WIPM Lectures on Models in Statistical Mechanics

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

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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

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

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,

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

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

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

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,

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

and

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

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

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

we find

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

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

or

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

We can rewrite this as

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

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

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* From this point we write $\langle O \rangle$ as short hand for $\langle O \rangle_{\mathcal{H}_c}$ 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,

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

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

We immediately get

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

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

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

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

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

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

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

Then

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

and

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

Having

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

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

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

and obtain

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

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 $T < T_c$), and the susceptibility χ behave as

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

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

$$f_s(t, B) = |t|^{2-\alpha} \Phi\left(\frac{B}{|t|^{\beta+\gamma}}\right), \qquad \text{as } t \text{ and } B \to 0,$$

so that $f_s/|t|^{2-\alpha}$ 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

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

where $\xi(T)$ is the correlation length, which diverges at the critical point, while at $T = T_\mathrm{c}$, 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 $T < T\mathrm{c}$ we have to take the 'connected pair correlation', subtracting the square of the magnetization. In two dimensions this behaves anomalously:

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

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

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

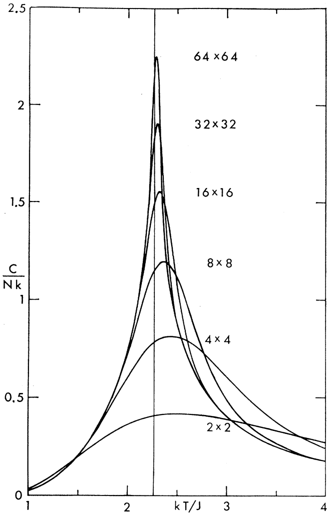
where $Q(x)$ is the scaling function while the scaled temperature is

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

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

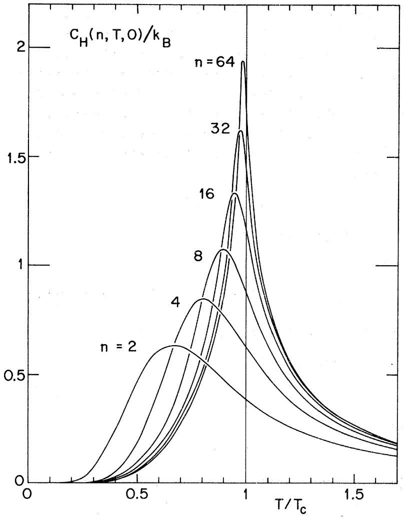
$$C(N;T) \approx N^{\alpha/\nu}[Q(x) - Q_0]/\alpha.$$

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.

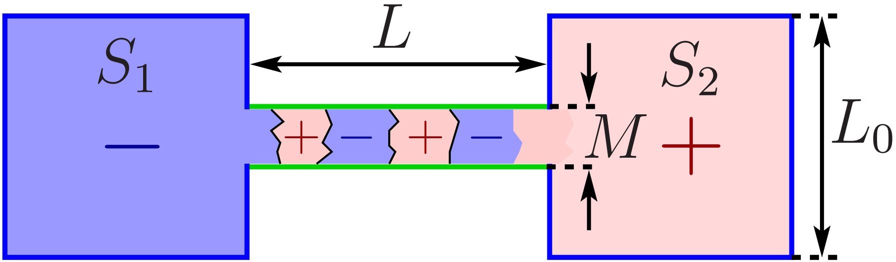
From Au-Yang and Fisher [Phys. Rev. **B 11**, 3469–3486 (1975)]: Specific heat of Ising model on an $n \times \infty$ strip.



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

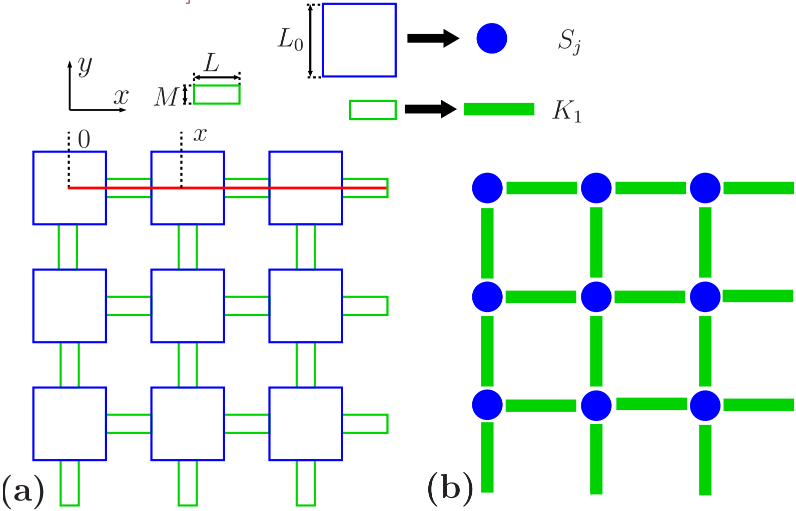
Hard homework:

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



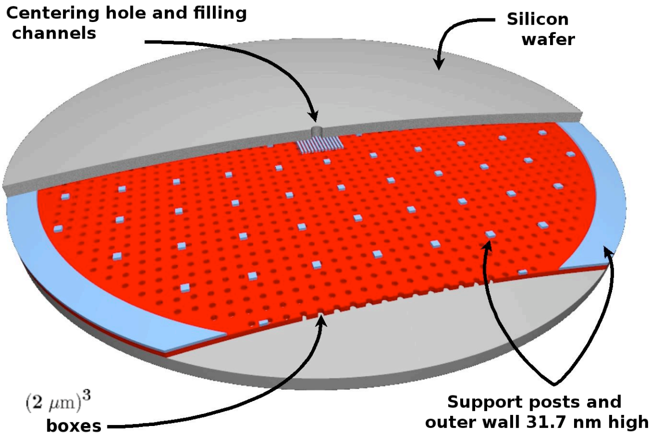
(Figure from the paper by Abraham and Maciołek [arXiv:1405.5367])

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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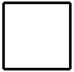
2. M.O. Kimball, K.P. Mooney, and F.M. Gasparini, "Three Dimensional Critical Behavior with 2D, 1D, and 0D Dimensionality Crossover: Surface and Edge Specific Heats" Phys. Rev. Lett. **92**, 115301 (2004).
3. J.K. Perron, M.O. Kimball, K.P. Mooney, and F.M. Gasparini, "Lack of Correlation-Length Scaling 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:

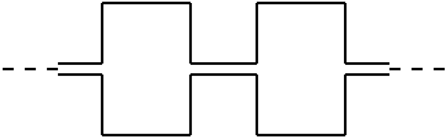
$M \times L$ square



$M \times L$ rectangle

$M \times L$ *or* $\infty \times L$ 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

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

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

where

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

and

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

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

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

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

We again use the KMS property:

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

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

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.