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

$$k_\beta^\alpha \left(x_k, x_j, T_k\right) = k_\beta^\alpha \left(x_k, x_j, \frac{x_{k+1} - x_k}{||x_k - x_{k+1}||} \right) \tag{3}$$

$$= \frac{\sqrt{||x_{k+1} - x_k||^2 ||x_k - x_j||^2 - \left((x_{k+1} - x_k) \cdot (x_k - x_j)\right)^2}^{\,\alpha}}{||x_k - x_j||^\beta ||x_k - x_{k+1}||^\alpha} \tag{4}$$

$$= \frac{\xi_{k,j}^{\alpha/2}}{\eta_{k,j}} \tag{5}$$

where $\xi_{k,j} \coloneqq ||x_{k+1} - x_k||^2 ||x_k - x_j||^2 - \left((x_{k+1} - x_k) \cdot (x_k - x_j)\right)^2$ and $\eta_{k,j} = ||x_k - x_j||^\beta ||x_k - x_{k+1}||^\alpha$.

Then we may write the derivative for this "kernel" as:

$$\frac{\partial k_\beta^\alpha \left(x_k, x_j, T_k\right)}{\partial x_k} = \frac{1}{\eta_{k,j}^2} \left(\frac{\alpha}{2} \xi_{k,j}^{\alpha/2-1} \frac{\partial \xi_{k,j}}{\partial x_k} \eta_{k,j} - \xi_{k,j}^{\alpha/2} \frac{\partial \eta_{k,j}}{\partial x_k} \right) \tag{6}$$

Where the derivative for ξ and η, are given by:

$$\begin{aligned}
\frac{\partial \xi_{k,j}}{\partial x_k} &= 2\left(x_k - x_{k+1}\right)||x_k - x_j||^2 + 2||x_{k+1} - x_k||^2(x_k - x_j) \\
&\quad - 2\left(\left(x_{k+1} - x_k\right)\cdot\left(x_k - x_j\right)\right)\left(x_j + x_{k+1} - 2x_k\right) && (7) \\
\frac{\partial \eta_{k,j}}{\partial x_k} &= \beta||x_k - x_j||^{\beta-2}(x_k - x_j)||x_k - x_{k+1}||^{\alpha} \\
&\quad + ||x_k - x_j||^{\beta}\alpha||x_k - x_{k+1}||^{\alpha-2}(x_k - x_{k+1}) && (8) \\
\frac{\partial \xi_{k-1,j}}{\partial x_k} &= 2||x_{k-1} - x_j||^2(x_k - x_{k-1}) - 2\left(\left(x_k - x_{k-1}\right)\cdot\left(x_{k-1} - x_j\right)\right)\left(x_{k-1} - x_j\right) && (9) \\
\frac{\partial \eta_{k-1,j}}{\partial x_k} &= ||x_{k-1} - x_j||^{\beta}\alpha||x_k - x_{k-1}||^{\alpha-2}(x_k - x_{k-1}) && (10) \\
\frac{\partial \xi_{j,k}}{\partial x_k} &= 2||x_{j+1} - x_j||^2(x_k - x_j) - 2\left(\left(x_{j+1} - x_j\right)\cdot\left(x_k - x_j\right)\right)\left(x_{j+1} - x_j\right) && (11) \\
\frac{\partial \eta_{j,k}}{\partial x_k} &= ||x_j - x_{j+1}||^{\alpha}\beta||x_k - x_j||^{\beta-2}\left(x_k - x_j\right) && (12) \\
& && (13)
\end{aligned}$$

and

$$\frac{\partial \eta_{j,k-1}}{\partial x_k} = \frac{\partial \xi_{j,k-1}}{\partial x_k} = 0 \qquad (14)$$

Now, the derivative of energy can be written as:

$$\frac{\partial E}{\partial x_k} = \sum\left(\frac{\partial k_{i,j}}{\partial x_k}||x_{i+1} - x_i||||x_{j+1} - x_j|| + k_{i,j}\frac{\partial}{\partial x_k}\left(||x_{i+1} - x_i||||x_{j+1} - x_j||\right)\right) \qquad (15)$$

where (i, j) are as enumerated in the beginning. Note that due to the "separation of i and j", one of the norms in the $\frac{\partial}{\partial x_k}\left(||x_{i+1} - x_i||||x_{j+1} - x_j||\right)$ term is a constant.