

Seth Dorfman

Prelims January 6, 2006

May 2004 SM

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

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

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

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

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

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

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

b. At  $T = 0$  energy considerations dominate

neighboring A's have lower energy than AB pairs.

$\therefore$  in the lowest energy configuration

$$\langle n \rangle = xN$$

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

$$H_1 = 2 \left[ -\frac{3E}{4} + \frac{1}{4} E \langle s \rangle \right]$$

$$Z_A H_1 = e^{-\frac{3E}{2T}} \left[ x e^{\frac{1}{2} \beta E \langle s \rangle} + (1-x) e^{-\frac{1}{2} \beta E \langle s \rangle} \right]$$

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

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

$$F_A = -N \ln Z_1$$

$$F_A = -N k_B T \ln Z_1 = -N k_B T \ln Z$$

$$F_A = -N k_B T \left[ -\frac{3}{2} \beta E + \ln \left( e^{-\frac{1}{2} \beta E \langle s \rangle} + 2x \sinh \left( \frac{\beta E}{2} \langle s \rangle \right) \right) \right]$$

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

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

$$\frac{\partial F}{\partial \langle s \rangle} = -N k_B T \left( \frac{\exp(-\beta E \langle s \rangle / 2) + 2x \cosh(\beta E \langle s \rangle / 2)}{e^{-\frac{1}{2} \beta E \langle s \rangle} + 2x \sinh(\frac{\beta E}{2} \langle s \rangle)} \right)$$

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

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

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

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

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

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

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

Exact calculation:

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

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

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

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

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

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

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

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

$$P(n_{AA} = 0) = (1-x)^2$$

$$P(n_{BB} = 0) = x^2$$

$$P(n_{AA} = 1) = 2(1-x)x$$

$$P(n_{BB} = 1) = 2(1-x)x$$

$$P(n_{AA} = 2) = x^2$$

$$P(n_{BB} = 2) = (1-x)^2$$

}  $A+$   
 $T=\infty$

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

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

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

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

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

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

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

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

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

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

$$F = -k_B T \ln Z$$

$$F = -N k_B T \left[ \frac{3}{2} \beta \epsilon + 2x \ln \left( e^{-\frac{1}{4}\beta \epsilon} + 2x \sinh\left(\frac{\beta \epsilon}{4}\right) \right) \right.$$

$$\left. + 2(1-x) \ln \left( e^{\frac{1}{4}\beta \epsilon} - 2x \sinh\left(\frac{\beta \epsilon}{4}\right) \right) \right]$$

$$F = -\frac{3}{2} N \epsilon - 2 N k_B T \left[ x \ln \left( e^{-\frac{1}{4}\beta \epsilon} + 2x \sinh\left(\frac{\beta \epsilon}{4}\right) \right) \right.$$

$$\left. + (1-x) \ln \left( e^{\frac{1}{4}\beta \epsilon} - 2x \sinh\left(\frac{\beta \epsilon}{4}\right) \right) \right]$$

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

Seth Dorfman

Prelims

January 6, 2006

May 2004 SM

#3 (continued)

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

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

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

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

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

$$A \Rightarrow T K_B T_c = \frac{E}{2}$$

$$T_c = \frac{E}{2K_B}$$

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

AAAA|BBBB|AAAAAAA|BBBBB

If an A and B by a domain wall switch all places there will be a net increase in energy.

Thus as T decreases, the system will stay in a local minimum of energy rather than condensing to the absolute minimum.