

4.

- (i) (a) The total energy for a system of  $N$  spins  $s_i = \pm 1$  with constant nearest-neighbour interactions  $J > 0$  placed in a uniform external field  $H$  is

$$E_{\{s_i\}} = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_{i=1}^N s_i,$$

where the notation  $\langle ij \rangle$  restricts the sum to run over all distinct nearest-neighbour pairs.

- (b) Let  $M_{\{s_i\}} = \sum_{i=1}^N s_i$  denote the total magnetisation and  $\langle M \rangle$  the average total magnetisation. The order parameter for the Ising model is defined as the magnetisation per spin

$$m(T, H) = \lim_{N \rightarrow \infty} \frac{\langle M \rangle}{N}.$$

- (c) The ratio of the average total energy,  $\langle E \rangle$ , to the temperature times entropy,  $TS$ , defines a dimensionless scale  $J/k_B T$ . A competition exists between the tendency to randomise the orientation of spins for  $J \ll k_B T$ , and a tendency to align spins for  $J \gg k_B T$ . In the former case, the free energy is minimised by maximising the entropic term: the magnetisation is zero because the spins point up and down randomly. In the latter case, the free energy is minimised by minimising the total energy: the magnetisation is non-zero because the spins tend to align. Since the entropy in the free energy is multiplied by temperature, for sufficiently low temperatures one could expect the minimisation of the free energy to be dominated by the minimisation of the total energy. Therefore, at least qualitatively, there is a possibility of a phase transition from a phase with zero magnetisation at relatively high temperatures, to a phase with non-zero magnetisation at relatively low temperatures.

- (ii) (a) The susceptibility is defined as the derivative of the average total magnetisation with respect to the external field at fixed temperature. Therefore, if  $\chi$  denotes the susceptibility per spin

$$N\chi = \left( \frac{\partial \langle M \rangle}{\partial H} \right)_T.$$

The susceptibility is related to the variance of the magnetisation through the fluctuation-dissipation theorem,

$$\begin{aligned} \chi &= \left( \frac{\partial \langle M \rangle}{\partial H} \right)_T \\ &= \frac{\partial}{\partial H} \left( \frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) M_{\{s_i\}} \right) \\ &= \frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) \beta M_{\{s_i\}}^2 - \frac{1}{Z^2} \frac{\partial Z}{\partial H} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) M_{\{s_i\}} \\ &= \beta \frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) M_{\{s_i\}}^2 - \beta \left( \frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) M_{\{s_i\}} \right)^2 \\ &= \beta \left( \langle M^2 \rangle - \langle M \rangle^2 \right). \end{aligned}$$

Therefore, the susceptibility per spin is related to the variance of the average total magnetisation by

$$k_B T \chi = \frac{1}{N} \left( \langle M^2 \rangle - \langle M \rangle^2 \right).$$

(b) The site-site correlation function  $g(\mathbf{r}_i, \mathbf{r}_j)$  is defined by

$$g(\mathbf{r}_i, \mathbf{r}_j) = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle.$$

According to the fluctuation-dissipation theorem

$$\begin{aligned} Nk_B T\chi &= \langle M^2 \rangle - \langle M \rangle^2 \\ &= \left\langle \sum_{k=1}^N s_k \sum_{j=1}^N s_j \right\rangle - \left\langle \sum_{k=1}^N s_k \right\rangle \left\langle \sum_{j=1}^N s_j \right\rangle \\ &= \sum_{k=1}^N \sum_{j=1}^N (\langle s_k s_j \rangle - \langle s_k \rangle \langle s_j \rangle) \\ &= \sum_{k=1}^N \sum_{j=1}^N g(\mathbf{r}_k, \mathbf{r}_j) \\ &= N \sum_{j=1}^N g(\mathbf{r}_i, \mathbf{r}_j) \end{aligned}$$

using translational invariance  $g(\mathbf{r}_k, \mathbf{r}_j) = g(\mathbf{r}_k + \mathbf{r}, \mathbf{r}_j + \mathbf{r})$ , and choosing an arbitrary site  $\mathbf{r}_i$  as a reference position.

(iii) (a) Replacing the sum over all sites by an integral over the whole system,

$$\int_V g(\mathbf{r}_i, \mathbf{r}_j) d\mathbf{r}_j = k_B T\chi. \quad (4.1)$$

At the critical point the correlation length  $\xi = \infty$  so the arguments of the scaling function are constant. Therefore the correlation function decays like a power law,

$$g(\mathbf{r}_i, \mathbf{r}_j) \propto r^{-(d-2+\eta)} \quad \text{at } t = 0, h = 0.$$

and we find

$$\int_V g(\mathbf{r}_i, \mathbf{r}_j) d\mathbf{r}_j \propto \int_0^\infty r^{-(d-2+\eta)} r^{d-1} dr = \int_0^\infty r^{1-\eta} dr \quad \text{for } t \rightarrow 0^\pm.$$

But since  $\eta \geq 0$ , the integral diverges and hence so does the susceptibility per spin for  $t \rightarrow 0, h \rightarrow 0$ .

(b) In zero external field, the right-hand side of Equation (4.1)

$$k_B T\chi \propto |t|^{-\gamma} \quad \text{for } t \rightarrow 0$$

while the left-hand side of Equation (4.1) yields

$$\begin{aligned} \int_V g(\mathbf{r}_i, \mathbf{r}_j) d\mathbf{r}_j &\propto \int_0^\infty r^{-(d-2+\eta)} \mathcal{G}_\pm(r/\xi, 0) r^{d-1} dr \\ &= \int_0^\infty r^{1-\eta} \mathcal{G}_\pm(r/\xi, 0) dr && \text{for } t \rightarrow 0^\pm \\ &= \int_0^\infty (u\xi)^{1-\eta} \mathcal{G}_\pm(u, 0) \xi du && \text{with } r = u\xi \\ &= \xi^{2-\eta} \int_0^\infty u^{1-\eta} \mathcal{G}_\pm(u, 0) du \\ &= |t|^{-\nu(2-\eta)} \int_0^\infty u^{1-\eta} \mathcal{G}_\pm(u, 0) du && \text{for } t \rightarrow 0. \end{aligned}$$

The integral is just a number so that by comparing exponents

$$\gamma = \nu(2 - \eta).$$