Solution 5

a) We calculate the average energy $< U >$:

$$
\begin{aligned}
U &= -J \sum_{\{\sigma\}} P(\{\sigma\}) \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} \\
&= -J \sum_{i=1}^{N-1} \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \cdots \sum_{\sigma_N=\pm 1} P(\sigma_1, ..., \sigma_N) \sigma_i \sigma_{i+1} \\
&= -J \sum_{i=1}^{N-1} \sum_{\sigma_i, \sigma_{i+1}=\pm 1} P(\sigma_i, \sigma_{i+1}) \sigma_i \sigma_{i+1} \\
&= -J(N-1)(\rho_{++} + \rho_{--} - \rho_{+-} - \rho_{-+}),
\end{aligned}
$$

using the identity $\sum_{\sigma_j=\pm 1} P(\sigma_1, ..., \sigma_N) = P(\sigma_1, ..., \sigma_{j-1}, \sigma_{j+1}, ..., \sigma_N)$.

The entropy (using the coupled mean field approximation) is:

$$
\begin{aligned}
S &= -k_B \sum_{\{\sigma\}} P(\{\sigma\}) \ln P(\{\sigma\}) \\
&= -k_B \sum_{\{\sigma\}} P(\{\sigma\}) \left(\sum_{i=1}^{N-1} \ln \frac{P(\sigma_i, \sigma_{i+1})}{P(\sigma_{i+1})} \right) \\
&= -k_B \sum_{i=1}^{N-1} \sum_{\{\sigma\}} P(\sigma_1, ..., \sigma_N)(\ln P(\sigma_i, \sigma_{i+1}) - \ln P(\sigma_{i+1})) \\
&= -k_B \sum_{i=1}^{N-1} \{\rho_{++}(\ln \rho_{++} - \ln P(1)) + \rho_{+-}(\ln \rho_{+-} - \ln P(1)) \\
&\qquad + \rho_{-+}(\ln \rho_{-+} - \ln P(-1)) + \rho_{--}(\ln \rho_{--} - \ln P(-1))\}
\end{aligned}
$$

We use the identity $P(\pm 1) = \rho_{\pm\pm} + \rho_{\pm\mp}$ to obtain:

$$
\begin{aligned}
S = -k_B(N-1) \Big\{ &\rho_{++}(\ln \rho_{++} - \ln(\rho_{++} + \rho_{+-})) + \rho_{+-}(\ln \rho_{+-} - \ln(\rho_{++} + \rho_{+-})) \\
&+ \rho_{-+}(\ln \rho_{-+} - \ln(\rho_{-+} + \rho_{--})) + \rho_{--}(\ln \rho_{--} - \ln(\rho_{-+} + \rho_{--})) \Big\}
\end{aligned}
$$

Also the probabilities ρ are normalized and by symmetry $\rho_{+-} = \rho_{-+}$, so:
$\rho_{+-} = \rho_{-+} = \frac{1}{2}(1 - \rho_{++} - \rho_{--})$.

$$\begin{aligned} S &= -k_B(N-1)\Big\{\rho_{++}\left(\ln\rho_{++}-\ln\left(\frac{1}{2}(1+\rho_{++}-\rho_{--})\right)\right) \\ &+\frac{1}{2}(1-\rho_{++}-\rho_{--})\left(\ln\left(\frac{1}{2}(1-\rho_{++}-\rho_{--})\right)-\ln\left(\frac{1}{2}(1+\rho_{++}-\rho_{--})\right)\right) \\ &+\frac{1}{2}(1-\rho_{++}-\rho_{--})\left(\ln\left(\frac{1}{2}(1-\rho_{++}-\rho_{--})\right)-\ln\left(\frac{1}{2}(1-\rho_{++}+\rho_{--})\right)\right) \\ &+\rho_{--}\left(\ln\rho_{--}-\ln\left(\frac{1}{2}(1-\rho_{++}+\rho_{--})\right)\right)\Big\} \end{aligned} \tag{1}$$

we define now the variables:

$$m = \rho_{++} - \rho_{--}$$
$$n = \rho_{++} + \rho_{--}$$

m is the average magnetization. In these variables the free energy is ($\frac{N-1}{N} \approx 1$ in the limit of big N):

$$\begin{aligned} f = \frac{F}{N} &= -J(2n-1) + k_BT\Big\{\frac{1}{2}(m+n)\left(\ln\left(\frac{1}{2}(m+n)\right)-\ln\left(\frac{1}{2}(1+m)\right)\right) \\ &+\frac{1}{2}(1-n)\left(\ln\left(\frac{1}{2}(1-n)\right)-\ln\left(\frac{1}{2}(1+m)\right)\right) \\ &+\frac{1}{2}(1-n)\left(\ln\left(\frac{1}{2}(1-n)\right)-\ln\left(\frac{1}{2}(1-m)\right)\right) \\ &+\frac{1}{2}(n-m)\left(\ln\left(\frac{1}{2}(n-m)\right)-\ln\left(\frac{1}{2}(1-m)\right)\right)\Big\} \end{aligned} \tag{2}$$

b) The state which minimizes the free energy is determined by the values of m and n for which the derivative of the free energy is zero.

$$\begin{aligned} \frac{\partial f}{\partial m} &= \frac{k_BT}{2}\Big\{\left(\ln\left(\frac{1}{2}(m+n)\right)-\ln\left(\frac{1}{2}(1+m)\right)\right) \\ &+\left(1-\frac{m+n}{1+m}\right)+\left(-\frac{1-n}{1+m}+\frac{1-n}{1-m}\right) \\ &-\left(\ln\left(\frac{1}{2}(n-m)\right)-\ln\left(\frac{1}{2}(1-m)\right)\right)+\left(-1+\frac{n-m}{1-m}\right)\Big\} \\ &= \frac{k_BT}{2}\left\{\frac{-m-n-1+n}{1+m}+\frac{n-m+1-n}{1-m}+\ln\left(\frac{(m+n)(1-m)}{(1+m)(n-m)}\right)\right\} \\ &= \frac{k_BT}{2}\left\{\ln\left(\frac{(m+n)(1-m)}{(1+m)(n-m)}\right)\right\} = 0 \end{aligned}$$

$$\Leftrightarrow (m+n)(1-m) = (1+m)(n-m) \Leftrightarrow 2m = 2mn \Leftrightarrow (m=0) \text{ OR } (n=1) \tag{3}$$

$$\begin{aligned}
\frac{\partial f}{\partial n} &= -2J+\frac{k_BT}{2}\Bigg\{\left(\ln\left(\frac{1}{2}(m+n)\right)-\ln\left(\frac{1}{2}(1+m))\right)\right)+1 \\
&\quad -\left(\ln\left(\frac{1}{2}(1-n)\right)-\ln\left(\frac{1}{2}(1+m)\right)\right)-1 \\
&\quad -\left(\ln\left(\frac{1}{2}(1-n)\right)-\ln\left(\frac{1}{2}(1-m)\right)\right)-1 \\
&\quad +\left(\ln\left(\frac{1}{2}(n-m)\right)-\ln\left(\frac{1}{2}(1-m)\right)\right)+1\Bigg\} \\
&= -2J+\frac{k_BT}{2}\left\{\ln\left(\frac{1}{2}(m+n)\right)-2\ln\left(\frac{1}{2}(1-n)\right)+\ln\left(\frac{1}{2}(n-m)\right)\right\}=0
\end{aligned}$$

$$\Leftrightarrow \frac{(m+n)(n-m)}{(1-n)^2}=\exp\left(\frac{4J}{k_BT}\right)=\lambda \qquad (4)$$

From (3) and (4), we see that $m=0$ for any $T\neq 0$. So the magnetization is zero at any temperature $T>0$. There is no transition phase, which is the same result as in the exact solution of the Ising model!

We obtain:

$$n^2 = (1-n)^2\lambda \Rightarrow n=\frac{-\lambda\pm\sqrt{\lambda}}{1-\lambda}=\frac{-\lambda+\sqrt{\lambda}}{1-\lambda}=\frac{-e^{2J\beta}+1}{e^{-2J\beta}-e^{2J\beta}}, \qquad (5)$$

because $0\leq n\leq 1$.

We notice that:

$$\lim_{T\to\infty} n = \lim_{\lambda\to 1} n = \frac{1}{2}$$

and $\rho_{++}=\rho_{--}=\rho_{+-}=\rho_{-+}=\frac{1}{4}$, which indicate a perfect mixing.

At $T=0$, the system minimizes its energy, that is $n=1$ and $m=\pm 1$ because $\rho_{+-}=0$.

c) We introduce m and n into (2).

$$\begin{aligned}
f &= -J(2n-1)+k_BT\left[n\left(\ln\frac{1}{2}n-\ln\frac{1}{2}\right)+(1-n)\left(\ln\frac{1}{2}(1-n)-\ln\frac{1}{2}\right)\right] \\
&= -J\left(2\frac{-e^{2J\beta}+1}{e^{-2J\beta}-e^{2J\beta}}-1\right)+k_BT\left[\frac{-e^{2J\beta}+1}{e^{-2J\beta}-e^{2J\beta}}\ln\left(\frac{n}{1-n}\right)+\ln\left(\frac{1}{2}\frac{-e^{2J\beta}+1}{e^{-2J\beta}-e^{2J\beta}}\right)-\ln\frac{1}{2}\right] \\
&= J-2J\left(\frac{-e^{2J\beta}+1}{e^{-2J\beta}-e^{2J\beta}}\right)+k_BT\left[\frac{-e^{2J\beta}+1}{e^{-2J\beta}-e^{2J\beta}}\ln e^{2J\beta}+\ln\left(\frac{1}{2}e^{-J\beta}\frac{e^{-J\beta}-e^{J\beta}}{e^{-2J\beta}-e^{2J\beta}}\right)-\ln\frac{1}{2}\right] \\
&= k_BT\ln\left(\frac{1}{e^{-J\beta}+e^{J\beta}}\right) \\
&= -k_BT\ln(2\cosh J\beta)
\end{aligned}$$

which is the exact result of the Ising model in 1 dimension. An approximation can also give an exact result! The mean field approximation does not give the exact answer for the Ising model in $D = 1$ but taking into account one step correlations was enough to obtain the correct result. In general we can often describe the exact behavior of a system only taking into account correlations at a finite number of steps. This is not possible when the correlations are infinite, as for example at the critical point.