Christian ... I did all exercises

Problem 2.1

we consider a lattice gas in d dimensions, with the Hamiltonian

$$H = -\lambda \sum_{\langle ij \rangle} n_i n_j \qquad n_i \in \{0,1\} \ \forall i$$

a) We calculate the grand canonical ensemble partition Function

$$Z_G = \sum_{\tilde{N}=0}^{\infty} e^{\beta\mu\tilde{N}} \underbrace{\sum_{n_1=0,1} \cdots \sum_{n_{|L|}=0,1}}_{\sum_i n_i = \tilde{N}} e^{-\beta H}$$

can be written as (with $|L| = N$

$$Z_G = \sum_{n_1=0,1} \cdots \sum_{n_N=0,1} e^{-\beta(H - \mu \sum_i n_i)}$$

we can write $H - \mu \sum_i n_i$ in a different form

by introducing the sublattices A and B we can write

the sum over nearest neighbours as $\sum_{\langle ij \rangle} = \sum_{\substack{i \in A \\ j \text{ nearest neighbours of } i \\ \text{in } B}} =: \sum_{\substack{i \in A \\ j n N}}$

when exchanging $n_i = \frac{1}{2}(1+s_i)$ $s_i \in \{-1,1\}$ we can write

$$H - \mu \sum_i n_i = -\lambda \sum_{\langle ij \rangle} n_i n_j - \mu \sum_i (n_i) = -\lambda \sum_{\langle ij \rangle} \frac{1}{4}(1+s_i)(1+s_j) - \mu \sum_i \frac{1}{2}(1+s_i)$$

$$= -\lambda \frac{1}{2} \Big(\sum_{\substack{i \in A \\ j n N}} \frac{1}{4}(1+s_i+s_j+s_i s_j) + \sum_{\substack{j \in B \\ i n N}} \frac{1}{4}(1+s_i+s_j+s_i s_j)$$

$$= -\lambda \frac{1}{2}\cdot\frac{1}{4}\Big(\gamma \frac{N}{2} + \gamma \sum_{i\in A} s_i + \gamma \sum_{j\in B} s_j + \sum_{\substack{i\in A\\ j nn}} s_i s_j + \gamma\frac{N}{2} + \gamma \sum_{i\in A} s_i$$

$$+ \gamma \sum_{j\in B} s_j + \sum_{\substack{j\in B\\ i nn}} s_i s_j \Big) - \mu \frac{1}{2} \sum_i (s_i + 1)$$

$$= -\lambda \left(\frac{1}{8}\gamma N + \frac{1}{4}\gamma \sum_i s_i + \frac{1}{4} \sum_{\langle i,j\rangle} s_i s_j \right) - \frac{\mu}{2} N - \frac{\mu}{2} \sum_i s_i$$

$$= \underbrace{-\mathcal{J} \sum_{\langle i,j\rangle} s_i s_j - H \sum_i s_i}_{=:\, H_y} - \left(\frac{\lambda \gamma}{8} + \frac{\mu}{2} \right) N$$

with $\mathcal{J} = \frac{1}{4}$ and $H = \frac{1}{4}\lambda\gamma + \frac{\mu}{2}$ (The symmetrization wouldn't have been necessary. But I wanted to show that it doesn't matter, whether I sum over $\sum_{\substack{i\in A\\ j nn}}$ or $\sum_{\substack{j\in B\\ i nn}}$)

$$\Rightarrow Z_G = e^{\beta\left(\frac{\lambda\gamma}{8} + \frac{\mu}{2}\right)N} \sum_{n_1=0,1} \cdots \sum_{n_N=0,1} e^{-\beta H_y} = Z_y \, e^{\beta\left(\frac{\lambda\gamma}{8} + \frac{\mu}{2}\right)N}$$

b) we now execute a mean field approximation

$m_A = \langle s_i \rangle_{i\in A}$ $\quad m_B = \langle s_i \rangle_{i\in B}$ $\quad$ we consider a small fluctuation

$s_i = m_A + \delta_i \quad i\in A \qquad s_i = m_B + \delta_i \quad i \in B$

$$\Rightarrow H_y = -\mathcal{J} \sum_{\substack{i\in A\\ j nn}} (m_A + \delta_i)(m_B + \delta_j) - H \sum_i s_i$$

neglecting δ^2 term $\rightarrow$
$$\approx -\mathcal{J} \sum_{\substack{i\in A\\ j nn}} m_A m_B + m_B \delta_i + m_A \delta_j - H s_i$$

$$= -J\gamma\frac{N}{2}m_A m_B - J\sum_{i\in A} m_B\delta_i\gamma - J\gamma\sum_{j\in B} m_A\delta_j - H\sum_{i\in A} S_i - H\sum_{j\in B} S_j$$

$$= -\frac{J\gamma N}{2}m_A m_B - \sum_{i\in A}(Jm_B\gamma + H)S_i - \sum_{j\in B}(Jm_A\gamma + H)S_j$$

using

$\delta_{i,j} = S_{i,j} - m_{A,B}$

$$+\sum_{i\in A} Jm_B m_A\gamma + \underbrace{\sum_{j\in B} Jm_B m_A\gamma}_{\frac{N}{2}Jm_A m_B\gamma}$$

$$= \frac{J\gamma N}{2}m_A m_B - \sum_{i\in A}(J\gamma m_B + H)S_i - \sum_{j\in B}(J\gamma m_A + H)S_j$$

$$\Rightarrow Z_J = \sum_{n_1=0,1}\cdots\sum_{n_N=0,1} e^{-\beta H_J} = \sum_{S_{A_1}=\pm1}\cdots\sum_{S_{A_{\frac{N}{2}}}=\pm1} e^{\beta\sum_{i\in A}(J\gamma m_B+H)S_i}$$

$$\cdot\sum_{S_{B_1}=\pm1}\cdots\sum_{S_{B_{\frac{N}{2}}}=\pm1} e^{\beta\sum_{j\in B}(J\gamma m_A+H)S_j}\; e^{-\beta\frac{J\gamma N}{2}m_A m_B}$$

$$= \left(\sum_{S=\pm1} e^{\beta(J\gamma m_B+H)S}\right)^{\frac{N}{2}}\left(\sum_{S=\pm1} e^{\beta(J\gamma m_A+H)S}\right)^{\frac{N}{2}} e^{-\beta\frac{J\gamma N}{2}m_A m_B}$$

$$= \left[2\cosh(\beta(J\gamma m_B+H))\right]^{\frac{N}{2}}\left[2\cosh(\beta(J\gamma m_A+H))\right]^{\frac{N}{2}} e^{-\beta\frac{J\gamma N}{2}m_A m_B}$$

$$m_A = \langle S_i\rangle_{i\in A} = \frac{1}{Z_J}\sum_{n_1=0,1}\cdots\sum_{n_N=0,1} S_i\, e^{-\beta H_J} = \frac{\sum_{S=\pm1} S\, e^{\beta(J\gamma m_B+H)S}}{2\cosh((J\gamma m_B+H)\beta)} = \tanh(\beta(J\gamma m_B + H))$$

analog

$$m_B = \tanh(\beta(J\gamma m_A + H))$$

c)

$$\Omega = -\frac{1}{\beta}\ln(Z_G) = -\frac{1}{\beta}\ln\left(Z_y\, e^{\beta\left(\frac{\lambda\gamma}{8}+\frac{\mu}{2}\right)N}\right)$$

$$= -\frac{1}{\beta}\Big[\frac{N}{2}\ln\left(2\cosh(\beta(J\gamma m_B + H))\right) + \frac{N}{2}\ln\left(2\cosh(\beta(J\gamma m_A + H))\right)$$

$$- \frac{N}{2}\beta J\gamma m_A m_B + N\beta\left(\frac{\lambda\gamma}{8} + \frac{\mu}{2}\right)\Big]$$

in order to determine $\varrho_A = \langle n_i \rangle_{i\in A}$ $\quad \varrho_B = \langle n_i \rangle_{i\in B}$

we use $\quad n_i = \frac{1}{2}(1+s_i) \Rightarrow \varrho_A = \frac{1}{2}(1+m_A)\; ; \; \varrho_B = \frac{1}{2}(1+m_B)$

mit $x_A = \beta(J\gamma m_B + H) = \beta\left(\frac{\lambda\gamma}{4}m_B + \frac{\lambda\gamma}{4} + \frac{\mu}{2}\right) = \beta\left(\frac{\lambda\gamma}{4}(m_B+1) + \frac{\mu}{2}\right)$

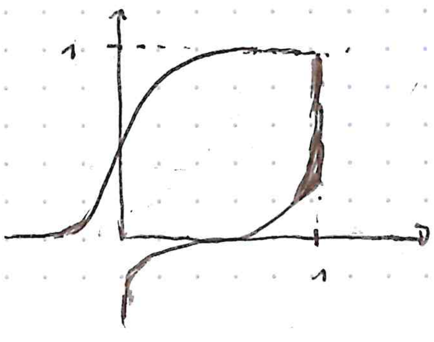
$= \frac{\beta}{2}(\lambda\gamma\varrho_B + \mu)$ $\quad$ and $\quad x_B := \frac{\beta}{2}(\lambda\gamma\varrho_A + \mu)$

$$\varrho_A = \frac{1}{2}(1+m_A) = \frac{1}{2}(1+\tanh(x_A)) = \frac{1}{2}\left(1 + \frac{e^{x_A} - e^{-x_A}}{e^{x_A}+e^{-x_A}}\right) = \frac{1}{2}\left(\frac{2e^{x_A}}{e^{x_A}+e^{-x_A}}\right)$$

$= \frac{1}{1+e^{-2x_A}} = \frac{1}{1+e^{-\beta(\lambda\gamma\varrho_B+\mu)}}$ and analog $\varrho_B = \frac{1}{1+e^{-2x_B}} = \frac{1}{1+e^{-\beta(\lambda\gamma\varrho_A+\mu)}}$

d) for $\lambda > 0$ $\phi(x)$ is strictly monoton increasing and it has to hold

$y = \phi(x)\; ; \; x = \phi(y)$



$x = y$

only one crossing point has to be where $x=y$ because the functions are mirrored.
($\Rightarrow$ has to be the same shape if it's mirrored again)

when we want to compare our results to the 1D Ising modell and from that discuss the critical temperature we have to set $\mu := -\frac{1}{2} J \gamma :: \mu_0$

in this case the self-consistency equation has the form

$m = \tanh(\beta J \gamma \cdot m)$ which leads to the condition

$T < T_c := \frac{J\gamma}{k_B}$ in order to get more solutions than $m = 0$

from the lecture we know $H = 0$ leads to approximated solutions for $T < T_c$

$m = 0 \quad m = \pm \sqrt{3(1 - \frac{T}{T_c})}$, which leads to the density

$\rho = \frac{1}{2}$, $\rho_g = \frac{1}{2}\left(1 - \sqrt{3(1 - \frac{T}{T_c})}\right)$, $\rho_e = \frac{1}{2}\left(1 + \sqrt{3(1 - \frac{T}{T_c})}\right)$

for $T > T_c$ only $m = 0 \Rightarrow \rho = \frac{1}{2}$ is a solution to the self-consistency equation.

$V = N$ e) with $p = -\frac{\partial \Omega}{\partial V} = -\frac{\partial \Omega}{\partial N} = \frac{1}{\beta}\Big\{ \ln\left(2\cosh\left[\beta\left(J\gamma(2\rho - 1) + H\right)\right]\right)$

$- \frac{\beta J \gamma}{2}(2\rho - 1)^2 + \beta\left(\frac{J\gamma}{2} + \frac{\mu}{2}\right)\Big\}$

$= \frac{1}{\beta} \ln\left(2\cosh\left[\beta\left(J\gamma\left(\frac{2-v}{v}\right) + H\right)\right]\right) - \frac{2J\gamma}{v^2} + \frac{2J\gamma}{v} + \frac{\mu}{2}$

$\Rightarrow p + \frac{2J\gamma}{v^2} = \frac{1}{\beta} \ln\left(2\cosh\left[\beta\left(J\gamma\left(\frac{2-v}{v}\right) + H\right)\right]\right) + \frac{2J\gamma\frac{2}{\mu} + v}{v\frac{2}{\mu}}$

$\Rightarrow \quad \left(p + \frac{2 J \gamma}{v^2}\right)(v-1) = \beta(v-1) \ln\left(2 \cosh\left[\beta\left(J\gamma\left(\frac{2-v}{v}\right)+H\right)\right]\right)$

$$-\frac{2J\gamma}{v} + v\frac{\mu}{2} + 2J\gamma - \frac{\mu}{2}$$

there is quite a difference between the result of our modell in comparison to the van der Waals-gas. One is that the density ρ always has to satisfy the self-consistency equation. Therefore v is either 2 for $T \geq T_c$ or v is a direct function of the time. Thus the degree of freedom is reduced and it makes not that much sense to analyze the behavior of p in dependence of v (this would lead to the fact that for very small p_G and p_{vW} behave the same)

For this reason p is only a function of time (considering $H=0$)

$$p(T) = \begin{cases} \text{for } T \geq T_c & p(T) = p(T, v=2) \\ \text{for } T < T_c & \begin{cases} p(T) = p(T, v_g(T)) \\ p(T) = p(T, v_e(T)) \end{cases} \end{cases}$$

but as seen from $\Omega(T,m)$ is a symetric function of m ($H=0$), it follows $p(T, v_g(T)) = p(T, v_e(T))$
this also shows that there is a phase coexsistance, where the two phases coexsist under the same pressure, while their density stays the same, only their relative volume distribution changes.
So for $T < T_c$ ($H=0$)

$$p(T, \rho(T)) = p(T) = \frac{1}{\beta} \ln\left(2 \cosh\left[\beta J \gamma \sqrt{3}\sqrt{1-\frac{T}{T_c}}\right]\right) - \frac{J\gamma}{2} 3\left(1 - \frac{T}{T_c}\right)$$

$$\underbrace{+\frac{J\gamma}{2} + \frac{\mu_0}{2}}_{} = -\frac{J\gamma}{2}$$

f) $p_c(T)$ is the critical pressure in dependence of T

for which for a certain T the coexistence of the two phases is possible. Because of the lack of stability of $\rho = \frac{1}{2}$ for $T<T_c$, what we earlier mentioned, every pressure from $T<T_c$ enables the coexistence. Therefore the curve $p(T)$ for $T<T_c$ is the ~~critical~~ temperature and depicts the coexistence line

$$p_c(T) = p(T) \quad \text{for } T<T_c$$

$$= \frac{1}{\beta} \ln\left(2\cosh\left[\beta J\gamma\sqrt{3(1-T/T_c)}\right]\right) - \frac{J\gamma}{2}\left(4-3\frac{T}{T_c}\right)$$

the critical point is at

$$(T_c, p_c(T_c)) = \left(T_c,\, k_B T_c \ln(2) - \frac{J\gamma}{2}\right)$$

$$= \left(\frac{J\gamma}{k_B},\, J\gamma\left(\ln(2) - \frac{1}{2}\right)\right)$$

addition to e)

for T very small $\qquad \ln(2\cosh(\beta\alpha)) \simeq \beta\alpha$

$$p(T) \simeq \frac{2J\gamma}{v} - J\gamma + H - \frac{2J\gamma}{v^2} + \frac{2J\gamma}{v} + \frac{\mu}{2}$$

$$= -\frac{2J\gamma}{v^2} + \frac{4J\gamma}{v} + \mu$$