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Total energy

$$E = K_B \sum_i E_i^H + \frac{K_B Z}{2AD^2} (AA - AA_0)^2$$

$$= E^H + E^{ADE}$$

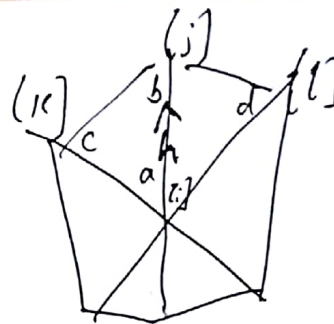
local Hdfrah energy.

$$E_i^H = \frac{1}{2} K_B (2H_i - 2H_0)^2 A_i \quad \text{with } H_0 = \frac{C_0}{2}$$

non-local ADE energy.

$$AA = 2D \sum_i H_i A_i \quad AA_0 = 2D H_0 A$$

$$E^{AD} = 2 \left[2D \left(\sum_i H_i A_i \right) - H_0 A \right]^2$$



$$H_i = \frac{1}{2} A_s X \cdot n$$

$$H_i^2 = \frac{1}{4} (A_s X)^2$$

$$\frac{\partial H_i}{\partial x_j} = \frac{1}{2H_i} \frac{\partial (H_i^2)}{\partial x_j} = \frac{1}{8H_i} \frac{\partial (A_s X^2)}{\partial x_j}$$

$$\frac{\partial E_i^H}{\partial x_j} = K_B (2H_i - 2H_0) A_i \cdot 2 \frac{\partial H_i}{\partial x_j} + \frac{1}{2} \frac{(2H_i - 2H_0)^2}{2(H_i - H_0)^2} \frac{\partial A_i}{\partial x_j}$$

$$F = - \frac{\partial E_i^H}{\partial x_{ik}}$$

$$= 2(H_i - H_0) K_B \left[2A_i \frac{\partial H_i}{\partial x_j} + (H_i - H_0) \frac{\partial A_i}{\partial x_j} \right]$$

$$= 2(H_i - H_0) K_B \left[\underbrace{\frac{A_i}{4H_i} \frac{\partial (A_s X^2)}{\partial x_j}}_{I, II} + \underbrace{(H_i - H_0) \frac{\partial A_i}{\partial x_j}}_{III} \right] \checkmark$$

$$\frac{\partial E^{AD}}{\partial x_j} = 22 \left[2D \left(\sum_i H_i A_i - H_0 A \right) \right] \left[2D \sum_i \left(\frac{\partial H_i}{\partial x_j} A_i + H_i \frac{\partial A_i}{\partial x_j} \right) \right]$$

$$= 82D^2 \left(\sum_i H_i A_i - H_0 A \right) \sum_i \left(\frac{\partial H_i}{\partial x_j} A_i + H_i \frac{\partial A_i}{\partial x_j} \right)$$

$$= \frac{4K_B Z}{A} \left(\sum_i H_i A_i - H_0 A \right) \sum_i \left[\underbrace{\frac{A_i}{8H_i} \frac{\partial (A_s X^2)}{\partial x_j}}_{I, II} + \underbrace{H_i \frac{\partial A_i}{\partial x_j}}_{III} \right] \checkmark$$

$$\Delta_s X_i = \frac{\sum_{ij} (\omega_{t_1}^{ij} + \omega_{t_2}^{ij}) (X_i - X_j)}{2 A_i = \frac{1}{4} \sum_{ij} (\omega_{t_1}^{ij} + \omega_{t_2}^{ij}) X_{ij}^2} = \frac{4 \sum_{ij} T_{ij} X_{ij}}{\sum_{ij} T_{ij} X_{ij}^2}$$

$$A_i = \frac{1}{8} \sum_{ij} (\omega_{t_1}^{ij} + \omega_{t_2}^{ij}) |X_i - X_j|^2 = \frac{1}{8} \sum_{ij} T_{ij} X_{ij}^2$$

$$(\Delta_s X_i)^2 = 16 \left[\frac{\sum_{ij} (T_{ij} X_{ij})}{\sum_{ij} T_{ij} X_{ij}^2} \right]^2$$

$$\frac{1}{8} \sum_{ij} T_{ij} X_{ij}^2 = A_i$$

$$\begin{cases} T_{ij} = (\omega_{t_1}^{ij} + \omega_{t_2}^{ij}) \\ X_{ij} = X_i - X_j \end{cases}$$

i, j, k are indices for position.
m direction such as x, y, z.

$$\frac{\partial (\Delta_s X_i)^2}{\partial X_k^m} = 32 \left(\frac{\sum_{ij} T_{ij} X_{ij}}{\sum_{ij} T_{ij} X_{ij}^2} \right) \cdot \left[\frac{\sum_{ij} \left(\frac{\partial X_{ij}}{\partial X_k^m} T_{ij} + \frac{\partial T_{ij}}{\partial X_k^m} X_{ij} \right)}{\sum_{ij} T_{ij} X_{ij}^2} - \frac{\left(\sum_{ij} T_{ij} X_{ij} \right) \left[\sum_{ij} T_{ij} X_{ij} \frac{\partial X_{ij}}{\partial X_k^m} + X_{ij}^2 \frac{\partial T_{ij}}{\partial X_k^m} \right]}{\left(\sum_{ij} T_{ij} X_{ij}^2 \right)^2} \right]$$

$$= 8 \Delta_s X_i \cdot \left[\frac{\sum_{ij} \frac{\partial X_{ij}}{\partial X_k^m} T_{ij} + \frac{\partial T_{ij}}{\partial X_k^m} X_{ij}}{8 A_i} \right] - 8 \Delta_s X_i \frac{1}{4} \cdot \Delta_s X_i \frac{1}{8 A_i} \left[\sum_{ij} 2 T_{ij} X_{ij} \frac{\partial X_{ij}}{\partial X_k^m} + X_{ij}^2 \frac{\partial T_{ij}}{\partial X_k^m} \right]$$

$$= \Delta_s X_i \cdot \frac{\sum_{ij} \frac{\partial X_{ij}}{\partial X_k^m} T_{ij}}{A_i} - \frac{(\Delta_s X_i)^2}{4 A_i} \sum_{ij} 2 T_{ij} X_{ij} \cdot \frac{\partial X_{ij}}{\partial X_k^m}$$

$$+ \Delta_s X_i \cdot \frac{\sum_{ij} \frac{\partial T_{ij}}{\partial X_k^m} X_{ij}}{A_i} - \frac{(\Delta_s X_i)^2}{4 A_i} \sum_{ij} X_{ij}^2 \frac{\partial T_{ij}}{\partial X_k^m}$$

$$\frac{\partial A_i}{\partial X_k^m} = \frac{1}{8} \sum_{ij} \frac{\partial T_{ij}}{\partial X_k^m} X_{ij}^2 + T_{ij} \frac{\partial X_{ij}^2}{\partial X_k^m} = \frac{1}{8} \sum_{ij} 2 T_{ij} X_{ij} \cdot \frac{\partial X_{ij}}{\partial X_k^m} + \frac{1}{8} \sum_{ij} X_{ij}^2 \frac{\partial T_{ij}}{\partial X_k^m}$$