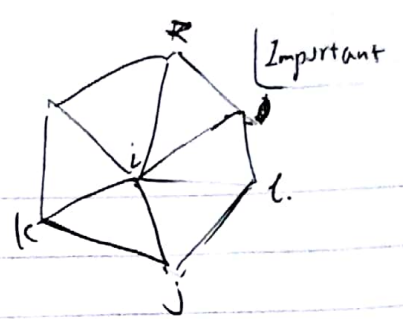


Force calculation



14.Sep.2018 and revised on 17.Sep.2018

Jülicher 1996

$$\checkmark E = K_b \sum_i^N E_i = K_b \sum_i 2(H_i - H_0)^2 A_i > E_i = 2 \left(\frac{H_i}{A_i} - H_0 \right)^2 A_i > E_i = 2 \left(\frac{1}{4A_i} \sum_e l_e \theta_e - H_0 \right)^2 A_i \checkmark$$

$$H_i = \frac{\hat{H}_i}{A_i} \quad \hat{H}_i = \frac{1}{4} \sum_e l_e \theta_e$$

$$E_i = 2 \left(\frac{1}{16A_i^2} \left(\sum_e l_e \theta_e \right)^2 - \frac{H_0}{2A_i} \sum_e l_e \theta_e + H_0^2 \right) A_i \checkmark$$

$$= \frac{1}{8A_i} \left(\sum_e l_e \theta_e \right)^2 - H_0 \sum_e l_e \theta_e + 2H_0^2 A_i \checkmark$$

$$A_i = \frac{1}{3} \sum_{t: i \in t} A_t \checkmark$$

$$- \frac{\partial E_i}{\partial s} \Bigg) = - \frac{2 \sum_e l_e \theta_e}{8A_i} \sum_e \left(\frac{\partial l_e}{\partial s} \theta_e + l_e \frac{\partial \theta_e}{\partial s} \right) + \left(\sum_e l_e \theta_e \right)^2 \frac{1}{8A_i^2} \frac{\partial A_i}{\partial s} + H_0 \sum_e \left(\frac{\partial l_e}{\partial s} \theta_e + l_e \frac{\partial \theta_e}{\partial s} \right) - 2H_0^2 \frac{\partial A_i}{\partial s}$$

$$= - \frac{\sum_e l_e \theta_e}{4A_i} \sum_e \left(\frac{\partial l_e}{\partial s} \theta_e + l_e \frac{\partial \theta_e}{\partial s} \right) + \frac{\left(\sum_e l_e \theta_e \right)^2}{8A_i^2} \frac{\partial A_i}{\partial s} + H_0 \sum_e \left(\frac{\partial l_e}{\partial s} \theta_e + l_e \frac{\partial \theta_e}{\partial s} \right) - 2H_0^2 \frac{\partial A_i}{\partial s}$$

Implementation: pseudo code.

loop 1: loop over each edge $e: \langle i, j \rangle$ and calculate l_e and θ_e so that at each vertex i and j , we have $\text{len}(\theta_e, l_i) \neq \text{len}(\theta_e, l_j) \neq l_e \cdot \theta_e$

loop 2: loop over each triangle t and calculate each A_t and split into $t: \langle i, j, k \rangle$ with $A_i = A_t$ $A_j = \frac{1}{3} A_t$ $A_k = \frac{1}{3} A_t$

loop 3: loop over each edge again. calculate $\frac{\partial l_e}{\partial s}$. calculate $\frac{\partial \theta_e}{\partial s}$: refer to Kohn-Sham force calculation

$$l_e = l_{ij} = \left[(x_i - x_j)^2 + (y_i - y_j)^2 \right]^{1/2}$$

$$\frac{\partial l_e}{\partial x_k} = \frac{1}{2} \frac{1}{l_e} \frac{\partial (x_i - x_j)^2}{\partial x_k} = \frac{(x_i - x_j)}{l_e} \frac{\partial (x_i - x_j)}{\partial x_k} = \frac{(x_i - x_j)}{l_e} (\delta_{ik} - \delta_{jk})$$

loop 4: loop over each triangle t and calculate $\frac{\partial A_t}{\partial s}$ and split contribution to i, j, k vertices

$$\frac{\partial A_i}{\partial s} = \frac{1}{3} \sum \frac{\partial A_t}{\partial s}$$