Appendix to the manual of four phi model program

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July 12, 2012

Potential function

$$V = V_{self} + V_{inter} \tag{1}$$

$$V_{self} = V_{iso} + V_{aniso1} + V_{aniso2} + V_{harm} \tag{2}$$

$$V_{iso} = c_1 \sum_i (|\bar{u}_i|^2 - 1)^2 \tag{3}$$

$$V_{aniso1} = c_2 \sum_i (u_{i1}^2 u_{i2}^2 + u_{i1}^2 u_{i3}^2 + u_{i2}^2 u_{i3}^2) \tag{4}$$

$$V_{aniso2} = c_3 \sum_i (u_{i1}^2 + u_{i2}^2) \tag{5}$$

$$V_{harm} = c_{harm} \sum_i |u_i|^2 \tag{6}$$

$$V_{inter} = V_{inter1} + V_{inter2} \tag{7}$$

$$V_{inter1} = c_4 \frac{1}{2} \sum_{\langle ij \rangle} (\bar{u}_i - \bar{u}_j)^2 \tag{8}$$

$$V_{inter2} = c_5 \frac{1}{2} \sum_{\alpha} \sum_{\langle ij,\alpha \rangle} (u_{i\alpha} - \bar{u}_{j\alpha})^2 \tag{9}$$

In total we then have

$$V_{self} = c_1 \sum_i (|\bar{u}_i|^2 - 1)^2 + c_2 \sum_i (u_{i1}^2 u_{i2}^2 + u_{i1}^2 u_{i3}^2 + u_{i2}^2 u_{i3}^2) + c_3 \sum_i (u_{i1}^2 + u_{i2}^2) + c_{harm} \sum_i |u_i|^2 \quad (10)$$

$$V_{inter} = c_4 \frac{1}{2} \sum_{\langle ij \rangle} (\bar{u}_i - \bar{u}_j)^2 + c_5 \frac{1}{2} \sum_{\alpha} \sum_{\langle ij,\alpha \rangle} (u_{i\alpha} - \bar{u}_{j\alpha})^2 \quad (11)$$

For V_{inter2} the nearest neighbors are taken only in the direction α, and the longitudinal force constant in this direction will thus be increased by c_5