2D Ising model – 2 × 2 with periodic boundary conditions

configurations — bonds — Energy (form $\sum_{\langle ij \rangle}^{NN} -\frac{1}{2} J \hat{S}_i \hat{S}_j$)

+ +
+ +

bonds:
+ + + +
+ + + +
+ + + +
+ + + +

$-8J$ $(M = 4)$

− +
+ +

bonds:
− − − −
+ + − −
− − + +
+ + + +

0 — 4× degenerate $(M = 2)$

equivalent to

+ −
+ +

+ +
− +

+ +
+ −

− −
+ +

bonds:
+ + − −
+ + − −
+ + − −
+ + − −

0 — 4× degenerate $(M = 0)$

equivalent to

+ +
− −

− +
− +

+ −
+ −

+ −
− +

bonds:
− − − −
− − − −
− − − −
− − − −

$+8J$ — 2× degenerate $(M = 0)$

equivalent to

− +
+ −

we then have:

~~M~~	~~E~~	~~Ω~~
~~4~~	~~$-8J$~~	~~1~~
~~0~~	~~0~~	~~4~~
~~0~~	~~$8J$~~	~~2~~

M	E	Ω
4	$-8J$	1
2	0	4
0	0	4
0	$8J$	2
−2	0	4
−4	$-8J$	1

(symmetry)

2 × 2 PBC

evaluating the partition function $Z = \sum_{\eta} e^{-\beta E_\eta}$

(η = states) $\beta = 1/k_B T$

$$Z = e^{8\beta J} + 4 + 4 + 2e^{-8\beta J} + 4 + e^{8\beta J}$$

$$= 12 + 2\left(e^{8\beta J} + e^{-8\beta J}\right)$$

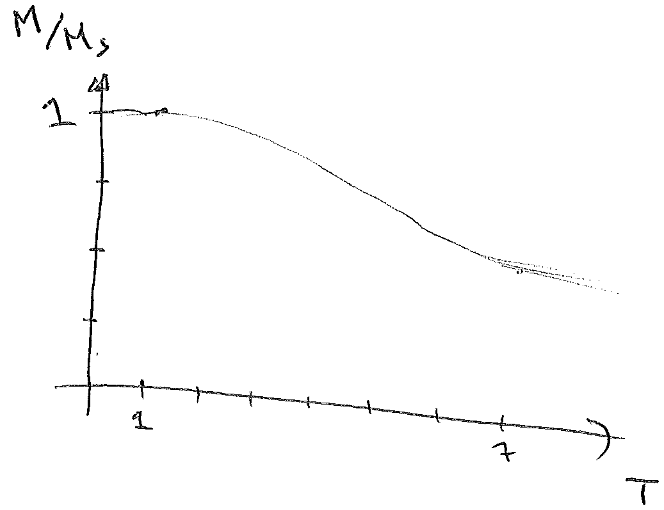
average absolute magnetization, $\langle |M| \rangle = \sum_{\eta} |M_\eta| e^{-\beta E_\eta} / Z$

$$\langle |M| \rangle = \left(4e^{8\beta J} + 4 \times 2 + 4 \times 2 + 4e^{8\beta J}\right) / Z$$

$$= \frac{16 + 8e^{8\beta J}}{12 + 2\left(e^{8\beta J} + e^{-8\beta J}\right)}$$

Temperature in units of J/k_B ; $J = 1$ (J in units of J)

T	$\langle \lvert M \rvert \rangle$
0,1	~ 4
1	~ 4
1,5	3,92
2	3,73
2,5	3,47
3	3,20
3,5	2,97
4	2,78
5	2,49
6	2,30
7	2,17



2 × 2 Ising model with PBC

Free energy $F = E - TS$

$S = k_B \log Z(M,T)$

for zero energy ; $S = k_B \log \Omega$

- for each M value, calculate Z, and then F expression

M	E	Ω	Z	F
4	$-8J$	1	$e^{8\beta J}$	$-8J$
2	0	4	4	$-T \ln 4$
0	0	4	$4 + 2e^{-8\beta J}$	$-T \ln [4 + 2e^{-8J\beta}]$
0	$8J$	2		
-2	0	4	4	$-T \ln 4$
-4	$-8J$	1	$e^{8\beta J}$	$-8J$

F(M) for T = 1 (J = 1); (k_B = 1)

M	F(M)
4	-8
2	1,3863
0	1,3865
-2	1,3863
4	~~[illegible]~~ -8

minimum free energy

T = 7

M	F(M)
4	-8
2	-9,70
0	-10,74
-2	-9,70
4	-8J

minimum free energy

2D Ising model – 2x2 no periodic boundary conditions

configurations | bonds | Energy (from $\sum_{i\neq j}^{NN} -\frac{1}{2} J \hat{S}_i \hat{S}_j$)

$$\begin{matrix} + & + \\ + & + \end{matrix} \qquad \begin{matrix} + & + \\ + & + \\ + & + \\ + & + \end{matrix} \qquad -4J \qquad (M=4)$$

$$\begin{matrix} - & + \\ + & + \end{matrix} \qquad \begin{matrix} - & - \\ - & + \\ + & - \\ + & + \end{matrix} \qquad 0$$

equivalent to $\begin{matrix} + & - \\ + & + \end{matrix} \quad \begin{matrix} + & + \\ - & + \end{matrix} \quad \begin{matrix} + & + \\ + & - \end{matrix}$

4x degenerate (M = 2)

$$\begin{matrix} - & - \\ + & + \end{matrix} \qquad \begin{matrix} + & - \\ + & - \\ + & - \\ + & - \end{matrix} \qquad 0$$

equivalent to $\begin{matrix} + & + \\ - & - \end{matrix} \quad \begin{matrix} - & + \\ - & + \end{matrix} \quad \begin{matrix} + & - \\ + & - \end{matrix}$

4x degenerate (M=0)

$$\begin{matrix} + & - \\ - & + \end{matrix} \qquad \begin{matrix} - & - \\ - & - \\ - & - \\ - & - \end{matrix} \qquad +4J$$

equivalent to $\begin{matrix} - & + \\ + & - \end{matrix}$

2x degenerate (M=0)

we then have:

M	E	Ω
4	-4J	1
2	0	4
0	0	4
0	4J	2
-2	0	4
-4	+4J	1

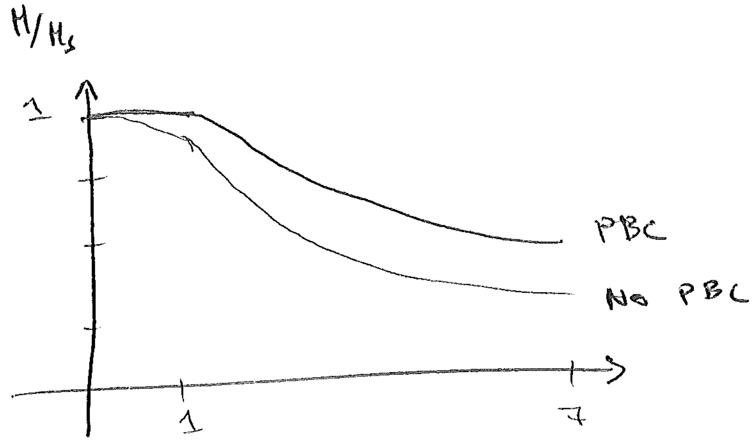
2x2 No PBC

similar to PBC but energy values are halved

$$Z = 12 + 2\left(e^{4\beta J} + e^{-4\beta J}\right)$$

$$\langle |M| \rangle = \frac{16 + 8e^{4\beta J}}{12 + 2\left(e^{4\beta J} + e^{-4\beta J}\right)}$$

T	$\langle \lvert M \rvert \rangle$
0,1	~4
1	3,73
1,5	3,20
2	2,72
2,5	2,49
3	2,30
3,5	2,17
4	2,08
5	1,95
6	1,87
7	1,81



Free energy 2×2 No PBC

M	F
4	$-4J$
2	$-T\ln 4$
0	$-T\ln(4+2e^{-4\beta J})$
-2	$-T\ln 4$
4	$-4J$

F(M) for $T=1$; $J=1$; $k_B=1$

M	F(M)
4	-4
2	-1,3863
0	-1,3954
-2	-1,3863
4	-4

$T=7$

M	F(M)
4	-4
2	-9,70
0	-11,45
-2	-9,70
4	-4

Disordered state more favorable compared to PBC lattice