Forces

Notation

Let r_i, v_i, m_i, q_i be position, velocity, mass and charge of ith particle, respectively. V is the potential of the force field. Let x^μ denote (0-indexed) μth component of x. Let $\partial_n^\mu := \partial/\partial(r_n)^\mu$ – in particular $(F_n)^\mu = -\partial_n^\mu V$. Let ε^μ be (somewhat incompatibly) unit vector for μth component.

Chirality

$$\begin{aligned} V &= \frac{1}{2} e_{chi} \sum (C_i - C_i^{nat})^2 \\ C_i &= \frac{(v_{i-1} \times v_i) \cdot v_{i+1}}{d_0^3} \end{aligned}$$

where $v_i = r_{i+1} - r_i$, d_0 is $|v_0|$ in the native state, and C_i^{nat} is C_i in the native state.

$$\begin{aligned} \partial_n^\mu V &= e_{chi} \sum (C_i - C_i^{nat}) \partial_n^\mu C_i \\ \partial_n^\mu C_i &= \frac{1}{d_0^3} \partial_n^\mu (\underbrace{(v_{i-1} \times v_i) \cdot v_{i+1}}_{f_i}) \end{aligned}$$

This vanishes for $n \neq i-1, i, i+1, i+2$. For these values,

$$\begin{aligned} \partial_{i-1}^\mu f_i &= (-\varepsilon^\mu \times v_i) \cdot v_{i+1} \\ &= -(v_i \times v_{i+1}) \cdot \varepsilon^\mu \\ \partial_i^\mu f_i &= (\varepsilon^\mu \times v_i - v_{i-1} \times \varepsilon^\mu) \cdot v_{i+1} \\ &= (v_i \times v_{i+1} + v_{i-1} \times v_{i+1}) \cdot \varepsilon^\mu \\ \partial_{i+1}^\mu f_i &= (v_{i-1} \times \varepsilon^\mu) \cdot v_{i+1} + (v_{i-1} \times v_i) \cdot (-\varepsilon^\mu) \\ &= -(v_{i-1} \times v_{i+1} + v_{i-1} \times v_i) \cdot \varepsilon^\mu \\ \partial_{i+2}^\mu f_i &= (v_{i-1} \times v_i) \cdot \varepsilon^\mu \end{aligned}$$

from the scalar triple product property; let us also recall, that $v \cdot \varepsilon^\mu = v^\mu$.