

Hubbard - Slater sum

- a) The energy needs to be extensive and $\sum_{i=1}^N \sum_{j=1}^N S_i S_j \sim O(N^2)$

Therefore J_{00} needs to be $O(1/N)$

- b) Completing the square:

$$-\frac{Na}{2} y^2 + axy = -\frac{Na}{2} \left[y^2 - \frac{2}{N} xy + \frac{x^2}{N^2} - \frac{x^2}{N^2} \right] = -\frac{Na}{2} \left(y - \frac{x}{N} \right)^2 + \frac{a}{2N} x^2$$

Hence:

$$\int dy \sqrt{\frac{Na}{2\pi}} e^{-\frac{Na}{2} y^2 + axy} = e^{\frac{a}{2N} x^2} \int dy \sqrt{\frac{Na}{2\pi}} e^{-\frac{Na}{2} \left(y - \frac{x}{N} \right)^2} =$$

$$\text{let } z = y - x/N \quad dz = dy$$

$$= e^{\frac{a}{2N} x^2} \int dz \sqrt{\frac{Na}{2\pi}} e^{-\alpha z^2} \quad \alpha = \frac{Na}{2}$$

$$\text{Since: } \int dz e^{-\alpha z^2} = \sqrt{\frac{\pi}{\alpha}}$$

$$\Rightarrow e^{\frac{a}{2N} x^2} = \int dy \sqrt{\frac{Na}{2\pi}} e^{-\frac{Na}{2} y^2 + axy}$$

- c) Let $x = \sum_{i=1}^N S_i$ so that the energy can be written: (introduce $J_0 = J/N$)

$$E = -\frac{J}{2N} \sum_i \sum_j S_i S_j - H \sum S_i = -\frac{J}{2N} x^2 - Hx$$

Hence the partition function:

$$Z = \sum_{S_1=-1}^1 \sum_{S_2} \dots \sum_{S_N} e^{-\beta E} = \sum \dots \int e^{\frac{\beta J}{2N} x^2 + \beta Hx} =$$

$$= \int dy \sqrt{\frac{JN}{2\pi k_B T}} e^{-\frac{J\beta N}{2} y^2} \left(\sum \dots \sum e^{\beta x(H+Jy)} \right)$$

$$= \int dy \sqrt{\frac{JN}{2\pi k_B T}} e^{-\frac{J\beta N}{2} y^2} \left(\sum_{S_i \text{ all } i} e^{\beta x(H+Jy)} \right)^N =$$

$$= \int dy \sqrt{\frac{JN}{2\pi k_B T}} e^{-\frac{J\beta N}{2} y^2} 2 \cosh^N \beta (H + Jy)$$

Then:

$$\begin{aligned} Z &= \int dy \sqrt{\frac{JN}{2\pi k_B T}} \cdot e^{-\frac{J\beta N}{2} y^2} e^{\ln 2 \cosh^N \beta (H + Jy)} = \\ &= \int dy \sqrt{\frac{JN}{2\pi k_B T}} e^{-N\beta \left[\frac{J}{2} y^2 - k_B T \ln (2 \cosh \beta (H + Jy)) \right]} \end{aligned}$$

$$\text{Finally: } Z = \int dy \sqrt{\frac{JN}{2\pi k_B T}} e^{-\beta N L(y)} \quad L(y) = \frac{J}{2} y^2 - k_B T \ln (2 \cosh \beta (H + Jy))$$

d) In the thermodynamic limit of $N \rightarrow \infty$ we approximate the integral by the value of the integrand at its (discrete) maximum:

$$Z = \sum_{\alpha} e^{-\beta N L(y_{\alpha})}$$

$$0 = \frac{\partial L(y)}{\partial y} = Jy_{\alpha} - k_B T \frac{2 \sinh \beta (H + Jy_{\alpha})}{2 \cosh \beta (H + Jy_{\alpha})} \quad \beta J \rightarrow 0$$

$$\Rightarrow \boxed{y_{\alpha} = \tanh \beta (Jy_{\alpha} + H)} \quad \text{Same expression found in mean field.}$$

There are potentially three solutions.

If we restrict $y_{\alpha} = y_0$, one minimum maximum of probability; i.e.,

$$m_0 = \frac{k_B T}{N} \frac{\partial \ln Z}{\partial H} = \langle y \rangle \approx y_0 \quad \text{since } \ln Z = \ln e^{-\beta N L(y_0)} = -\beta N L(y_0)$$

$$\Rightarrow \frac{\partial \ln Z}{\partial H} = -\beta \left[-\frac{1}{\beta} \frac{2 \sinh \beta (H + Jy)}{2 \cosh \beta (H + Jy)} \right] =$$

$$= N \beta \tanh \beta (H + Jy)$$

$$\rightarrow m_0 = y_0.$$

f) y_0 is a function of H :

$$\frac{\partial y_0}{\partial H} = \operatorname{sech}^2 \rho(H + Jy_0) \left[\rho + \rho J \frac{\partial y_0}{\partial H} \right] \quad \text{from } y_0 = \tanh \rho(H + Jy_0)$$

$$\Rightarrow \frac{\partial y_0}{\partial H} [1 - \rho J \operatorname{sech}^2 \rho(H + Jy_0)] = \rho \operatorname{sech}^2 \rho(H + Jy_0)$$

$$\Rightarrow \chi = \frac{\partial y_0}{\partial H} = \rho \frac{\operatorname{sech}^2 \rho J y_0}{1 - \rho J \operatorname{sech}^2 \rho J y_0} \quad \text{which diverges as } y_0 \rightarrow 0 \text{ at } \rho J = 1, \text{ the critical point.}$$