FYS3150 Project 4

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2.1 Example: Analytical expression for the 2×2 case

For a 2×2 lattice, the thermodynamic quantities can be found analytically without too much work. To find the partition function, we need to write out all possible microstates and calculate their energies. Using the periodic boundary conditions, we get

Microstate	Energy	Magnetization
$\begin{array}{cccc} & \downarrow & \downarrow & \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \downarrow & \downarrow & \downarrow & \downarrow \\ & \downarrow & \downarrow & \end{array}$	$E = -8J$	$M = -4$

Microstate	Energy	Magnetization
$\begin{array}{cccc} & \downarrow & \uparrow & \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ & \downarrow & \downarrow & \end{array}$	$E = 0$	$M = -2$
$\begin{array}{cccc} & \uparrow & \downarrow & \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ & \downarrow & \downarrow & \end{array}$	$E = 0$	$M = -2$
$\begin{array}{cccc} & \uparrow & \uparrow & \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ & \downarrow & \downarrow & \end{array}$	$E = 0$	$M = 0$
$\begin{array}{cccc} & \downarrow & \downarrow & \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \downarrow & \downarrow & \downarrow \\ & \downarrow & \uparrow & \end{array}$	$E = 0$	$M = -2$
$\begin{array}{cccc} & \downarrow & \uparrow & \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ & \downarrow & \uparrow & \end{array}$	$E = 0$	$M = 0$
$\begin{array}{cccc} & \uparrow & \downarrow & \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ & \downarrow & \uparrow & \end{array}$	$E = 8J$	$M = 0$
$\begin{array}{cccc} & \uparrow & \uparrow & \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ & \downarrow & \uparrow & \end{array}$	$E = 0$	$M = 2$
$\begin{array}{cccc} & \downarrow & \downarrow & \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \downarrow & \downarrow & \downarrow & \downarrow \\ & \uparrow & \downarrow & \end{array}$	$E = 0$	$M = -2$
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Microstate	Energy	Magnetization
$\begin{array}{cccc} & \uparrow & \uparrow & \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ & \uparrow & \downarrow & \end{array}$	$E = 0$	$M = 2$
$\begin{array}{cccc} & \downarrow & \downarrow & \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \downarrow & \downarrow & \downarrow & \downarrow \\ & \uparrow & \uparrow & \end{array}$	$E = 0$	$M = 0$
$\begin{array}{cccc} & \downarrow & \uparrow & \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ & \uparrow & \uparrow & \end{array}$	$E = 0$	$M = 2$
$\begin{array}{cccc} & \uparrow & \downarrow & \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ & \uparrow & \uparrow & \end{array}$	$E = 0$	$M = 2$
$\begin{array}{cccc} & \uparrow & \uparrow & \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ & \uparrow & \uparrow & \end{array}$	$E = -8J$	$M = 4$

To summarise, we have

Number of $\uparrow$	Multiplicity	Energy	Magnetisation
4	1	$-8J$	4
3	4	0	2
2	2	$8J$	0
2	4	0	0
1	4	0	-2
0	1	$-8J$	-4

Summing over all microstates, we get the partition function

$$Z = \sum_{\substack{\text{all}\\\text{micro-}\\\text{states}}} \mathrm{e}^{-\beta E_i} = 2\mathrm{e}^{8J\beta} + 2\mathrm{e}^{-8J\beta} + 12$$

The expectation value of the energy can then be found from

$$
\begin{aligned}
\langle E\rangle = \frac{\partial \ln(Z)}{\partial \beta} &= \frac{\partial}{\partial \beta}\left(\ln\left(2\mathrm{e}^{8J\beta}+2\mathrm{e}^{-8J\beta}+12\right)\right) \\
&= \frac{1}{2\mathrm{e}^{8J\beta}+2\mathrm{e}^{-8J\beta}+12}\left(16J\mathrm{e}^{8J\beta}-16J\mathrm{e}^{-8J\beta}\right) \\
&= \frac{8J\left(\mathrm{e}^{8J\beta}-\mathrm{e}^{-8J\beta}\right)}{\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}+6}
\end{aligned}
$$

yielding the heat capacity

$$
\begin{aligned}
C_V &= \frac{\partial}{\partial T}(\langle E\rangle) = \frac{\partial \beta}{\partial T}\frac{\partial}{\partial \beta}(\langle E\rangle) = -\frac{1}{kT^2}\frac{\partial}{\partial \beta}(\langle E\rangle) \\
&= -\frac{1}{kT^2}\frac{\partial}{\partial \beta}\left(\frac{8J\left(\mathrm{e}^{8J\beta}-\mathrm{e}^{-8J\beta}\right)}{\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}+6}\right) \\
&= -\frac{8J}{kT^2}\frac{8J\left(\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}\right)(\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}+6)-\left(\mathrm{e}^{8J\beta}-\mathrm{e}^{-8J\beta}\right)8J\left(\mathrm{e}^{8J\beta}-\mathrm{e}^{-8J\beta}\right)}{\left(\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}+6\right)^2} \\
&= -\frac{64J^2}{kT^2}\frac{6\left(\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}\right)+\left(\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}\right)^2-\left(\mathrm{e}^{8J\beta}-\mathrm{e}^{-8J\beta}\right)^2}{\left(\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}+6\right)^2} \\
&= -\frac{64J^2}{kT^2}\frac{6\left(\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}\right)+\mathrm{e}^{16J\beta}+2+\mathrm{e}^{-16J\beta}-\left(\mathrm{e}^{16J\beta}-2+\mathrm{e}^{-16\beta}\right)}{\left(\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}+6\right)^2} \\
&= -\frac{64J^2}{kT^2}\frac{6\left(\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}\right)+4}{\left(\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}+6\right)^2}
\end{aligned}
$$

To find the various quantities connected to magnetization, we use the general formula

$$
\langle A\rangle = \frac{1}{Z}\sum_{\substack{\text{all}\\ \text{micro-}\\ \text{states}}} A_i \mathrm{e}^{-\beta E_i}
$$

Mean magnetic moment(s):

$$
\begin{aligned}
\langle M\rangle &= \frac{1}{2\mathrm{e}^{8J\beta}+2\mathrm{e}^{-8J\beta}+12}\left(-4\mathrm{e}^{8J\beta}+4\cdot(-2)+0+0+4\cdot 2+4\mathrm{e}^{8J\beta}\right)=0 \\
\langle M^2\rangle &= \frac{1}{2\mathrm{e}^{8J\beta}+2\mathrm{e}^{-8J\beta}+12}\left((-4)^2\mathrm{e}^{8J\beta}+4\cdot(-2)^2+0+0+4\cdot 2^2+4^2\mathrm{e}^{8J\beta}\right) \\
&= \frac{32\left(\mathrm{e}^{8J\beta}+1\right)}{2\mathrm{e}^{8J\beta}+2\mathrm{e}^{-8J\beta}+12} = \frac{16\left(\mathrm{e}^{8J\beta}+1\right)}{\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}+6} \\
\langle |M|\rangle &= \frac{1}{2\mathrm{e}^{8J\beta}+2\mathrm{e}^{-8J\beta}+12}\left(|-4|\mathrm{e}^{8J\beta}+4\cdot|-2|+0+0+4\cdot 2+4\mathrm{e}^{8J\beta}\right) \\
&= \frac{8\left(\mathrm{e}^{8J\beta}+2\right)}{2\mathrm{e}^{8J\beta}+2\mathrm{e}^{-8J\beta}+12} = \frac{4\left(\mathrm{e}^{8J\beta}+2\right)}{\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}+6}
\end{aligned}
$$

Magnetic susceptibility:

$$
\chi = \beta\left(\langle M^2\rangle - \cancel{\langle M\rangle^2}\right) = \frac{16\beta\left(\mathrm{e}^{8J\beta}+1\right)}{\mathrm{e}^{8J\beta}+\mathrm{e}^{-8J\beta}+6}
$$