STATISTICAL MECHANICS of SUPERCOILING-INDUCED B-TO-Z TRANSITIONS IN A CLOSED CIRCULAR DNA: S. Miyazawa and A. Sarai, (Intr. by), Lab. of Math. Biol., NCI, NIH, Bethesda, MD 20205

A configurational partition function for transitions from the right handed B helix to left handed Z helix in a closed circular double stranded DNA is formulated on the basis of an idealized model. A double quadratic twisting potential with minima at the B- and Z-forms for base pair twists and a harmonic potential for nearest neighbor interactions between twists are assumed. Long range interactions among the twists, which are attributable to the conservation of linking number (L_k) between two closed DNA strands, are approximated to be a harmonic potential with regard to the writhing number (W_r); $L_k=T_w+W_r$; the twisting number T_w is equal to the total twists. Interactions between phonon and structures such as B- and Z- regions and B-Z junctions are neglected. The configurational partition functions are formulated for two cases; one that all base pair can take the Z form, and another that only part of DNA can take the Z- and B-forms. These partition functions are consistent with the fact that the equilibrium ensemble of B-form closed DNAs over L_k obeys the Gaussian distribution with the variance of L_k, kTN/κ; N is the total length of DNA. It is proved that the variance of T_w in a closed DNA is smaller than that of a linear DNA, because of the long range interactions. The characteristics of B-to-Z transitions induced by reducing L_k of a closed circular DNA are examined in details; the dependences of the transition linking number on external variables such as the total length of DNA and the length of a DNA segment that can take the Z form are analytically derived among others. Also, the relative energy of Z-form to B-form, the energy for forming a B-Z junction, and $\kappa/2$ have been estimated by curve-fitting of transition curves to the experimental data (Peck & Wang, 1983) to be 0.84•kT, 8.28•kT and 1490•kT.