$\boxed{A13}$ (HW 2010 3.2)

N atoms, N sites, M atoms shifted to alternative sites numbered N'. Each such defect costs w energy. $N' \sim N$.

a) # of defects:

$$Z_M = \underbrace{\binom{N}{M}}_{\text{choose } M \text{ atoms from the } N \text{ available}} \underbrace{\binom{N'}{M}}_{\text{chose } M \text{ defect sites from the } N' \text{ available}} e^{-\beta w M} \leftarrow \text{canonical: } \left(\text{Assume } M \text{ is known}\right)$$

$$\ln Z = N\ln N - \cancel{N} - M\ln M - (N-M)\ln(N-M) + N'\ln N' - M\ln M - (N'-M)\ln(N'-M) - \beta w M$$

extremize the free energy with respect to M

$$\frac{\partial \ln Z}{\partial M} = 0 \rightarrow -\ln M \cancel{-1} + \ln(N-M) \cancel{+1} - \ln M \cancel{-1} + \ln(N'-M) \cancel{+1} - \beta w = 0$$

$$\rightarrow \ln\left(\frac{(N-M)(N'-M)}{M^2}\right) = \beta w$$

for $\left\{\begin{matrix} M \ll \{N, N'\} \\ e^{-\beta w} \ll 1 \end{matrix}\right\}$

$$\beta w \approx \ln\left(\frac{NN'}{M^2}\right)$$

$$M = \sqrt{NN'}\, e^{-\beta w/2}$$

Grand Canonically: $N_{defect} \longleftrightarrow N_{site} + w$ פקס ספים

$$\Omega_1 = 1 + e^{\beta(\mu - w)}$$

ספק פגם טיס

$$\Omega_{N'} = \Omega_1^{N'}, \quad M = kT \frac{\partial \ln \Omega_{N'}}{\partial \mu} = N' \frac{e^{\beta(\mu-w)}}{e^{\beta(\mu-w)} + 1} = N' \frac{1}{1 + e^{-\beta(\mu - w)}}$$

$$\tilde{\Omega}_1 = 1 + e^{\beta\mu} \rightarrow \tilde{\Omega}_N = \tilde{\Omega}_1^{N}$$

לא פגמים

$$(N - M) = \frac{N}{1 + e^{-\beta\mu}} \rightarrow \boxed{e^{-\beta\mu} = \frac{N}{(N-M)} - 1 = \frac{M}{N}}$$

$$M = \frac{N'}{1 + \frac{M}{N}e^{\beta w}} = \frac{NN'}{1 + Me^{\beta w}} \approx \frac{NN'}{Me^{\beta w}} \rightarrow \boxed{M = \sqrt{NN'}\, e^{-\frac{\beta w}{2}}}$$