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

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

where

$$\xi_{p,q,r} = ||x_{r+1} - x_r||^2 ||x_p - x_q||^2 - \left((x_{r+1} - x_r) \cdot (x_p - x_q)\right)^2 \tag{4}$$

$$\eta_{p,q,r} = ||x_p - x_q||^\beta ||x_r - x_{r+1}||^\alpha \tag{5}$$

Derivative with respect to x_k can now be written as:

$$\frac{\partial}{\partial x_k} \left(\frac{\xi^{\alpha/2}}{\eta} \right) = \frac{1}{\eta^2} \left(\frac{\alpha}{2} \xi^{\alpha/2 - 1} \frac{\partial \xi}{\partial x_k} \eta - \xi^{\alpha/2} \frac{\partial \eta}{\partial x_k} \right) \tag{6}$$

where p, q, r are omitted.

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

$$\xi_{k,j,k} = ||x_{k+1} - x_k||^2 ||x_k - x_j||^2 - \left((x_{k+1} - x_k) \cdot (x_k - x_j)\right)^2 \tag{7}$$

$$\eta_{k,j,k} = ||x_k - x_j||^\beta ||x_k - x_{k+1}||^\alpha \tag{8}$$

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

$$\frac{\partial \xi_{k,j,k}}{\partial x_k} = 2\left(x_k - x_{k+1}\right)||x_k - x_j||^2 \tag{9}$$
$$+ 2||x_{k+1} - x_k||^2 \left(x_k - x_j\right) \tag{10}$$
$$- 2\left(x_{k+1} - x_k\right) \cdot \left(x_k - x_j\right)\left(x_j + x_{k+1} - 2x_k\right) \tag{11}$$

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

$$\frac{\partial \eta_{k,j,k}}{\partial x_k} = \beta||x_k - x_j||^{\beta-2}||x_k - x_{k+1}||^{\alpha}\left(x_k - x_j\right) \tag{12}$$
$$+ \alpha||x_k - x_j||^{\beta}||x_k - x_{k+1}||^{\alpha-2}\left(x_k - x_{k+1}\right) \tag{13}$$

2 $(p,q,r) = (i,j,k)$ where $i \neq k$ or $i \neq k-1$

$$\xi_{i,j,k} = ||x_{k+1} - x_k||^2||x_i - x_j||^2 - \left(\left(x_{k+1} - x_k\right) \cdot \left(x_i - x_j\right)\right)^2 \tag{14}$$
$$\eta_{i,j,k} = ||x_i - x_j||^{\beta}||x_k - x_{k+1}||^{\alpha} \tag{15}$$

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

$$\frac{\partial \xi_{i,j,k}}{\partial x_k} = 2||x_i - x_j||^2\left(x_k - x_{k+1}\right) \tag{16}$$
$$- 2\left(x_{k+1} - x_k\right) \cdot \left(x_i - x_j\right)\left(x_j - x_i\right) \tag{17}$$

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

$$\frac{\partial \eta_{i,j,k}}{\partial x_k} = \alpha||x_i - x_j||^{\beta}||x_k - x_{k+1}||^{\alpha-2}\left(x_k - x_{k+1}\right) \tag{18}$$

3 $(p,q,r) = (k-1,j,k-1)$

$$\xi_{k-1,j,k-1} = ||x_k - x_{k-1}||^2||x_{k-1} - x_j||^2 - \left(\left(x_k - x_{k-1}\right) \cdot \left(x_{k-1} - x_j\right)\right)^2 \tag{19}$$
$$\eta_{k-1,j,k-1} = ||x_{k-1} - x_j||^{\beta}||x_{k-1} - x_k||^{\alpha} \tag{20}$$

Taking derivative of $\xi_{k-1,j,k-1}$ with respect to x_k,

$$\frac{\partial \xi_{k-1,j,k-1}}{\partial x_k} = 2||x_{k-1} - x_j||^2\left(x_k - x_{k-1}\right) \tag{21}$$
$$- 2\left(x_k - x_{k-1}\right) \cdot \left(x_{k-1} - x_j\right)\left(x_{k-1} - x_j\right) \tag{22}$$

Taking derivative of $\eta_{k-1,j,k-1}$ with respect to x_k,

$$\frac{\partial \eta_{k-1,j,k-1}}{\partial x_k} = \alpha||x_{k-1} - x_j||^{\beta}||x_k - x_{k-1}||^{\alpha-2}\left(x_k - x_{k-1}\right) \tag{23}$$