Problem 1:

or the single two-state spin $s = \pm 1$, with energy described by Eq. 8.1, find the entropy as a function of the temperature T and applied field H.

Solution:For a single two-state spin, the partition function is

$$Z = \sum_{s=\pm 1} e^{-\beta E_s} = e^{\beta H} + e^{-\beta H}$$
 (1)

The entropy is given by

$$S = -k_B \sum_{s=\pm 1} p_s \ln p_s$$

$$= -k_B \sum_{s=\pm 1} \frac{e^{-\beta E_s}}{Z} \ln \frac{e^{-\beta E_s}}{Z}$$

$$= -k_B \sum_{s=\pm 1} \frac{e^{-\beta E_s}}{Z} \left(-\beta E_s - \ln Z\right)$$

$$= k_B \left(\beta H e^{\beta H} + \beta H e^{-\beta H} - \ln \left(e^{\beta H} + e^{-\beta H}\right)\right)$$

where $\beta = \frac{1}{k_B T}$.

Problem 2:

Calculate expressions for the free energy and mean magnetization of a system of three coupled two-state spins s_1, s_2 and $s_3 = \pm 1$, with Hamiltonian (total energy)

 $E = -J(s_1s_2 + s_2s_3) - H(s_1 + s_2 + s_3)$. Show that the mean magnetization of this system vanishes in the absence of an applied field H.

Solution:

Using the transfer matrix, the partition function is

$$Z = \sum_{s_1 = \pm 1} \sum_{s_2 = \pm 1} \sum_{s_3 = \pm 1} e^{-\beta E}$$
$$= \mathbf{Tr}(\mathbf{T}^3)$$

where

$$\mathbf{T} = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}$$
 (2)

Evaluating the trace of \mathbf{T}^3 , we have

$$\mathbf{T}^{3} = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}^{3}$$

$$= \begin{pmatrix} e^{3\beta(J+H)} + e^{3\beta(J-H)} + 2e^{\beta J}e^{-\beta H} & e^{3\beta(J-H)} + e^{3\beta(J+H)} - 2e^{\beta J}e^{-\beta H} \\ e^{3\beta(J-H)} + e^{3\beta(J+H)} - 2e^{\beta J}e^{-\beta H} & e^{3\beta(J+H)} + e^{3\beta(J-H)} + 2e^{\beta J}e^{-\beta H} \end{pmatrix}$$

The partition function is then

$$Z = \mathbf{Tr}(\mathbf{T}^{3})$$

$$= e^{3\beta(J+H)} + e^{3\beta(J-H)} + 2e^{\beta J}e^{-\beta H} + e^{3\beta(J-H)} + e^{3\beta(J+H)} - 2e^{\beta J}e^{-\beta H}$$

$$= 2e^{3\beta(J+H)} + 2e^{3\beta(J-H)}$$

The free energy is given by

$$F = -k_B T \ln Z$$
$$= -k_B T \ln \left(2e^{3\beta(J+H)} + 2e^{3\beta(J-H)} \right)$$

When H=0, the mean magnetization is given by

$$\langle s_1 + s_2 + s_3 \rangle = \frac{\partial(-\beta F)}{\partial(\beta H)}$$

$$= \frac{6e^{3\beta(J+H)} - 6e^{3\beta(J-H)}}{2e^{3\beta(J+H)} + 2e^{3\beta(J-H)}} \Big|_{H=0}$$

$$= 0$$

Problem 3:

Let

$$\mathbf{T} = \begin{pmatrix} e^{\beta(J'+H')} & e^{-\beta J'} \\ e^{-\beta J'} & e^{\beta(J'-H')} \end{pmatrix}$$
 (3)

(b) If H' = 0, show that $\mathbf{U}^{-1}\mathbf{T}\mathbf{U}$ is diagonal for the unitary rotation matrix

$$\mathbf{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1\\ 1 & -1 \end{pmatrix} \tag{4}$$

Solution::

Since H'=0,

$$\mathbf{T} = \begin{pmatrix} e^{\beta J'} & e^{-\beta J'} \\ e^{-\beta J'} & e^{\beta J'} \end{pmatrix} \tag{5}$$

The eigenvalues of ${f T}$ are

$$\lambda_1 = e^{\beta J'} + e^{-\beta J'}, \quad \lambda_2 = e^{\beta J'} - e^{-\beta J'}$$
 (6)

The corresponding eigenvectors are

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \mathbf{v}_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{7}$$

Thus the diagonal matrix is

$$\mathbf{D} = \begin{pmatrix} e^{\beta J'} + e^{-\beta J'} & 0\\ 0 & e^{\beta J'} - e^{-\beta J'} \end{pmatrix} \tag{8}$$

Therefore $\mathbf{U}^{-1}\mathbf{T}\mathbf{U}$ is diagonal. And

$$\mathbf{U}^{-1}\mathbf{T}\mathbf{U} = \begin{pmatrix} e^{\beta J'} + e^{-\beta J'} & 0\\ 0 & e^{\beta J'} - e^{-\beta J'} \end{pmatrix}$$
(9)

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Solution:

$$\frac{\lambda_1^{N-r}\lambda_2^r + \lambda_2^{N-r}\lambda_1^r}{\lambda_1^N + \lambda_2^N} = \frac{\lambda_1^N \frac{\lambda_2}{\lambda_1} + \lambda_2^N \frac{\lambda_1}{\lambda^2}}{\lambda_1^N + \lambda_2^N}$$
$$= \frac{\left(\frac{\lambda_1}{\lambda_2}\right)^N}{\left(\frac{\lambda_1}{\lambda_2}\right)^N + 1}$$

Problem 5:

In the chiral clock model, a one-dimensional chain of sites each carries an integer variable ni that can take values 0, 1 or 2, representing three equally-spaced directions around a clock-face. Nearest neighbours interact so that their lowest-energy states occur when each site is one position further round the clock-face than its neighbour to the left, so that the energy is given by

$$E = -J \sum_{i=1}^{N} \cos \left(\frac{2\pi (n_i - n_{i-1} + 1)}{3} \right)$$
 (10)

with a coupling constant J and periodic boundary conditions $n_{N+1} = n_1$. Show that the transfer matrix for this model has only one eigenvalue, equal to $2 \exp(-\beta J/2) + \exp(\beta J)$, and hence write down the free energy per site.

Solution:

The partition function is

$$Z =$$

Problem 6:

Problem 7: (Page 90-91)

A mean field theory of a particular thermodynamic system yields an expression for the free energy density f as a function of volume fraction ϕ of conserved particles as

$$f = \frac{1}{\phi^2 (1 - \phi)^2} + 250\phi (1 - \phi) \tag{11}$$

Use the common-tangent construction to discover the binodal values, for which this system exhibits coexistence. [Hint: You may find it helpful to re-write this function in a more symmetrical way by making a substitution for ϕ .]

Solution:Here we make a substitution for ϕ :

$$\phi = \varphi + \frac{1}{2} \tag{12}$$

where α is a new variable. Then

$$f = \frac{1}{\phi^2 (1 - \phi)^2} + 250\phi (1 - \phi)$$

$$= \frac{1}{\left(\alpha + \frac{1}{2}\right)^2 \left(1 - \alpha - \frac{1}{2}\right)^2} + 250\left(\alpha + \frac{1}{2}\right)\left(1 - \alpha - \frac{1}{2}\right)$$

$$= \frac{1}{(\alpha^2 - 1/4)^2} + 250\left(\alpha^2 - \frac{1}{4}\right)$$

We set up two equations:

$$\left. \frac{\partial f}{\partial \alpha} \right|_{\alpha = \alpha_1} = \left. \frac{\partial f}{\partial \alpha} \right|_{\alpha = \alpha_2} \tag{13}$$

which is equivalent to

$$-\frac{4\alpha_1}{(\alpha_1^2 - 1/4)^3} + 500\alpha_1 = -\frac{4\alpha_2}{(\alpha_2^2 - 1/4)^3} + 500\alpha_2 \tag{14}$$

and

$$\alpha_1 \frac{\partial f}{\partial \alpha} \Big|_{\alpha = \alpha_1} - f(\alpha_1) = \alpha_2 \frac{\partial f}{\partial \alpha} \Big|_{\alpha = \alpha_2} - f(\alpha_2)$$
 (15)

which is equivalent to

$$-\frac{4\alpha_1^2}{(\alpha_1^2 - 1/4)^3} + 500\alpha_1^2 - \frac{1}{(\alpha_1^2 - 1/4)^2} - 250\alpha_1^2 + 125 = -\frac{4\alpha_2^2}{(\alpha_2^2 - 1/4)^3} + 500\alpha_2^2 - \frac{1}{(\alpha_2^2 - 1/4)^2} - 250\alpha_2^2 + 125$$

$$(16)$$

Solving the equations, we have

Assume that f(x) is integrable over any interval (a, b), and g(x) is the probability density function of X within the interval (a, b), with $\int_a^b g(x) = 1$. We need to prove that after repeating the sampling process n times (where n is sufficiently large), the mean of $\frac{f(x_i)}{g(x_i)}$ converges to $\int_a^b f(x)dx$, i.e.,

$$\lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \frac{f(x_i)}{g(x_i)} = \int_{a}^{b} f(x) dx$$
 (17)

According to the Law of Large Numbers, if X_1, X_2, \ldots, X_n are independent and identically distributed random variables with finite mean μ and variance σ^2 , then for any given positive number ϵ , when n is sufficiently large, we have

$$\Pr\left(\left|\frac{1}{n}\sum_{i=1}^{n}X_{i}-\mu\right|<\epsilon\right)\approx 1.$$
(18)

Now let's prove that the mean of $\frac{f(x_i)}{g(x_i)}$ converges to $\int_a^b f(x)dx$ after repeating the sampling process n times.

Assume that we perform n independent samples, resulting in random variables X_1, X_2, \ldots, X_n , where each X_i has the probability density function g(x).

Define the random variable $Y_i = \frac{f(X_i)}{g(X_i)}$, and the expectation of Y_i is

$$E[Y_i] = \int_{-\infty}^{\infty} \frac{f(x)}{g(x)} g(x) dx = \int_{-\infty}^{\infty} f(x) dx.$$
 (19)

According to the Law of Large Numbers, for any given positive number ϵ , when n is sufficiently large, we have

$$\Pr\left(\left|\frac{1}{n}\sum_{i=1}^{n}Y_{i}-\int_{-\infty}^{\infty}f(x)dx\right|<\epsilon\right)\approx 1.$$
 (20)

Since f(x) is integrable over any interval (a,b), we can transform the integral $\int_{-\infty}^{\infty} f(x)dx$ into $\int_{a}^{b} f(x)dx$, as the values of f(x) outside (a,b) do not affect the integral result.

Therefore, when n is sufficiently large, we have

$$\Pr\left(\left|\frac{1}{n}\sum_{i=1}^{n}Y_{i}-\int_{a}^{b}f(x)dx\right|<\epsilon\right)\approx 1.$$
(21)

In other words, when n is sufficiently large, $\frac{1}{n}\sum_{i=1}^{n}Y_{i}$ is highly likely to fall within an ϵ