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Boundary conditions subtleties in plaquette spin models (and the $1d$ Ising model)

Marco Müller[1], Wolfhard Janke[1], Desmond A. Johnston[2]

[1] Institut für Theoretische Physik, Universität Leipzig, Germany

[2] Department of Mathematics, Heriot-Watt University, Edinburgh, United Kingdom

Outline

We explore the use of a product spin transformation

$$\tau_1 = \sigma_1 \sigma_2$$

where $\sigma_{1,2}$ are adjacent spins at both ends of a bond, in solving the standard nearest-neighbour $1d$ Ising model and plaquette Ising models (1, 2, 3) in $2d$ and $3d$.

The exact solutions facilitated by this transformation highlight the role of boundary conditions in inducing correlations in the case of periodic boundaries and their potential impact on finite-size scaling (4).

$1d$ Ising, free BCs

- Free boundary conditions, partition function

$$Z_{1d,\,\text{free}} = \sum_{\{\sigma\}} \exp\left(\beta \sum_{i=1}^{L-1} \sigma_i \sigma_{i+1}\right)$$

- Evaluate using the variable transformation

$$\{\sigma_1, \sigma_2, \ldots \sigma_L\} \to \{\tau_1, \tau_2, \ldots \tau_L\}$$

where in this case

$$\tau_1 = \sigma_1\sigma_2,\ \tau_2 = \sigma_2\sigma_3,\ \ldots,\ \tau_{L-1} = \sigma_{L-1}\sigma_L$$

- Setting $\tau_L = \sigma_L$ the mapping $\{\sigma\} \to \{\tau\}$ is one-to-one.
- This allows us to write Z in factorized form as

$$Z_{1d,\,\text{free}} = \sum_{\{\tau\}} \exp\left(\beta \sum_{i=1}^{L-1} \tau_i\right)$$

- May then trivially be evaluated to give

$$Z_{1d,\,\text{free}} = 2 \prod_{i=1}^{L-1} \sum_{\tau_i = \pm 1} \exp(\beta \tau_i) = 2(2\,\mathrm{ch}(\beta))^{L-1}$$

$1d$ Ising, periodic BCs

- Periodic BCs $\implies$ the constraint

$$\prod_{i=1}^{L} \tau_i = \prod_{i=1}^{L} \sigma_i^2 = 1$$

must be imposed on the τ-variables.

- This can be implemented in the partition function as

$$Z_{1d,\,\text{periodic}} = \sum_{\{\tau\}} \exp\left(\beta \sum_{i=1}^{L} \tau_i\right)\left(1 + \prod_{i=1}^{L} \tau_i\right)$$

- Giving

$$\begin{aligned} Z_{1d,\,\text{periodic}} &= \left[\prod_{i=1}^{L} \sum_{\tau_i = \pm 1} \exp(\beta\tau_i) + \prod_{i=1}^{L} \sum_{\tau_i = \pm 1} \tau_i \exp(\beta\tau_i)\right] \\ &= 2^L \left[\mathrm{ch}(\beta)^L + \mathrm{sh}(\beta)^L\right] \\ &= 2^L\,\mathrm{ch}(\beta)^L \left[1 + \mathrm{th}(\beta)^L\right] \end{aligned}$$

- This is the well known result for periodic BCs, usually obtained via a transfer matrix calculation.
- The constraint arising from PBCs induces an additional $\mathrm{th}(\beta)^L$

$2d$ Plaquette, free+various BCs

- $L_x \times L_y$ lattice, free boundaries in the y-direction
- Define $\tau_{x,y} = \sigma_{x,y}\sigma_{x,y+1}$, with the condition $\tau_{x,L_y} = \sigma_{x,L_y}$
- Free boundaries in x-direction also

$$\begin{aligned} Z_{\text{free, free}} &= \sum_{\{\sigma\}} \exp\left(\beta \sum_{x=1}^{L_x-1} \sum_{y=1}^{L_y-1} \sigma_{x,y}\sigma_{x,y+1}\sigma_{x+1,y}\sigma_{x+1,y+1}\right) \\ &= \sum_{\{\tau\}} \exp\left(\beta \sum_{x=1}^{L_x-1} \sum_{y=1}^{L_y-1} \tau_{x,y}\tau_{x+1,y}\right) \\ &= 2^{L_x}(Z_{1d,\,\text{Ising}})^{L_y-1} \end{aligned}$$

- Using the free boundary $1d$ solution

$$Z_{\text{free, free}} = 2^{L_x L_y}\,\mathrm{ch}(\beta)^{(L_x-1)(L_y-1)}$$

- Periodic boundary conditions in x-direction

$$\begin{aligned} Z_{\text{free, periodic}} &= 2^{L_x L_y}\,\mathrm{ch}(\beta)^{L_x(L_y-1)} \left(1 + \mathrm{th}(\beta)^{L_x}\right)^{L_y-1} \\ &= 2^{L_x L_y}\,\mathrm{ch}(\beta)^{L_x(L_y-1)} \sum_{h=0}^{L_y-1} \binom{L_y-1}{h} \mathrm{th}(\beta)^{L_x h} \end{aligned}$$

- Free and periodic BCs equivalent in thermodynamic limit, but finite-size corrections differ (as with $1d$ ising)

$2d$ Plaquette, periodic+periodic BCs

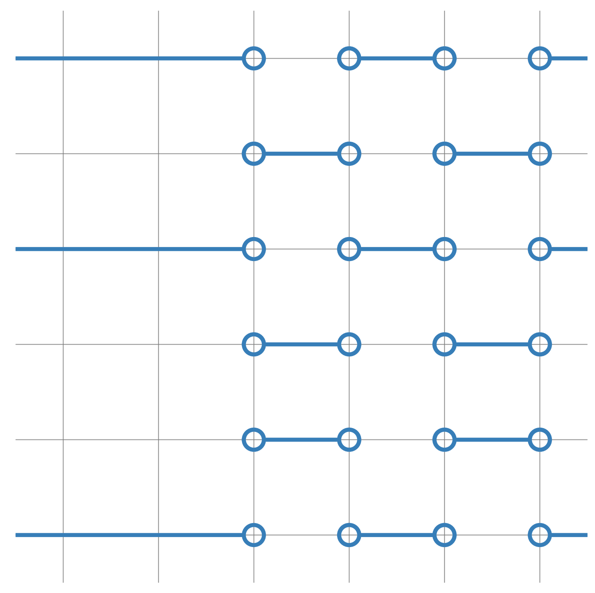
- Transformation $\tau_{x,y} = \sigma_{x,y}\sigma_{x,y+1}$ imposes the L_x constraints $\prod_y \tau_{x,y} = 1$
- Partition function is now

$$\begin{aligned} Z &= \sum_{\{\sigma\}} \exp\left(\beta \sum_{x=1}^{L_x} \sum_{y=1}^{L_y} \sigma_{x,y}\sigma_{x,y+1}\sigma_{x+1,y}\sigma_{x+1,y+1}\right) \\ &= 2^{L_x} \sum_{\{\tau\}} \exp\left(\beta \sum_{x=1}^{L_x} \sum_{y=1}^{L_y} \tau_{x,y}\tau_{x+1,y}\right) \prod_{x=1}^{L_x} \delta\left(\prod_{y=1}^{L_y} \tau_{x,y}, 1\right) \end{aligned}$$

- Convenient to use high-T expansion

$$\begin{aligned} Z &= 2^{L_x}\,\mathrm{ch}(\beta)^{L_x L_y} \sum_{\{\tau\}} \left[\prod_{y=1}^{L_y} \prod_{x=1}^{L_x} \left(1 + \mathrm{th}(\beta)\,\tau_{x,y}\tau_{x+1,y}\right)\right] \\ &\times \prod_{x=1}^{L_x} \delta\left(\prod_{y=1}^{L_y} \tau_{x,y}, 1\right) \end{aligned}$$

- Graphically the factors of $\mathrm{th}(\beta)\tau_{x,y}\tau_{x+1,y}$, which appear when expanding the product are represented as horizontal dimers.



- Gaps in the filled rows of dimers may also be present due to δ's Both a horizontal configuration of dimers and its "dual", where shaded and unshaded bonds are swapped, may appear.
- Gives (4):

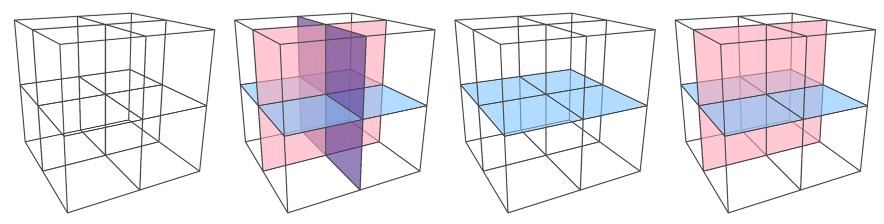
$$Z = \left(\frac{1}{2}\right) 2^{L_x L_y}\,\mathrm{ch}(\beta)^{L_x L_y} \sum_{v=0}^{L_x} \binom{L_x}{v} \left(\mathrm{th}(\beta)^v + \mathrm{th}(\beta)^{L_x - v}\right)^{L_y}$$

$3d$ Plaquette

- **Isotropic** Hamiltonian:

$$\mathcal{H} = -\frac{1}{2} \sum_{\square} \sigma\sigma\sigma\sigma$$

- Zero-temperature: elementary ground state composed of:



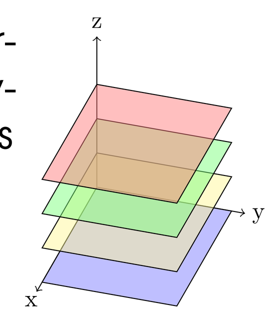
- Flip of whole planes parallel to either one of the xy, yz, zx-planes allowed
- Strong first-order phase transition (3)

$3d$ Plaquette, anisotropic

- **Anisotropic** variant no interaction in z-direction, so-called "Fuki-Nuke" model (1):

$$\mathcal{H} = -\frac{1}{2}\left(\sum_{\square_{xz}} \sigma\sigma\sigma\sigma + \sum_{\square_{yz}} \sigma\sigma\sigma\sigma\right)$$

- Also solvable by the transformation $\tau = \sigma\sigma$, reduces to layers of standard $2d$ Ising models



- Free BCs in z-direction

$$\begin{aligned} Z &= 2^{L^2} \prod_{z=1}^{L_z-1} \sum_{\{\tau_{x,y,z \neq L_z}\}} \exp\left(\beta \sum_{x=1}^{L} \sum_{y=1}^{L} \left(\tau_{x,y,z}\tau_{x+1,y,z} + \tau_{x,y,z}\tau_{x,y+1,z}\right)\right) \\ &= 2^{L^2} \prod_{z=1}^{L_z-1} Z_{2d\text{ Ising}} = 2^{L^2} \left(Z_{2d\text{ Ising}}\right)^{L_z-1} \end{aligned}$$

- Periodic BCs in z-direction induce correlations

$$Z = \sum_{\{\tau\}} \exp\left(-\beta\mathcal{H}(\{\tau\})\right) \prod_{x=1}^{L} \prod_{y=1}^{L} \left(1 + \prod_{z=1}^{L_z} \tau_{x,y,z}\right)$$

- Gives additional 1-point correlations C_1 (and higher) by comparison with free boundaries (4):

$$Z = \left(Z_{2d,\,\text{Ising}}\right)^{L_z} \left(1 + C_1^{L_z} + \ldots\right)$$

Conclusions

The key point to be drawn from the various exact solutions discussed here is that correlations may be induced in finite systems as a consequence of the choice of boundary conditions.

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