

## Supporting Appendix: Energy Terms

The total energy of the nucleosomal array system includes stretching, twisting, bending energy, electrostatic interaction, and excluded volume effect:

$$E = E_S + E_T + E_B + E_C + E_V \quad [1]$$

The first three terms describe the elastic energy: stretching ( $E_S$ ), twisting ( $E_T$ ), and bending ( $E_B$ ) of the system:

$$E_S = \frac{h}{2} \sum_{i=1}^{N-1} (l_i - l_0)^2, \quad [2]$$

$$E_T = \frac{C}{2l_0} \sum_{i=1}^{N-1} (\alpha_i + \gamma_i)^2, \quad [3]$$

$$E_B = \frac{g}{2} \sum_{i=1}^{N-1} \beta_i^2 + \frac{g}{2} \sum_{i \in I_C} (\beta_i^+)^2, \quad [4]$$

where  $l_i$  is the segment length between bead  $i$  and bead  $i + 1$ ,  $l_0$  is the equilibrium segment length, and  $\alpha$ ,  $\beta$ , and  $\gamma$  are the Euler angles describing the transformation from one bead to the next (see ref. 1 for details). The parameters describing the energy terms of stretching, bending, and twisting of the linker DNA are adopted from the study of superhelical DNA (2). We assume that the linker DNA has similar properties as free DNA, as adopted in other macroscopic models of chromatin (1, 3, 4). The values for the stretching constant  $h$ , twisting constant  $C$ , and bending constant  $g$  are listed in Table 3.

The electrostatic interaction includes linker–linker, linker DNA–nucleosome and internucleosome terms

$$E_C = \sum_{\substack{j>i+1 \\ i,j \in I_l}} \frac{q_l^2 e^{-\kappa r_{ij}}}{\epsilon r_{ij}} + \sum_{\substack{j>i+1 \\ i \in I_l, j \in I_C}} \sum_{k=1}^{N_C} \frac{q_l q_C^k e^{-\kappa r_{i\{jk\}}}}{\epsilon r_{i\{jk\}}} + \sum_{\substack{j>i \\ i,j \in I_C}} \sum_{k=1}^{N_C} \sum_{l=1}^{N_C} \frac{q_C^k q_C^l e^{-\kappa r_{\{ik\}\{jl\}}}}{\epsilon r_{\{ik\}\{jl\}}} \quad [5]$$

where  $q_l$  and  $q_C$  represent the effective charges of the linker DNA beads ( $I_l$ ) and the DiSCO charges of the nucleosome ( $I_C$ ), respectively, and  $r$  is the distance between these charges. The electrostatic interactions between linker DNA beads are calculated with a Debye–Hückel potential by setting an effective charge on the corresponding linker bead, where the effective charges were derived by Stigter (5). The internucleosome electrostatic interaction is described by the Debye–Hückel potential from DiSCO (6, 7). The linker DNA–nucleosome interaction also is described by the Debye–Hückel potential between the DiSCO charges of the nucleosome and the effective charge of the linker DNA bead.

Excluded volume effects are treated with a van der Waals-type interaction that includes linker DNA–nucleosome and internucleosome terms to prevent the overlap between them

$$E_V = k_{ex} k_B T \sum_{\substack{j>i+1 \\ i \in I_l, j \in I_C}} \left[ \sum_{k=1}^{N_C} \left( \frac{\sigma_1}{r_{i\{jk\}}} \right)^{12} - \left( \frac{\sigma_1}{r_{i\{jk\}}} \right)^6 \right] + k_{ex} k_B T \sum_{\substack{j>i \\ i,j \in I_C}} \left[ \sum_{k=1}^{N_C} \sum_{l=1}^{N_C} \left( \frac{\sigma_2}{r_{\{ik\}\{jl\}}} \right)^{12} - \left( \frac{\sigma_2}{r_{\{ik\}\{jl\}}} \right)^6 \right] \quad [6]$$

The values for  $k_{ex}$ ,  $\sigma_1$  and  $\sigma_2$  are listed in Table 3. (The linker–linker excluded volume effect is not necessary because the uniformly negatively charged linker DNA beads repulse each other.)

Thus, interactions between nucleosomes and linker DNA include mechanical coupling, electrostatic interaction, and excluded volume effects. The mechanical coupling between a nucleosome and linker DNA constrains the way in which the linker DNA enters and exits from the nucleosome and requires extra energy terms to describe this effect, as described in ref. 1.

All energy parameters are listed in Table 3. Except for the excluded volume parameters ( $\sigma_1$  and  $\sigma_2$ ), which are reduced by 0.5 nm to accommodate the inclusion of the histone tails, all parameters are the same as in ref. 1.

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