Exercise: 8-14 ***(Statistical Mechanics and Thermodynamics, Claude Garrod)***

Apply the Bethe-Peierls approximation to an Ising model, with no external field, on a 2D hexagonal lattice?

Solution

Fig.1 shows a portion of a hexagonal lattice. A central spin σ_1 and its three neighboring spins σ_2, σ_3 and σ_4, are isolated from the rest of the lattice by replacing all the shaded spins by some yet to be determined average value $\bar{\sigma}$. Although the external field is zero, it is very convenient first to include an external field term H' for spin 1 and different value H for spins 2, 3, and 4. Then, at the end we will set H and H' equal to zero.

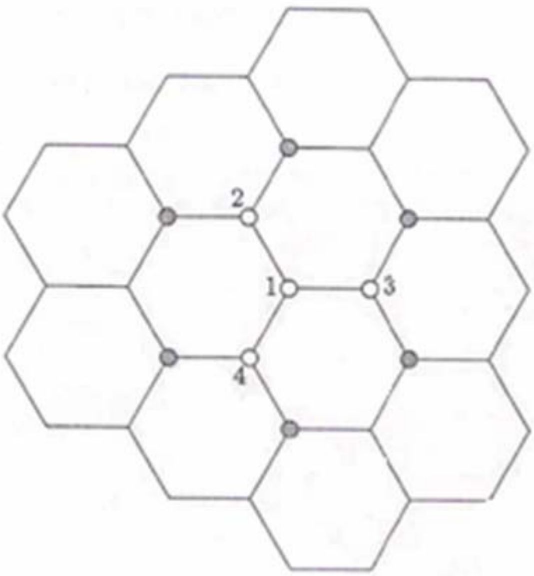

Fig.1 A section of a hexagonal lattice.

The Hamiltonian of the system is given by:

$$\beta E = -J\sum_{i=1}^{N}\sigma_i\sigma_{i+1} - H\sum_{i=1}^{N}\sigma_i$$

$$\beta E = -H'\sigma_1 - H(\sigma_2+\sigma_3+\sigma_4) - J(2\bar{\sigma}+\sigma_1)(\sigma_2+\sigma_3+\sigma_4)$$

With the definitions

$$j = \beta J,\, h = \beta H \ and \ h' = \beta H'$$

$$\beta E = -h'\sigma_1 - h(\sigma_2+\sigma_3+\sigma_4) - j(\bar{\sigma}\sigma_2+\bar{\sigma}\sigma_2+\bar{\sigma}\sigma_3+\bar{\sigma}\sigma_3+\bar{\sigma}\sigma_4+\bar{\sigma}\sigma_4+\sigma_1\sigma_2+\sigma_1\sigma_3+\sigma_1\sigma_4)$$

$$\Rightarrow \beta E = -h'\sigma_1 - h(\sigma_2+\sigma_3+\sigma_4) - j(2\bar{\sigma}+\sigma_1)(\sigma_2+\sigma_3+\sigma_4)$$

The partition function of the system is given by summing $e^{\beta E}$ over all possible values of the four spin values.

$$Z = \sum_{\sigma_1}\sum_{\sigma_2}\sum_{\sigma_3}\sum_{\sigma_4} \exp[h'\sigma_1 + h(\sigma_2 + \sigma_3 + \sigma_4) + j(2\overline{\sigma} + \sigma_1)(\sigma_2 + \sigma_3 + \sigma_4)]$$

$$Z = \sum_{\sigma_1}\sum_{\sigma_2}\sum_{\sigma_3}\sum_{\sigma_4} \exp[h'\sigma_1 + (h + 2j\overline{\sigma} + j\sigma_1)(\sigma_2 + \sigma_3 + \sigma_4)]$$

$$Z = \sum_{\sigma_1} \exp(h'\sigma_1)\sum_{\sigma_2}\sum_{\sigma_3}\sum_{\sigma_4} \exp[(h + 2j\overline{\sigma} + j\sigma_1)(\sigma_2 + \sigma_3 + \sigma_4)]$$

$$Z = \sum_{\sigma_1} \exp(h'\sigma_1)\sum_{\sigma_2} \exp[(h + 2j\overline{\sigma} + j\sigma_1)\sigma_2]\sum_{\sigma_3} \exp[(h + 2j\overline{\sigma} + j\sigma_1)\sigma_3]\sum_{\sigma_4} \exp[(h + 2j\overline{\sigma} + j\sigma_1)\sigma_4]$$

$$Z = \sum_{\sigma_1} \exp(h'\sigma_1)\sum_{\sigma} \exp[(h + 2j\overline{\sigma} + j\sigma_1)\sigma]\sum_{\sigma} \exp[(h + 2j\overline{\sigma} + j\sigma_1)\sigma]\sum_{\sigma} \exp[(h + 2j\overline{\sigma} + j\sigma_1)\sigma]$$

$$Z = \sum_{\sigma_1} \exp(h'\sigma_1)[\sum_{\sigma} \exp[(h + 2j\overline{\sigma} + j\sigma_1)\sigma]^3$$

$$Z = \sum_{\sigma_1} \exp(h'\sigma_1)[\exp(h + 2j\overline{\sigma} + j\sigma_1) + \exp(-h - 2j\overline{\sigma} - j\sigma_1)]^3$$

$$Z = \sum_{\sigma_1} \exp(h'\sigma_1)[2\cosh(h + 2j\overline{\sigma} + j\sigma_1)]^3$$

$$Z = 8\sum_{\sigma_1} \exp(h'\sigma_1)[\cosh^3(h + 2j\overline{\sigma} + j\sigma_1)]$$

$$Z = 8[\exp(h')\cosh^3(h + 2j\overline{\sigma} + j) + \exp(-h')\cosh^3(h + 2j\overline{\sigma} - j)]$$

Since,

$$\langle\sigma_1\rangle = \frac{1}{Z}\frac{\partial Z}{\partial h'} \quad and \quad \langle\sigma_2 + \sigma_3 + \sigma_4\rangle = \frac{1}{Z}\frac{\partial Z}{\partial h}$$

$$\Rightarrow \langle\sigma_1\rangle = \frac{8}{Z}[\exp(h')\cosh^3(h + 2j\overline{\sigma} + j) - \exp(-h')\cosh^3(h + 2j\overline{\sigma} - j)]$$

Define: $cc = h + 2j\overline{\sigma} - j$, then

$$\langle\sigma_2 + \sigma_3 + \sigma_4\rangle = \frac{24}{Z}[\exp(h')\cosh^2(cc)\sinh(h + 2j\overline{\sigma} + j) + \exp(-h')\cosh^2(cc)\sinh(cc)]$$

Thus, the partial derivatives at $h' = h = 0$,

$$\langle\sigma_1\rangle = \frac{8}{Z}[\cosh^3(2j\overline{\sigma} + j) - \cosh^3(2j\overline{\sigma} - j)]$$

$$\langle\sigma_2 + \sigma_3 + \sigma_4\rangle = \frac{24}{Z}[\cosh^2(2j\overline{\sigma} + j)\sinh(2j\overline{\sigma} + j) + \cosh^2(2j\overline{\sigma} - j)\sinh(2j\overline{\sigma} - j)]$$

Setting $\langle\sigma_2 + \sigma_3 + \sigma_4\rangle = 3\langle\sigma_1\rangle$

$$\Rightarrow [\cosh^2(2j\overline{\sigma} + j)\sinh(2j\overline{\sigma} + j) + \cosh^2(2j\overline{\sigma} - j)\sinh(2j\overline{\sigma} - j)] = [\cosh^3(2j\overline{\sigma} + j) - \cosh^3(2j\overline{\sigma} - j)]$$

$$\Rightarrow [\frac{\exp(2j\bar{\sigma}+j)+\exp(-2j\bar{\sigma}-j)}{2}]^2 \; [\frac{\exp(2j\bar{\sigma}+j)-\exp(-2j\bar{\sigma}-j)}{2}]$$
$$+[\frac{\exp(2j\bar{\sigma}-j)+\exp(-2j\bar{\sigma}+j)}{2}]^2 \; [\frac{\exp(2j\bar{\sigma}-j)-\exp(-2j\bar{\sigma}+j)}{2}]$$
$$=[\frac{\exp(2j\bar{\sigma}+j)+\exp(-2j\bar{\sigma}-j)}{2}]^3 - [\frac{\exp(2j\bar{\sigma}-j)+\exp(-2j\bar{\sigma}+j)}{2}]^3$$

Making the substitutions,

$$x = \exp(2j\bar{\sigma}) \;\; and \;\; y = \exp(j)$$

One can take the formidable-looking polynomial equation,

$$(xy + x^{-1}y^{-1})^2\,(xy - x^{-1}y^{-1}) + (xy^{-1} + x^{-1}y)^2\,(xy^{-1} - x^{-1}y) = (xy + x^{-1}y^{-1})^3 - (xy^{-1} + x^{-1}y)^3$$

Multiplying the above equation by x^3y^3 and collecting the terms gives the equation,

$$x^6 - (y^4 - 2y^2)x^4 + (y^4 - 2y^2)x^2 - 1 = 0$$

Letting $u = x^2$ *and* $A = y^4 - 2y^2$, we see that this is a cubic equation for u,

$$u^3 - Au^2 + Au - 1 = 0$$

The above cubic equation can be written as,

$$u - 1\,(u^2 - (A-1)u + 1) = 0$$

Comparing the trivial solution of this equation with that of the mean-field theory, one can observe that this equation has a trivial solution at $u = 1$ while the mean-field theories always have the trivial solution $\bar{\sigma} = 0$. On the other hand, the non-trivial solution of this equation can be obtained from the simple quadratic equation, $u^2 - (A-1) + 1 = 0$ which is,

$$u = \frac{1}{2}(A-1) \pm \frac{1}{2}\sqrt{(A-1)^2 - 4}$$

Since $u = x^2$, u must be positive. Thus, the acceptable solution is,

$$u = \frac{1}{2}(A-1) + \frac{1}{2}\sqrt{(A-1)^2 - 4}$$

This solution is real if and only if $A \geq 3$, which implies that $y \geq \sqrt{3}$. Thus, the Bethe-Peierls approximation predicts a ferromagnetic phase transition at a Curie temperature given by setting, $e^j = \sqrt{3}$.

Since, $$j = \beta J = \frac{J}{kT} \Rightarrow e^{\frac{J}{kT_c}} = 3^{\frac{1}{2}} \Rightarrow \frac{J}{kT_c} = \frac{1}{2}\log(3)$$

Thus, $$T_c = 2J / \log(3) \approx 1.82J$$

The exact relation, known from the Onsager solution, $T_c = 1.518649J$. Since the coordination number of the hexagonal lattice is three; simple mean-field theory would predict that the phase transition occurs at $T_c = 3J$. Thus, we see that the Bethe-Peierls approximation is a substantial improvement on the results of simple mean-field theory.