# Symmetry and elastic deformation of corpuscle rings – formulae for the elastic spring model

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If a deformation of a corpuscle structure leads to new edge lengths $D_{\alpha\beta}$, the deformation energy is given by

$$E = \frac{1}{2} \sum_{\mathrm{pairs}(\alpha,\beta)} (D_{\alpha\beta} - L_{\alpha\beta})^2 = \frac{1}{2} \sum_{\mathrm{pairs}(\alpha,\beta)} \left( \sqrt{||x_\alpha - x_\beta||^2} - L_{\alpha\beta} \right)^2 \tag{1}$$

where we assume a standard edge length $L_{\alpha\beta} = 1$ for all pairs and $x_\gamma$ is the position vector of the $\gamma^{\mathrm{th}}$ node. The partial derivatives of the deformed edge lengths with respect to the node positions read

$$\begin{aligned} \frac{\partial D_{\alpha\beta}}{\partial x_{i\gamma}} &= \frac{\partial}{\partial x_{i\gamma}} \sqrt{\sum_j (x_{j\alpha} - x_{j\beta})^2} = \frac{1/2}{D_{\alpha\beta}} \frac{\partial}{\partial x_{i\gamma}} \sum_j (x_{j\alpha} - x_{j\beta})^2 \\ &= \frac{1/2}{D_{\alpha\beta}} \frac{\partial}{\partial x_{i\gamma}} (x_{i\alpha} - x_{i\beta})^2 = \frac{1/2}{D_{\alpha\beta}} 2(x_{i\alpha} - x_{i\beta}) \frac{\partial}{\partial x_{i\gamma}} (x_{i\alpha} - x_{i\beta}) = \frac{x_{i\alpha} - x_{i\beta}}{D_{\alpha\beta}} (\delta_{\gamma\alpha} - \delta_{\gamma\beta}) \end{aligned} \tag{2}$$

Likewise, the derivatives of the deformation energy read

$$\frac{\partial E}{\partial x_{i\gamma}} = \frac{1}{2} \sum_{\mathrm{pairs}(\alpha,\beta)} 2\,(D_{\alpha\beta} - L_{\alpha\beta}) \frac{\partial D_{\alpha\beta}}{\partial x_{i\gamma}} = \sum_{\mathrm{pairs}(\alpha,\beta)} \frac{D_{\alpha\beta} - L_{\alpha\beta}}{D_{\alpha\beta}} (x_{i\alpha} - x_{i\beta})(\delta_{\gamma\alpha} - \delta_{\gamma\beta}) \tag{3}$$

with Kronecker's $\delta_{\alpha\beta} = 1$ if $\alpha = \beta$, and 0 otherwise. The second $\delta$ term can be omitted if all pairs are counted in both directions.

$$\frac{\partial E}{\partial x_{i\gamma}} = \sum_{\mathrm{directedpairs}(\gamma,\beta)} \frac{D_{\gamma\beta} - L_{\gamma\beta}}{D_{\gamma\beta}} (x_{i\gamma} - x_{i\beta}) = \sum_{\mathrm{directedpairs}(\gamma,\beta)} (1 - \frac{L_{\gamma\beta}}{D_{\gamma\beta}})(x_{i\gamma} - x_{i\beta}) \tag{4}$$

The second derivatives of the energy function read (consider only first term and then consider pairs in both directions)

$$
\begin{aligned}
\frac{\partial E}{\partial x_{r\kappa} x_{i\gamma}} &= \sum_{\mathrm{directedpairs}(\gamma,\beta)} \left[\frac{\partial}{\partial x_{r\kappa}}(1-\frac{L_{\gamma\beta}}{D_{\gamma\beta}})\right](x_{i\gamma}-x_{i\beta}) + (1-\frac{L_{\gamma\beta}}{D_{\gamma\beta}})\left[\frac{\partial}{\partial x_{r\kappa}}(x_{i\gamma}-x_{i\beta})\right] \\
&= \sum_{\mathrm{directedpairs}(\gamma,\beta)} -\left[\frac{\partial}{\partial x_{r\kappa}}\frac{L_{\gamma\beta}}{D_{\gamma\beta}}\right](x_{i\gamma}-x_{i\beta}) + (1-\frac{L_{\gamma\beta}}{D_{\gamma\beta}})\delta_{ri}(\delta_{\kappa\gamma}-\delta_{\kappa\beta}) \\
&= \sum_{\mathrm{directedpairs}(\gamma,\beta)} \frac{L_{\gamma\beta}}{D_{\gamma\beta}^2}\left[\frac{\partial}{\partial x_{r\kappa}}D_{\gamma\beta}\right](x_{i\gamma}-x_{i\beta}) + (1-\frac{L_{\gamma\beta}}{D_{\gamma\beta}})\delta_{ri}(\delta_{\kappa\gamma}-\delta_{\kappa\beta}) \\
&= \sum_{\mathrm{directedpairs}(\gamma,\beta)} \frac{L_{\gamma\beta}}{D_{\gamma\beta}^2}\left[\frac{(x_{r\gamma}-x_{r\beta})}{D_{\gamma\beta}}(\delta_{\kappa\gamma}-\delta_{\kappa\beta})\right](x_{i\gamma}-x_{i\beta}) + (1-\frac{L_{\gamma\beta}}{D_{\gamma\beta}})\delta_{ri}(\delta_{\kappa\gamma}-\delta_{\kappa\beta}) \\
&= \sum_{\mathrm{directedpairs}(\gamma,\beta)} (\delta_{\kappa\gamma}-\delta_{\kappa\beta})\left(\frac{L_{\gamma\beta}(x_{r\gamma}-x_{r\beta})(x_{i\gamma}-x_{i\beta})}{D_{\gamma\beta}^3} + \delta_{ri}(1-\frac{L_{\gamma\beta}}{D_{\gamma\beta}})\right) \qquad (5)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial E}{\partial x_{r\kappa} x_{i\gamma}} &= \delta_{\kappa\gamma}\sum_{\mathrm{directedpairs}(\gamma,\beta)}\left(\frac{L_{\gamma\beta}(x_{r\gamma}-x_{r\beta})(x_{i\gamma}-x_{i\beta})}{D_{\gamma\beta}^3} + \delta_{ri}(1-\frac{L_{\gamma\beta}}{D_{\gamma\beta}})\right) \\
&\quad -\left(\frac{L_{\gamma\kappa}(x_{r\gamma}-x_{r\kappa})(x_{i\gamma}-x_{i\kappa})}{D_{\gamma\kappa}^3} + \delta_{ri}(1-\frac{L_{\gamma\kappa}}{D_{\gamma\kappa}})\right) \qquad (6)
\end{aligned}
$$