For an function

$$V(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sum_{\text{pairs}} r_{ij}^n \tag{1}$$

that defines the energy where atoms $\{i\}$ can be rotated with a rotation matrix R the derivative with respect to a vector $\boldsymbol{\omega} = [\omega_1, \omega_2, \omega_3]$ defining R is derived as follows. Atoms $\{j\}$ are fixed and r_{ij} is the Euclidan distance between a pair of atoms i, j.

From [G. Terzakis, M. Lourakis and D. Ait-Boudaoud, J. Math Imaging Vis., 2018, 60, 422]

$$[\omega]_\times = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix} \tag{2}$$

$$R = \exp([\omega]_\times) = I_3 + \frac{\sin(\theta)}{\theta}[\omega]_\times + \frac{1-\cos(\theta)}{\theta^2}[\omega]_\times^2 \tag{3}$$

where I_3 is the 3×3 identity matrix and $\theta = |\boldsymbol{\omega}|$.

$$\frac{\partial V}{\partial \omega_1} = \sum_{\text{pairs}} \frac{\partial}{\partial \omega_1} r_{ij}^n = \sum_{\text{pairs}} n r_{ij}^{n-1} \frac{\partial r_{ij}}{\partial \omega_1} \tag{4}$$

$$\begin{aligned} \frac{\partial r_{ij}}{\partial \omega_1} &= \frac{\partial}{\partial \omega_1}[(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2]^{1/2} \\ &= r_{ij}^{-1}\Big[\frac{\partial (x_i - x_j)}{\partial \omega_1}(x_i - x_j) + \frac{\partial (y_i - y_j)}{\partial \omega_1}(y_i - y_j) + \frac{\partial (z_i - z_j)}{\partial \omega_1}(z_i - z_j)\Big] \\ &= r_{ij}^{-1}\Big[\frac{\partial x_i}{\partial \omega_1}(x_i - x_j) + \frac{\partial y_i}{\partial \omega_1}(y_i - y_j) + \frac{\partial z_i}{\partial \omega_1}(z_i - z_j)\Big] \end{aligned} \tag{5}$$

$$\frac{\partial x_i}{\partial \omega_1} = \frac{\partial}{\partial \omega_1}\{R\boldsymbol{c}\}_x = \frac{\partial R_{00}}{\partial \omega_1} c_1 + \frac{\partial R_{01}}{\partial \omega_1} c_2 + \frac{\partial R_{02}}{\partial \omega_1} c_3 \tag{6}$$

where $\boldsymbol{c} = [c_1, c_2, c_3]$ is the coordinate of atom i and R_{nm} are elements of the rotation matrix. From [G. Gallego, A. Yezzi, J. Math. Imag. Vis., 2015, 51, 378]

$$\frac{\partial R}{\partial \omega_k} = \frac{\omega_k[\omega]_\times + \boldsymbol{\omega} \times (I_3 - R)e_k}{\theta^2} R \tag{7}$$

where e_k is the kth component basis vector e.g. $\{\hat{\boldsymbol{\imath}}, \hat{\boldsymbol{\jmath}}, \hat{\boldsymbol{k}}\}$.