The **discretized energy** E can be expressed as:

$$E = \sum_{i=1}^{J} \sum_{\substack{j=1 \\ |j-i|>1}} k_{i,j} ||x_{i+1} - x_i|| \, ||x_{j+1} - x_j|| \tag{1}$$

$$k_{i,j} = \frac{1}{4} \left(k_\beta^\alpha \left(x_i, x_j, T_i \right) + k_\beta^\alpha \left(x_i, x_{j+1}, T_i \right) + k_\beta^\alpha \left(x_{i+1}, x_j, T_i \right) + k_\beta^\alpha \left(x_{i+1}, x_{j+1}, T_i \right) \right) \tag{2}$$

where we index cyclically.

For derivative with respect to x_k (note that it is a vector), the only terms indexed by (i, j) that involves x_k are enumerated by the following indices:

- $(k, 1), \cdots, (k, k-2), (k, k+2), \cdots, (k, J)$
- $(k-1, 1), \cdots, (k-1, k-3), (k-1, k+1), \cdots, (k-1, J)$
- $(1, k), \cdots, (k-2, k), (k+2, k), \cdots, (J, k)$
- $(1, k-1), \cdots, (k-3, k-1), (k+1, k-1), \cdots, (J, k-1)$

We now attempt to construct derivative (in a "modular fashion"). Write

$$\begin{aligned} k_\beta^\alpha \left(x_p, x_q, T_r \right) &= k_\beta^\alpha \left(x_p, x_q, \frac{x_{r+1} - x_r}{||x_r - x_{r+1}||} \right) && (3) \\ &= \frac{\sqrt{||x_{r+1} - x_r||^2 ||x_p - x_q||^2 - \left((x_{r+1} - x_r) \cdot (x_p - x_q) \right)^2}^{\,\alpha}}{||x_p - x_q||^\beta ||x_r - x_{r+1}||^\alpha} && (4) \\ &= \frac{\xi_{p,q,r}^{\alpha/2}}{\eta_{p,q,r}} && (5) \end{aligned}$$

where

$$\xi_{p,q,r} = ||x_{r+1} - x_r||^2 ||x_p - x_q||^2 - \left((x_{r+1} - x_r) \cdot (x_p - x_q) \right)^2 \tag{6}$$

$$\eta_{p,q,r} = ||x_p - x_q||^\beta ||x_r - x_{r+1}||^\alpha \tag{7}$$

Derivative with respect to x_k can now be written as:

$$\frac{\partial}{\partial x_k} \left(\frac{\xi^{\alpha/2}}{\eta} \right) = \frac{1}{\eta^2} \left(\frac{\alpha}{2} \xi^{\alpha/2-1} \frac{\partial \xi}{\partial x_k} \eta - \xi^{\alpha/2} \frac{\partial \eta}{\partial x_k} \right) \tag{8}$$

where p, q, r are omitted.

1 $(p, q, r) = (k, j, k)$

$$\xi_{k,j,k} = ||x_{k+1} - x_k||^2 ||x_k - x_j||^2 - \left((x_{k+1} - x_k) \cdot (x_k - x_j) \right)^2 \tag{9}$$

$$\eta_{k,j,k} = ||x_k - x_j||^\beta ||x_k - x_{k+1}||^\alpha \tag{10}$$

Taking derivative of $\xi_{k,j,k}$ with respect to x_k,

$$\begin{aligned} \frac{\partial \xi_{k,j,k}}{\partial x_k} &= 2 \left(x_k - x_{k+1} \right) ||x_k - x_j||^2 && (11) \\ &+ 2 ||x_{k+1} - x_k||^2 \left(x_k - x_j \right) && (12) \\ &- 2 \left(x_{k+1} - x_k \right) \cdot \left(x_k - x_j \right) \left(x_j + x_{k+1} - 2x_k \right) && (13) \end{aligned}$$