WIPM Lectures on Models in Statistical Mechanics Lecture 5: 2D Ising Model and 1D Quantum Ising Model III

Jacques H. H. Perk, Oklahoma State University

Last lecture we solved the fermion equal-time correlation function, internal energy and free energy of the quantum Ising chain in transverse field. We also gave a discussion of finite-size scaling, a related experiment, and calculations that could be tried. We ended with a little bit of 2-dimensional Ising model. Today:

- * We shall finish the discussion of the 2D zero-field Ising model, deriving the pair correlation of two Gamma operators in the thermodynamic limit.
- * Next we shall show how to extend this result to cases with two Gamma operators in different rows. This can be used to get the internal energy and free energy per site by integration.
- * Finally we shall briefly discuss an identity for pair correlations.

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Two-Dimensional Ising Model

In an earlier lecture we found the transfer matrices of the 2D Ising model to be

$$\mathsf{T}_{n+\frac{1}{2}} = \mathsf{T}_1 = \left(2\sinh(2K')\right)^{M/2} \exp\left(K'^* \sum_{m=1}^M \sigma_m^z\right),$$
$$\mathsf{T}_n = \mathsf{T}_2 = \exp\left(K \sum_{m=1}^M \sigma_m^x \sigma_{m+1}^x\right),$$

where

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

so that

$$Z = \text{Tr} \left(\mathsf{T}_{1} \mathsf{T}_{2} \right)^{N} = \text{Tr} \left(\mathsf{T}_{2} \mathsf{T}_{1} \right)^{N} = \text{Tr} \left(\mathsf{T}_{2}^{\frac{1}{2}} \mathsf{T}_{1} \mathsf{T}_{2}^{\frac{1}{2}} \right)^{N} = \text{Tr} \left(\mathsf{T}_{1}^{\frac{1}{2}} \mathsf{T}_{2} \mathsf{T}_{1}^{\frac{1}{2}} \right)^{N}$$

One may change the order or symmetrize in two ways. It is all the same.

After the Jordan–Wigner transformation, we get

$$\begin{aligned} \mathsf{T}_{n+\frac{1}{2}} &= \mathsf{T}_1 = \left(2\sinh(2K')\right)^{M/2} \exp\left(K'^*\sum_{m=1}^M \mathrm{i}\Gamma_{2m-1}\Gamma_{2m}\right) \\ \\ \mathsf{T}_n &= \mathsf{T}_2 = \exp\left(K\sum_{m=1}^M \mathrm{i}\Gamma_{2m}\Gamma_{2m+1}\right), \qquad \Gamma_{2M+1} \equiv \Gamma_1, \end{aligned}$$

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

We define

$$G_{i,j} = \left\langle \Gamma_i \Gamma_j \right\rangle = \frac{\operatorname{Tr} \left[\Gamma_i \Gamma_j \mathsf{T}^N \right]}{\operatorname{Tr} \mathsf{T}^N}, \quad \mathsf{T} \equiv \mathsf{T}_1^{\frac{1}{2}} \mathsf{T}_2 \mathsf{T}_1^{\frac{1}{2}},$$

in analogy with was done before. Compared to last time we have symmetrized the transfer matrix.

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We again use the KMS property:

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

In place of T^N here, before we had $\mathrm{e}^{-\beta\mathcal{H}_c}$ with the cyclic (periodic) fermion Hamiltonian

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

This $\mathcal{H}_{\rm c}$ had been written more compactly as

$$\mathcal{H}_{c} = i \sum_{k=1}^{2M} \sum_{l=1}^{2M} C_{k,l} \Gamma_{k} \Gamma_{l} = i \mathbf{\Gamma} \cdot \mathbf{C} \cdot \mathbf{\Gamma} = -i J \mathbf{\Gamma} \cdot \mathbf{A} \cdot \mathbf{\Gamma} + i B \mathbf{\Gamma} \cdot \mathbf{B} \cdot \mathbf{\Gamma},$$

where we now have introduced constant matrices A and B via

$$\mathsf{C} = -J\mathsf{A} + B\mathsf{B},$$

as we now have to deal with the two transfer matrices T_1 and T_2 .

	$\begin{pmatrix} 0 \end{pmatrix}$	B	0	0	0	0	0	0	0	0	0	J
2C =	-B	0	-J	0	0	0	0	0	0	0	0	0
	0	J	0	В	0	0	0	0	0	0	0	0
	0	0	-B	0	-J	0	0	0	0	0	0	0
	0	0	0	J	0	В	0	0	0	0	0	0
	0	0	0	0	-B	0	-J	0	0	0	0	0
	0	0	0	0	0	J	0	В	0	0	0	0
	0	0	0	0	0	0	-B	0	-J	0	0	0
	0	0	0	0	0	0	0	J	0	В	0	0
	0	0	0	0	0	0	0	0	-B	0	-J	0
	0	0	0	0	0	0	0	0	0	J	0	В
	$\setminus -J$	0	0	0	0	0	0	0	0	0	-B	0 /

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

Note that for J = -B the matrix is cyclic: $B = \pm J$ is the critical case.

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Matrix ${\sf A}$ shows up in ${\sf T}_2,$ i.e.,

$$\Gamma_2 = \exp(\mathrm{i}K\,\mathbf{\Gamma}\cdot\mathbf{A}\cdot\mathbf{\Gamma}),\,$$

with matrix block-cyclic A. We give here the case M = 6 as an example:

	$\left(0 \right)$	0	0	0	0	0	0	0	0	0	0	-1
2A =	0	0	1	0	0	0	0	0	0	0	0	0
	0	-1	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	1	0	0	0	0	0	0	0
	0	0	0	-1	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	1	0	0	0	0	0
	0	0	0	0	0	-1	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	1	0	0	0
	0	0	0	0	0	0	0	-1	0	0	0	0
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	$-1 \\ 0$	0 0	0 0	0 1	0 0
	$\begin{array}{c} 0\\ 0\\ \hline 0\\ \end{array}$	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0	-1 0	0 0 0	$\begin{array}{c} 0 \\ 0 \\ -1 \end{array}$	0 1 0	0 0 0

Matrix ${\sf B}$ shows up in ${\sf T}_1,$ i.e.,

$$\mathsf{T}_1 = \left(2\sinh(2K')\right)^{M/2}\exp(\mathrm{i}K^*\,\mathbf{\Gamma}\cdot\mathsf{B}\cdot\mathbf{\Gamma}),\,$$

with matrix B block-diagonal. Again we give the case M = 6 as an example:

	$\begin{pmatrix} 0 \end{pmatrix}$	1	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	1	0	0	0	0	0	0	0	0
	0	0	-1	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	1	0	0	0	0	0	0
	0	0	0	0	-1	0	0	0	0	0	0	0
2D =	0	0	0	0	0	0	0	1	0	0	0	0
	0	0	0	0	0	0	-1	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	1	0	0
	0	0	0	0	0	0	0	0	-1	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	1
	0	0	0	0	0	0	0	0	0	0	-1	0/
						7						

Just like C, matrices A and B are block-cyclic with 2-by-2 blocks, allowing us to reduce the problem to 2-by-2 matrices using discrete Fourier transform. Let

$$b_{0} = b_{\pm M} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad a_{1} = a_{1-M} = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}, \quad a_{-1} = a_{M-1} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

$$a_{k} = b_{k} = 0_{2} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \text{ for all other } k \text{ with } -M \leqslant k \leqslant M, \quad \mathbf{1}_{2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$
Then we have, when $M = 6$ for example,
$$2A = \begin{pmatrix} 0_{2} & a_{-1} & 0_{2} & 0_{2} & 0_{2} & a_{1} \\ a_{1} & 0_{2} & a_{-1} & 0_{2} & 0_{2} & 0_{2} \\ 0_{2} & a_{1} & 0_{2} & a_{-1} & 0_{2} & 0_{2} \\ 0_{2} & 0_{2} & a_{1} & 0_{2} & a_{-1} & 0_{2} \\ 0_{2} & 0_{2} & 0_{2} & a_{1} & 0_{2} & a_{-1} \\ a_{-1} & 0_{2} & 0_{2} & 0_{2} & a_{1} & 0_{2} \end{pmatrix}, \quad 2B = \begin{pmatrix} b_{0} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} \\ 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} \\ 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} \\ 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} \\ 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} \\ 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} \\ 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} \\ 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} & 0_{2} \\ 0_{2} & 0_{2}$$

$$\frac{2A_{2(k-1)+p,2(l-1)+q} = (\mathbf{a}_{k-l})_{p,q}}{2B_{2(k-1)+p,2(l-1)+q} = (\mathbf{b}_{k-l})_{p,q}} \right\} \qquad (k,l=1,\cdots,M,\ p,q=1,2).$$

Again we apply discrete Fourier transform by unitary similarity transform $\mathsf{U}:$

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

Then, as before for C,

$$2\hat{A}_{2(k-1)+p,2(k'-1)+q} = \sum_{l=1}^{M} \sum_{l'=1}^{M} \frac{e^{2\pi i k l/M}}{\sqrt{M}} (a_{l-l'})_{p,q} \frac{e^{-2\pi i l'k'/M}}{\sqrt{M}}$$
$$= \frac{1}{M} \sum_{l'=1}^{M} e^{2\pi i l'(k-k')/M} \sum_{l=1}^{M} e^{2\pi i k (l-l')/M} (a_{l-l'})_{p,q}$$
$$= \delta_{k,k'} \sum_{l=1}^{M} e^{2\pi i k l/M} (a_l)_{p,q} = \delta_{k,k'} \left(\hat{a}(\phi_k)\right)_{p,q}, \quad \phi_k = \frac{2\pi k}{M},$$

while

$$2\hat{\mathsf{B}}_{2(k-1)+p,2(k'-1)+q} = \delta_{k,k'} \sum_{l=1}^{M} e^{2\pi i k l/M} (\mathsf{b}_l)_{p,q} = \delta_{k,k'} \left(\hat{\mathsf{b}}(\phi_k) \right)_{p,q} = \delta_{k,k'} \left(\mathsf{b}_0 \right)_{p,q}.$$

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Both $\hat{\mathsf{A}}$ and $\hat{\mathsf{B}}$ are block diagonal with the 2-by-2 blocks

$$\hat{\mathsf{a}}(\phi_k) = e^{\mathrm{i}\phi_k} \mathsf{a}_1 + e^{-\mathrm{i}\phi_k} \mathsf{a}_{-1} = \begin{pmatrix} 0 & -e^{\mathrm{i}\phi_k} \\ e^{-\mathrm{i}\phi_k} & 0 \end{pmatrix} = -\mathrm{i}(\sin\phi_k)\sigma^x - \mathrm{i}(\cos\phi_k)\sigma^y,$$
$$\hat{\mathsf{b}}(\phi_k) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \mathrm{i}\,\sigma^y.$$
on the diagonal for $k = 1, \cdots, M$.

Now we are in a position to simplify the KMS property,

$$G_{j,i} = \left\langle \Gamma_j \Gamma_i \right\rangle = \left\langle \left(\mathsf{T}_1^{\frac{1}{2}} \mathsf{T}_2 \mathsf{T}_1^{\frac{1}{2}} \right)^{-N} \Gamma_i \left(\mathsf{T}_1^{\frac{1}{2}} \mathsf{T}_2 \mathsf{T}_1^{\frac{1}{2}} \right)^N \Gamma_j \right\rangle.$$

Remember that we had shown

$$\boldsymbol{\Gamma}(t) \equiv \mathrm{e}^{-t\boldsymbol{\Gamma}\cdot\boldsymbol{\mathsf{C}}\cdot\boldsymbol{\Gamma}} \,\boldsymbol{\Gamma} \,\mathrm{e}^{t\boldsymbol{\Gamma}\cdot\boldsymbol{\mathsf{C}}\cdot\boldsymbol{\Gamma}} = \mathrm{e}^{4t\boldsymbol{\mathsf{C}}}\cdot\boldsymbol{\Gamma},$$

Therefore,

$$\begin{cases} \mathsf{T}_2^{-1}\Gamma\mathsf{T}_2 = \mathrm{e}^{-\mathrm{i}K\,\Gamma\cdot\mathsf{A}\cdot\Gamma}\,\Gamma\,\mathrm{e}^{\mathrm{i}K\,\Gamma\cdot\mathsf{A}\cdot\Gamma} = \mathrm{e}^{4\mathrm{i}K\mathsf{A}}\cdot\Gamma,\\ \mathsf{T}_1^{-1}\Gamma\mathsf{T}_1 = \mathrm{e}^{-\mathrm{i}K^*\Gamma\cdot\mathsf{B}\cdot\Gamma}\,\Gamma\,\mathrm{e}^{\mathrm{i}K^*\Gamma\cdot\mathsf{B}\cdot\Gamma} = \mathrm{e}^{4\mathrm{i}K^*\mathsf{B}}\cdot\Gamma\end{cases}$$

as the factor $(2\sinh(2K'))^{M/2}$ in T_1 cancels out.

Therefore,

$$\left(\mathsf{T}_{1}^{\frac{1}{2}}\mathsf{T}_{2}\mathsf{T}_{1}^{\frac{1}{2}}\right)^{-N}\boldsymbol{\Gamma}\left(\mathsf{T}_{1}^{\frac{1}{2}}\mathsf{T}_{2}\mathsf{T}_{1}^{\frac{1}{2}}\right)^{N} = \left(\mathrm{e}^{2\mathrm{i}K^{*}\mathsf{B}}\mathrm{e}^{4\mathrm{i}K\mathsf{A}}\mathrm{e}^{2\mathrm{i}K^{*}\mathsf{B}}\right)^{N}\cdot\boldsymbol{\Gamma},$$

and using

$$2\delta_{i,j} = \left\langle \Gamma_i \Gamma_j \right\rangle + \left\langle \Gamma_j \Gamma_i \right\rangle = \left\langle \Gamma_i \Gamma_j \right\rangle + \left\langle \left(\mathsf{T}_1^{\frac{1}{2}} \mathsf{T}_2 \mathsf{T}_1^{\frac{1}{2}} \right)^{-N} \Gamma_i \left(\mathsf{T}_1^{\frac{1}{2}} \mathsf{T}_2 \mathsf{T}_1^{\frac{1}{2}} \right)^N \Gamma_j \right\rangle,$$

we arrive at

$$\langle \mathbf{\Gamma} \mathbf{\Gamma} \rangle = 2 \left(\mathbf{1} + \left(e^{2iK^*\mathsf{B}} e^{4iK\mathsf{A}} e^{2iK^*\mathsf{B}} \right)^N \right)^{-1}$$

Taking the block-Fourier transformation with U we get

$$\langle \widehat{\mathbf{\Gamma} \mathbf{\Gamma}} \rangle \equiv \mathsf{U} \langle \mathbf{\Gamma} \mathbf{\Gamma} \rangle \mathsf{U}^{-1} = 2 \left(\mathbf{1} + \left(\mathrm{e}^{2\mathrm{i}K^*\hat{\mathsf{B}}} \mathrm{e}^{4\mathrm{i}K\hat{\mathsf{A}}} \mathrm{e}^{2\mathrm{i}K^*\hat{\mathsf{B}}} \right)^N \right)^{-1},$$

which is block-diagonal with 2-by-2 blocks

$$\left\langle \widehat{\mathbf{\Gamma}\mathbf{\Gamma}} \right\rangle (\phi_k) = 2 \left(\mathbf{1} + \left(\mathrm{e}^{2\mathrm{i}K^* \hat{\mathsf{b}}(\phi_k)} \mathrm{e}^{4\mathrm{i}K \hat{\mathsf{a}}(\phi_k)} \mathrm{e}^{2\mathrm{i}K^* \hat{\mathsf{b}}(\phi_k)} \right)^N \right)^{-1}$$

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It takes a little algebra here:

$$e^{2iK^*\hat{b}(\phi_k)}e^{4iK\hat{a}(\phi_k)}e^{2iK^*\hat{b}(\phi_k)} = e^{-K^*\sigma^y}e^{2K(\sigma^x\sin\phi_k + \sigma^y\cos\phi_k)}e^{-K^*\sigma^y} = (\cosh K^* - \sigma^y\sinh K^*)(\cosh 2K + (\sigma^x\sin\phi_k + \sigma^y\cos\phi_k)\sinh 2K)(\cosh K^* - \sigma^y\sinh K^*) = (\cosh 2K\cosh 2K^* - \sinh 2K\sinh 2K^*\cos\phi_k) + \sigma^x\sinh 2K\sin(\phi_k) - \sigma^y(\cosh 2K\sinh 2K^* - \sinh 2K\cosh 2K^*\cos\phi_k) + \sigma^x\sinh 2K\sin(\phi_k) = \cosh \gamma_k + \sinh \gamma_k(\sigma^x\sin\delta_k - \sigma^y\cos\delta_k) = e^{\gamma_k(\sigma^x\sin\delta_k - \sigma^y\cos\delta_k)},$$

where †

$$\cosh \gamma_k = \cosh 2K \cosh 2K^* - \sinh 2K \sinh 2K^* \cos \phi_k,$$

$$\sinh \gamma_k \sin \delta_k = \sinh 2K \sin(\phi_k),$$

$$\sinh \gamma_k \cos \delta_k = \cosh 2K \sinh 2K^* - \sinh 2K \cosh 2K^* \cos \phi_k$$

[†] Compare eq. (89) of L. Onsager, Phys. Rev. **65**, 117–149 (1944), and eqs. (51) and (52) of B. Kaufman, Phys. Rev. **76** 1232–1243 (1949).

Putting this result into the blocks of $\langle \widehat{\Gamma \Gamma} \rangle$ we get

$$\langle \widehat{\mathbf{\Gamma}} \widehat{\mathbf{\Gamma}} \rangle (\phi_k) = 2 \left(\mathbf{1} + e^{N\gamma_k (\sigma^x \sin \delta_k - \sigma^y \cos \delta_k)} \right)^{-1}$$

= $\mathbf{1} + \tanh \left[N\gamma_k (\sigma^x \sin \delta_k - \sigma^y \cos \delta_k) \right]$
= $\mathbf{1} + (\sigma^x \sin \delta_k - \sigma^y \cos \delta_k) \tanh(N\gamma_k).$

Thus, in the thermodynamic limit we have $N \to \infty$ and thus we find

$$\langle \Gamma \Gamma \rangle (\phi_k) = \mathbf{1} + (\sigma^x \sin \delta_k - \sigma^y \cos \delta_k),$$

where

$$\tan \delta_k = \frac{\sinh 2K \sin(\phi_k)}{\cosh 2K \sinh 2K^* - \sinh 2K \cosh 2K^* \cos \phi_k}$$

From this result $\langle \Gamma \Gamma \rangle$ is obtained by inverse Fourier transform, which in the limit $M \to \infty$ turns into the well-known Fourier integral with a square root, as

$$\langle \widehat{\mathbf{\Gamma}} \widehat{\mathbf{\Gamma}} \rangle (\phi_k) = \mathbf{1} + \frac{\sigma^x \tan \delta_k - \sigma^y}{\sqrt{1 + \tan^2 \delta_k}}.$$

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More precisely,*

$$\begin{aligned} \mathsf{G}_{2(k-1)+p,2(k'-1)+q} &= \left\langle \Gamma_{2(k-1)+p} \Gamma_{2(k'-1)+q} \right\rangle \\ &= \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\phi \,\mathrm{e}^{\mathrm{i}(k'-k)\phi} \left(\left\langle \widehat{\mathbf{\Gamma} \mathbf{\Gamma}} \right\rangle(\phi_k) \right)_{p,q}. \end{aligned}$$

with

$$\langle \widehat{\mathbf{\Gamma} \mathbf{\Gamma}} \rangle (\phi_k) = \begin{pmatrix} 1 & \mathrm{i} \, \mathrm{e}^{-\mathrm{i} \delta_k} \\ -\mathrm{i} \, \mathrm{e}^{\mathrm{i} \delta_k} & 1 \end{pmatrix}.$$

Besides this result for the equal-row pair correlation of Γ 's, we also need a result with the two Γ 's in different rows. This then allows us to calculate the internal energy per site. After that, we can continue as for the transverse-field Ising chain (and the more general XY chain which we did not do).

^{*} A variation of the method presented here was used for the 'Bariev' problem with one line of horizontal couplings modified, see B.M. McCoy and J.H.H. Perk, "Continuous exponents of spin correlation functions of inhomogeneous layered Ising models," Lecture Notes in Mathematics, Vol. 925, (Springer, Berlin, 1982), pp. 12–27.

<u>Remarks</u>:

- Since we worked with periodic boundary conditions, we had to deal with the complication of the operator P involving the product of all Gamma operators. For the calculations done we could replace \mathcal{H} and T by their fermion-cyclic versions \mathcal{H}_c and T_c , which is only valid in the limit $M \to \infty$.
- For finite M we have to work with both the fermion-cyclic and fermionanticyclic versions of \mathcal{H} and T , as done first by Kaufman in 1949. Then all traces have to be replaced by half the sum of four traces, as we work with the two projection operators $\frac{1}{2}(\mathbf{1} \pm \mathsf{P})$.
- If we use open boundary conditions in the horizontal direction, putting the system on a cylinder rather than a torus, we do not have the operator P. But then we lose translation invariance, which is only restored in the bulk after taking the thermodynamic limit. Closer to the boundaries we then have boundary effects.
- With open boundary conditions we can still use the methods used for the periodic system, provided we find the proper modification of the discrete block-Fourier transform.

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Modification for open boundary condition, bosonic case

Let us introduce the function

$$S(j,k) \equiv \sqrt{\frac{2}{M+1}} \sin\left(\frac{\pi jk}{M+1}\right) = S(k,j).$$

Then,

$$\begin{split} &\sum_{k=1}^{M} S(j,k) S(j',k) = \delta_{j,j'}, \\ &\sum_{k=1}^{M-1} [S(j,k) S(j',k+1) + S(j,k+1) S(j',k)] = 2\delta_{j,j'} \cos\left(\frac{\pi j}{M+1}\right), \end{split}$$

etc. We can then do the discrete block-Fourier-sine transform in certain bosonic cases. Its inverse now has the identical form.

Note that this involved a 'replacement' $M \to M + 1$.

The different fundamental operators

Consider one square of the 2d Ising model and the objects we want to define in it within the transfer matrix formalism:

At the four corners live four spin operators; in the center a dual spin on the dual lattice; and connecting these are four fermion operators. Let now

$$\mathsf{T} = \mathsf{T}_2^{1/2} \mathsf{T}_1 \mathsf{T}_2^{1/2}.$$

Then, in the transfer matrix formalism, we can associate

$$\sigma_{m,n} \longrightarrow \mathsf{T}^n \sigma_m^x \mathsf{T}^{-n} = \mathsf{T}^n \mathsf{T}_2^{\pm 1/2} \sigma_m^x \mathsf{T}_2^{\pm 1/2} \mathsf{T}^{-n},$$

as T_2 commutes with σ_m^x .

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Remember the Jordan–Wigner transformation:

$$\sigma_j^x = \begin{bmatrix} j^{-1}(i\Gamma_{2k-1}\Gamma_{2k}) \\ k=1 \end{bmatrix} \Gamma_{2j-1}, \quad \sigma_j^y = \begin{bmatrix} j^{-1}(i\Gamma_{2k-1}\Gamma_{2k}) \\ k=1 \end{bmatrix} \Gamma_{2j}, \quad \sigma_j^z = -i\Gamma_{2j-1}\Gamma_{2j}$$

We can define dual spin operators

$$\sigma_j^{*x} = \left[\prod_{k=0}^{j-1} (i\,\Gamma_{2k}\Gamma_{2k+1})\right] \Gamma_{2j}, \quad \sigma_j^{*y} = \left[\prod_{k=0}^{j-1} (i\,\Gamma_{2k}\Gamma_{2k+1})\right] \Gamma_{2j+1}, \quad \sigma_j^{*z} = -i\,\Gamma_{2j}\Gamma_{2j+1},$$

introducing an extra 'ghost' operator Γ_0 . This allows us to identify

$$\mu_{m+\frac{1}{2},n+\frac{1}{2}} \longrightarrow \mathsf{T}^{n}\mathsf{T}_{2}^{1/2}\mathsf{T}_{1}^{1/2}\sigma_{m}^{*x}\mathsf{T}_{1}^{-1/2}\mathsf{T}_{2}^{-1/2}\mathsf{T}^{-n},$$

transferring it half a row up further than $\sigma_{m,n}$.

The four Gamma's in the square can also be similarly defined, e.g.

$$\Gamma_{m+\frac{1}{4},n+\frac{1}{4}},\ \Gamma_{m+\frac{3}{4},n+\frac{1}{4}} \longrightarrow \mathsf{T}^{n}\mathsf{T}_{2}^{1/2}\Gamma_{2m}\mathsf{T}_{2}^{-1/2}\mathsf{T}^{-n},\ \mathsf{T}^{n}\mathsf{T}_{2}^{1/2}\Gamma_{2m+1}\mathsf{T}_{2}^{-1/2}\mathsf{T}^{-n}.$$

Comparing we find the duality relations

$$\sigma_{j}^{x}\sigma_{j+1}^{x} = -\sigma_{j}^{*z}, \qquad \sigma_{j}^{*x}\sigma_{j+1}^{*x} = -\sigma_{j+1}^{z},$$

where one also can remove the two minuses using slightly different definitions.⁺

In fermion language we just have $\Gamma_j \to \Gamma_{j+1}$ giving the duality transformation, connecting the high-and low-temperature regimes of the 2d Ising model.

For the Ising chain in transverse field,

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

transforms to

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

+ For example, we can use a different representation of the Pauli matrices, rotating $\vec{\sigma}_j = (\sigma_j^x, \sigma_j^y, \sigma_j^z)$ 180° about the *x*-axis for odd *j* and 180° about the *y*-axis for even *j*.

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With the two-dimensional picture we can do a lot more. Look at

$$\begin{split} & \Gamma_{m+\frac{1}{4},n+\frac{3}{4}} & \longrightarrow & \mathsf{T}^{n}\mathsf{T}_{2}^{1/2}\mathsf{T}_{1}\Gamma_{2m}\mathsf{T}_{1}^{-1}\mathsf{T}_{2}^{-1/2}\mathsf{T}^{-n}, \\ & \Gamma_{m-\frac{1}{4},n+\frac{3}{4}} & \longrightarrow & \mathsf{T}^{n}\mathsf{T}_{2}^{1/2}\mathsf{T}_{1}\Gamma_{2m-1}\mathsf{T}_{1}^{-1}\mathsf{T}_{2}^{-1/2}\mathsf{T}^{-n}. \end{split}$$

Now

$$\begin{aligned} \mathsf{T}_{1}\Gamma_{2m}\mathsf{T}_{1}^{-1} &= \mathrm{e}^{\mathrm{i}K'^{*}\Gamma_{2m-1}\Gamma_{2m}}\Gamma_{2m}\mathrm{e}^{-\mathrm{i}K'^{*}\Gamma_{2m-1}\Gamma_{2m}}\\ &= \mathrm{e}^{2\mathrm{i}K'^{*}\Gamma_{2m-1}\Gamma_{2m}}\Gamma_{2m}\\ &= \left(\cosh(2K'^{*}) + \mathrm{i}\Gamma_{2m-1}\Gamma_{2m}\sinh(2K'^{*})\right)\Gamma_{2m}, \end{aligned}$$

or

$$\mathsf{T}_{1}\Gamma_{2m}\mathsf{T}_{1}^{-1} = \cosh(2K'^{*})\Gamma_{2m} + \mathrm{i}\sinh(2K'^{*})\Gamma_{2m-1},$$

$$\mathsf{T}_{1}\Gamma_{2m-1}\mathsf{T}_{1}^{-1} = \cosh(2K'^{*})\Gamma_{2m-1} - \mathrm{i}\sinh(2K'^{*})\Gamma_{2m}.$$

With such relations we can express the Γ 's in one row in terms of those in another row. Applying this and $[\mathsf{T}_1, \mathsf{i}\,\Gamma_{2k-1}\Gamma_{2k}] = 0$, we find

$$\begin{split} \mathsf{T}_1 \sigma_m^x \mathsf{T}_1^{-1} &= \mathsf{T}_1 \left[\prod_{k=1}^{m-1} (\mathrm{i}\,\Gamma_{2k-1}\Gamma_{2k}) \right] \mathsf{T}_1^{-1} \big(\mathsf{T}_1 \Gamma_{2m-1} \mathsf{T}_1^{-1} \big) \\ &= \cosh(2K'^*) \sigma_m^x - \mathrm{i} \sinh(2K'^*) \sigma_m^y. \end{split}$$

We are now in a situation to apply the general Wick theorem to $\langle \sigma_{m+1,n} \sigma_{m'+1,n'} \rangle$. Let us introduce the notations

$$C(m,n) = \langle \sigma_{p,q} \sigma_{p+m,q+n} \rangle, \qquad C^*(m,n) = \langle \sigma^*_{p,q} \sigma^*_{p+m,q+n} \rangle,$$

where $C^*(m, n)$ is the value of C(m, n) at the dual temperature. These notations explicitly use translational invariance.

Then we can derive the equations

$$\sinh^{2}(2K)[C(m+1,n)C(m-1,n) - C(m,n)^{2}] + [C^{*}(m,n+1)C^{*}(m,n-1) - C^{*}(m,n)^{2}] = 0,$$

$$\sinh^{2}(2K')[C(m,n+1)C(m,n-1) - C(m,n)^{2}] + [C^{*}(m+1,n)C^{*}(m-1,n) - C^{*}(m,n)^{2}] = 0.$$

From such equations one can calculate many pair correlations by iteration, using results only on special lines, for which we have other recurrences. (See, e.g., Y. Chan, A.J. Guttmann, B.G. Nickel and J.H.H. Perk, J. Stat. Phys. **145**, 549–590 (2011) [arXiv:1012.5272] and references cited.)

To derive one of these quadratic recurrence relations we start with $\langle \sigma_{m+1,n} \sigma_{m'+1,n'} \rangle$ with $n' \ge n$, which can be expressed in the transfer matrix formalism as:

$$C(m'-m,n'-n) = \langle \sigma_{m+1}^{x}(\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n}\sigma_{m'+1}^{x}(\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'} \rangle = \langle \sigma_{m}^{x}(\mathrm{i}\,\Gamma_{2m}\Gamma_{2m+1})(\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n}\sigma_{m'}^{x}(\mathrm{i}\,\Gamma_{2m'}\Gamma_{2m'+1})(\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'} \rangle.$$

From the general Wick theorem we then have

$$\langle \sigma_{m}^{x}(i\Gamma_{2m}\Gamma_{2m+1})(\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n}\sigma_{m'}^{x}(i\Gamma_{2m'}\Gamma_{2m'+1})(\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'}\rangle \times \langle \sigma_{m}^{x}i(\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n}\sigma_{m'}^{x}i(\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'}\rangle = \langle \sigma_{m}^{x}(i\Gamma_{2m}\Gamma_{2m+1})(\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n}\sigma_{m'}^{x}i(\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'}\rangle \times \langle \sigma_{m}^{x}i(\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n}\sigma_{m'}^{x}(i\Gamma_{2m'}\Gamma_{2m'+1})(\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'}\rangle - \langle \sigma_{m}^{x}(i\Gamma_{2m})(\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n}\sigma_{m'}^{x}(i\Gamma_{2m'})(\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'}\rangle \times \langle \sigma_{m}^{x}(i\Gamma_{2m+1})(\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n}\sigma_{m'}^{x}(i\Gamma_{2m'+1})(\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'}\rangle + \langle \sigma_{m}^{x}(i\Gamma_{2m})(\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n}\sigma_{m'}^{x}(i\Gamma_{2m'+1})(\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'}\rangle \times \langle \sigma_{m}^{x}(i\Gamma_{2m+1})(\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n}\sigma_{m'}^{x}(i\Gamma_{2m'})(\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'}\rangle,$$

or

$$- \langle \sigma_{m+1}^{x} (\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n} \sigma_{m'+1}^{x} (\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'} \rangle \langle \sigma_{m}^{x} (\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n} \sigma_{m'}^{x} (\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'} \rangle = - \langle \sigma_{m+1}^{x} (\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n} \sigma_{m'}^{x} (\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'} \rangle \langle \sigma_{m}^{x} (\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n} \sigma_{m'+1}^{x} (\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'} \rangle - \langle \sigma_{m}^{*x} (\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n} \sigma_{m'}^{*x} (\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'} \rangle \langle \sigma_{m}^{*y} (\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n} \sigma_{m'}^{*y} (\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'} \rangle + \langle \sigma_{m}^{*x} (\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n} \sigma_{m'}^{*y} (\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'} \rangle \langle \sigma_{m}^{*y} (\mathsf{T}_{2}\mathsf{T}_{1})^{n'-n} \sigma_{m'}^{*x} (\mathsf{T}_{2}\mathsf{T}_{1})^{n-n'} \rangle.$$

One can easily derive

$$(\mathsf{T}_{2}\mathsf{T}_{1})\sigma_{m}^{*x}(\mathsf{T}_{2}\mathsf{T}_{1})^{-1} = \mathsf{T}_{2}\sigma_{m}^{*x}\mathsf{T}_{2}^{-1}$$

$$= \mathsf{T}_{2} \left[\prod_{k=0}^{m-1} (i\,\Gamma_{2k}\Gamma_{2k+1})\right] \mathsf{T}_{2}^{-1} (\mathsf{T}_{2}\Gamma_{2m}\mathsf{T}_{2}^{-1})$$

$$= \left[\prod_{k=0}^{m-1} (i\,\Gamma_{2k}\Gamma_{2k+1})\right] (\cosh(2K)\Gamma_{2m} - i\sinh(2K)\Gamma_{2m+1})$$

$$= \cosh(2K)\sigma_{m}^{*x} - i\sinh(2K)\sigma_{m}^{*y}.$$

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If we now multiply (*) by $(i \sinh(2K))^2$ and eliminate σ_m^{*y} from it, we get

$$\sinh^{2}(2K) C(m'-m,n'-n)^{2} = \sinh^{2}(2K) C(m'-m+1,n'-n)C(m'-m-1,n'-n) - C^{*}(m'-m,n'-n)[2C^{*}(m'-m,n'-n) - C^{*}(m'-m,n'-n+1) - C^{*}(m'-m,n'-n-1)]] [C^{*}(m'-m,n'-n) - C^{*}(m'-m,n'-n-1)] [C^{*}(m'-m,n'-n) - C^{*}(m'-m,n'-n+1)].$$

We arrive thus at

$$\sinh^2(2K)[C(m+1,n)C(m-1,n) - C(m,n)^2] + [C^*(m,n+1)C^*(m,n-1) - C^*(m,n)^2] = 0.$$

Many more equations can be derived and much more can be said, but time is up. Some more information can be found from my papers listed at my website at http://physics.okstate.edu/perk/vperk.html .