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

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

where

$$\begin{aligned} \xi_{p,q,r} &= ||x_{r+1} - x_r||^2 ||x_p - x_q||^2 - \left(\left(x_{r+1} - x_r\right) \cdot \left(x_p - x_q\right)\right)^2 && (6) \\ \eta_{p,q,r} &= ||x_p - x_q||^\beta ||x_r - x_{r+1}||^\alpha && (7) \end{aligned}$$

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.