Seth Dorfman Prelims January 6, 2006

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3) a. At $T=\infty$ entropy considerations dominate

$P(\text{cluster of } n \text{ A's}) = x^n$

$$\langle n \rangle = \frac{\sum n x^n}{\sum x^n} = x \frac{\partial}{\partial x} \ln\left(\sum_{n=1}^{\infty} x^n\right)$$

$$= x \frac{\partial}{\partial x} \ln\left(\frac{x}{1-x}\right)$$

$$= x \frac{1-x}{x}\left[\frac{1}{1-x} + \frac{x}{(1-x)^2}\right]$$

$$\langle n \rangle = 1 + \frac{x}{1-x}$$

$$\langle n \rangle = \frac{1}{1-x}$$

b. At $T=0$ energy considerations dominate

neigboring A's have lower energy than AB pairs.

$\therefore$ in the lowest energy configuration

$\langle n \rangle = xN$

c. Let $A \Leftrightarrow s=1$ $B \Leftrightarrow s=-1$

$$\mathcal{H}_1 = 2\left[\frac{-3\varepsilon}{4} - \frac{1}{4}\varepsilon s \langle s \rangle\right]$$

$$\mathcal{H}_1 = \frac{-3\varepsilon}{2} - \frac{1}{2}\varepsilon s\langle s \rangle$$

$$Z_1 = e^{\beta\frac{3\varepsilon}{2}}\left[x e^{\frac{1}{2}\beta\varepsilon\langle s \rangle} + (1-x)e^{-\frac{1}{2}\beta\varepsilon\langle s \rangle}\right]$$

$$Z_1 = e^{\frac{3}{2}\beta\varepsilon}\left[e^{-\frac{1}{2}\beta\varepsilon\langle s \rangle} + 2x\sinh\left(\frac{\beta\varepsilon}{2}\langle s \rangle\right)\right]$$

$$Z = Z_1^N$$

$$F = -k_B T \ln(Z_1) = -Nk_B T \ln(Z)$$

$$F = -Nk_B T\left[\frac{3}{2}\beta\varepsilon + \ln\left(e^{-\frac{1}{2}\beta\varepsilon\langle s \rangle} + 2x\sinh\left(\frac{\beta\varepsilon}{2}\langle s \rangle\right)\right)\right]$$

$$F = -\frac{3}{2}N\varepsilon - Nk_B T \ln\left(e^{-\frac{1}{2}\beta\varepsilon\langle s \rangle} + 2x\sinh\left(\frac{\beta\varepsilon}{2}\langle s \rangle\right)\right)$$

Minimizing with respect to $\langle s \rangle$:

$$\frac{\partial F}{\partial \langle s \rangle} = -Nk_B T\left(\frac{1}{\exp(-\beta\varepsilon\langle s \rangle/2) + 2x\sinh(\beta\varepsilon\langle s \rangle/2)}\right)$$

$$\left(-\frac{1}{2}\beta\varepsilon e^{-\frac{1}{2}\beta\varepsilon\langle s \rangle} + 2x\frac{\beta\varepsilon}{2}\cosh\left(\frac{\beta\varepsilon}{2}\langle s \rangle\right)\right) = 0$$

$$\Rightarrow -e^{\frac{1}{2}\beta\varepsilon\langle s \rangle} + x\left(e^{\frac{1}{2}\beta\varepsilon\langle s \rangle} + e^{-\frac{1}{2}\beta\varepsilon\langle s \rangle}\right) = 0$$

$$(x-1)e^{\frac{1}{2}\beta\varepsilon\langle s \rangle} = -x e^{-\frac{1}{2}\beta\varepsilon\langle s \rangle}$$

$$e^{\beta\varepsilon\langle s \rangle} = \frac{x}{1-x}$$

$$\beta\varepsilon\langle s \rangle = \ln\left(\frac{x}{1-x}\right)$$

$$\langle s \rangle = \frac{k_B T}{\varepsilon}\ln\left(\frac{x}{1+x}\right)$$

$$\therefore F = -\frac{3}{2}N\varepsilon - Nk_B T \ln\left(x\sqrt{\frac{x}{1-x}} + (1-x)\sqrt{\frac{1-x}{x}}\right)$$

Exact calculation:

c. $\mathcal{H}_A = -\varepsilon n_{AA} - \frac{\varepsilon}{2} n_{AB}$

$\mathcal{H}_B = -\varepsilon n_{BB} - \frac{\varepsilon}{2} n_{BA}$

n_{xy} = number of y's that are x's neighbor

$n_{AA} + n_{AB} = 2 \Rightarrow n_{AB} = 2 - n_{AA}$

$n_{BB} + n_{BA} = 2 \Rightarrow n_{BA} = 2 - n_{BA}$

$\mathcal{H}_A = -\frac{\varepsilon}{2} n_{AA} + \varepsilon = -\varepsilon\left(\frac{n_{AA}}{2} + 1\right)$

$\mathcal{H}_B = -\frac{\varepsilon}{2} n_{BB} - \varepsilon = -\varepsilon\left(\frac{n_{BB}}{2} + 1\right)$

$Z_A = \sum_{\text{states}} e^{\beta\varepsilon(n_{AA}/2+1)}$

$$\left.\begin{array}{ll} P(n_{AA}=0) = (1-x)^2 & P(n_{BB}=0) = x^2 \\ P(n_{AA}=1) = 2(1-x)x & P(n_{BB}=1) = 2(1-x)x \\ P(n_{AA}=2) = x^2 & P(n_{BB}=2) = (1-x)^2 \end{array}\right\} \begin{array}{l} A+ \\ T=\infty \end{array}$$

$Z_A = (1-x)^2 e^{\beta\varepsilon} + 2(1-x)x\, e^{\frac{3}{2}\beta\varepsilon} + x^2 e^{2\beta\varepsilon}$

$= e^{\frac{3}{2}\beta\varepsilon}\left[(1-x)^2 e^{-\frac{1}{2}\beta\varepsilon} + 2(1-x)x + x^2 e^{\frac{1}{2}\beta\varepsilon}\right]$

$= e^{\frac{3}{2}\beta\varepsilon}\left[(1-x)e^{-\frac{1}{4}\beta\varepsilon} + x e^{\frac{1}{4}\beta\varepsilon}\right]^2$

$Z_A = e^{\frac{3}{2}\beta\varepsilon}\left[e^{-\frac{1}{4}\beta\varepsilon} + 2x\sinh\left(\frac{\beta\varepsilon}{4}\right)\right]^2$

$Z_B = \sum_{\text{states}} e^{\beta\varepsilon(n_{BB}/2+1)}$

$= x^2 e^{\beta\varepsilon} + 2(1-x)x\, e^{\frac{3}{2}\beta\varepsilon} + (1-y)^2 e^{2\beta\varepsilon}$

$= e^{\frac{3}{2}\beta\varepsilon}\left[x e^{-\frac{1}{4}\beta\varepsilon} + (1-x)e^{\frac{1}{4}\beta\varepsilon}\right]^2$

$Z_B = e^{\frac{3}{2}\beta\varepsilon}\left[e^{\frac{1}{4}\beta\varepsilon} - 2x\sinh\left(\frac{\beta\varepsilon}{4}\right)\right]^2$

$Z = Z_A^{Nx} Z_B^{N(1-x)}$ atoms independenty distributed

$Z = \left[e^{\frac{3}{2}\beta\varepsilon}\left(e^{-\frac{1}{4}\beta\varepsilon} + 2x\sinh\left(\frac{\beta\varepsilon}{4}\right)\right)^{2x}\left(e^{\frac{1}{4}\beta\varepsilon} - 2x\sinh\left(\frac{\beta\varepsilon}{4}\right)\right)^{2(1-x)}\right]^N$

$F = -k_B T \ln Z$

$F = -Nk_BT\left[\frac{3}{2}\beta\varepsilon + 2x\ln\left(e^{-\frac{1}{4}\beta\varepsilon} + 2x\sinh\left(\frac{\beta\varepsilon}{4}\right)\right) + 2(1-x)\ln\left(e^{\frac{1}{4}\beta\varepsilon} - 2x\sinh\left(\frac{\beta\varepsilon}{4}\right)\right)\right]$

$F = -\frac{3}{2}N\varepsilon - 2Nk_BT\left[x\ln\left(e^{-\frac{1}{4}\beta\varepsilon} + 2x\sinh\left(\frac{\beta\varepsilon}{4}\right)\right) + (1-x)\ln\left(e^{\frac{1}{4}\beta\varepsilon} - 2x\sinh\left(\frac{\beta\varepsilon}{4}\right)\right)\right]$

d. The value in part (c) is a variational upper limit on the free energy.

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#3 (continued)

e. $Z_1(x=\frac{1}{2}) = e^{\beta\frac{3\epsilon}{2}} \cdot 2\cosh\left(\frac{\beta\epsilon}{2}\langle s\rangle\right)$ Let $\alpha = \frac{\beta\epsilon}{2}\langle s\rangle$

$= e^{\beta\frac{3\epsilon}{2}} \sum_{\text{states}} e^{\frac{1}{2}\beta\epsilon s\langle s\rangle}$

$\therefore \langle s\rangle = \frac{\partial}{\partial\alpha}\ln(2\cosh(\alpha))$

$\langle s\rangle = \tanh(\alpha)$

$\langle s\rangle = \tanh\left(\frac{\beta\epsilon}{2}\langle s\rangle\right)$

$\frac{\partial\langle s\rangle}{\partial\langle s\rangle} = \frac{\beta\epsilon}{2}\operatorname{sech}^2\left(\frac{\beta\epsilon}{2}\langle s\rangle\right) = 1$ at T_c

$\Rightarrow k_B T_c = \frac{\epsilon}{2}$

$T_c = \frac{\epsilon}{2k_B}$

f. If we have a set of domains at small T:

AAAA | BBB | AAAAAAA | BBBBB

If an A and B by a domain wall switch places there will be a net <u>increase</u> in energy. Thus as T decreases, the system will stay in a local minimum of energy rather than condensing to the absolute minimum.