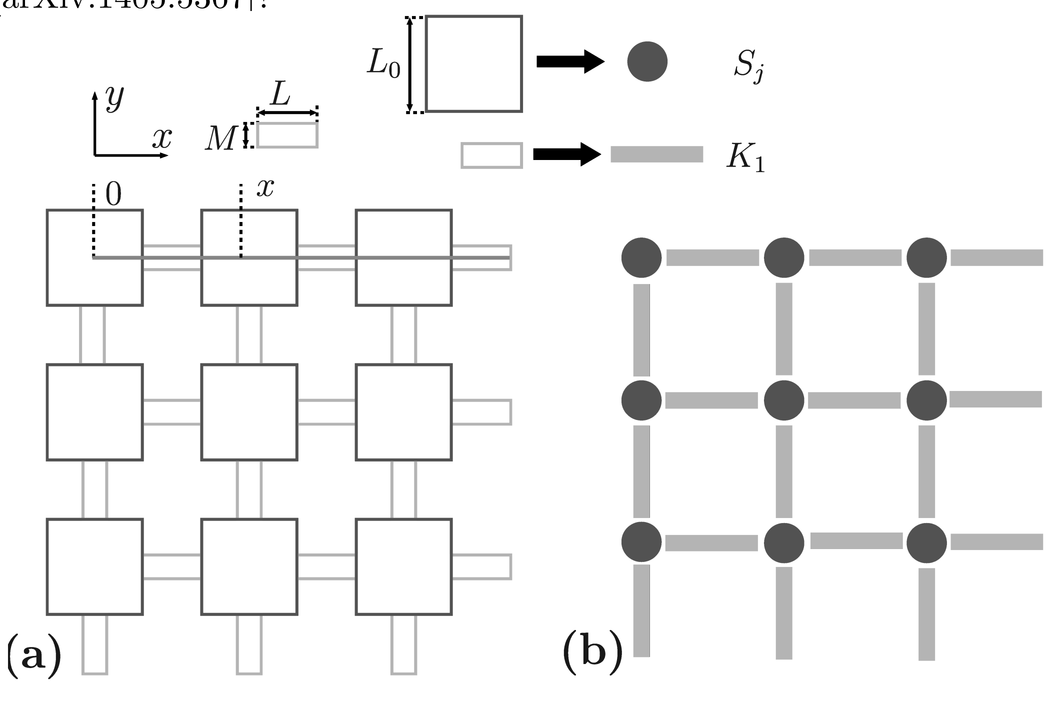
Hard homework:

Can you calculate the specific heat of an Ising system like this?



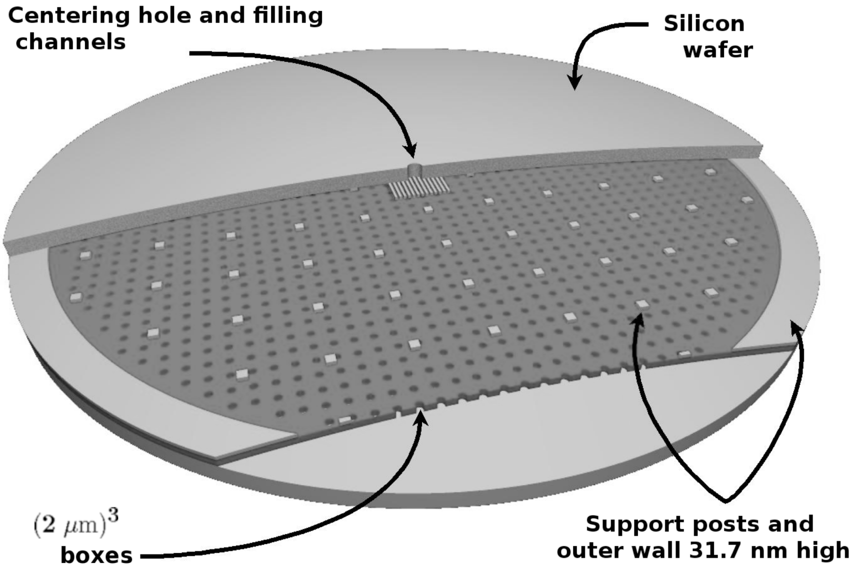
(Figure from the paper by Abraham and Maciołek [arXiv:1405.5367])

Also [arXiv:1405.5367]?



This is more like the experiment:

Reason for the calculation is the liquid helium experiment of Gasparini:



(Figure provided by Gasparini)

Further references:

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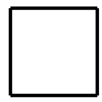
3. J.K. Perron, M.O. Kimball, K.P. Mooney, and F.M. Gasparini, "Lack of Correlation-Length Scaling for an Array of Boxes," J. Phys.: Conf. Ser. **150**, 032082 (2009).
4. J.K. Perron, M.O. Kimball, K.P. Mooney, and F.M. Gasparini, "Coupling and Proximity Effects in the Superfluid Transition in ^{4}He Dots," Nature Physics **6**, 499–502 (2010).
5. M.E. Fisher, "Superfluid Transitions: Proximity Eases Confinement," Nature Physics **6**, 483–484 (2010). News & Views: Comment on Perron *et al.*
6. J.K. Perron, and F.M. Gasparini, "Critical Point Coupling and Proximity Effects in ^{4}He at the Superfluid Transition," Phys. Rev. Lett. **109**, 035302 (2012).
7. J.K. Perron, M.O. Kimball, K.P. Mooney and F.M. Gasparini, "Critical Behavior of Coupled ^{4}He Regions near the Superfluid Transition," Phys. Rev. B **87**, 094507 (2013).
8. H. Au-Yang and M.E. Fisher, "Criticality in Alternating Layered Ising Models. I. Effects of Connectivity and Proximity," Phys. Rev. E **88**, 032147 (2013).

Some other geometries for hard homework:

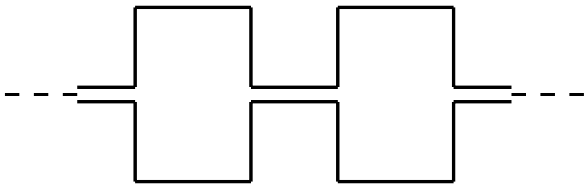
$M \times L$ square



$M \times L$ rectangle

$M \times L \quad or \quad \infty \times L$ cylindrical strip

Infinite strip repeatedly wide and narrow



Two-Dimensional Ising Model

Two-Dimensional Ising Model

We can now do the analogous calculation for the 2D Ising model, for which

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

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

where

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

and

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

After the Jordan–Wigner transformation, we get

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

$$\boxed{\mathsf{T}_n = \mathsf{T}_2 = \exp\left(K \sum_{m=1}^{M} \mathrm{i}\Gamma_{2m}\Gamma_{2m+1}\right)}, \qquad \Gamma_{2M+1} \equiv \Gamma_1,$$

where we can again justify the use of cyclic fermion boundary conditions using the calculations that follow.

We define

$$G_{i,j} = \big\langle \Gamma_i \Gamma_j \big\rangle = \frac{\operatorname{Tr}\left[\Gamma_i \Gamma_j (\mathsf{T}_2 \mathsf{T}_1)^N\right]}{\operatorname{Tr}(\mathsf{T}_2 \mathsf{T}_1)^N}$$

in analogy with was done before. We again use the KMS property:

We again use the KMS property:

$$G_{j,i} = \langle \Gamma_j \Gamma_i \rangle = \frac{\mathrm{Tr}\left[\Gamma_j \Gamma_i (\mathsf{T}_2 \mathsf{T}_1)^N\right]}{\mathrm{Tr}\,(\mathsf{T}_2 \mathsf{T}_1)^N} = \frac{\mathrm{Tr}\left[\Gamma_i (\mathsf{T}_2 \mathsf{T}_1)^N \Gamma_j\right]}{\mathrm{Tr}\,(\mathsf{T}_2 \mathsf{T}_1)^N}$$
$$= \frac{\mathrm{Tr}\left[(\mathsf{T}_2 \mathsf{T}_1)^{-N} \Gamma_i (\mathsf{T}_2 \mathsf{T}_1)^N \Gamma_j (\mathsf{T}_2 \mathsf{T}_1)^N\right]}{\mathrm{Tr}\,(\mathsf{T}_2 \mathsf{T}_1)^N} = \left\langle (\mathsf{T}_2 \mathsf{T}_1)^{-N} \Gamma_i (\mathsf{T}_2 \mathsf{T}_1)^N \Gamma_j \right\rangle.$$

Here T_1 and T_2 have the same form as $\mathrm{e}^{-\beta \mathcal{H}_\mathrm{c}}$ for the transverse-field Ising chain.

We finish this next time.