Packing of charged chains on toroidal geometries

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We study a strongly adsorbed flexible polyelectrolyte chain on tori. In this generalized Thomson problem, the patterns of the adsorbed chain are analyzed in the space of the toroidal coordinates and in terms of the orientation of each chain segment. Various patterns are found, including double spirals, disclination-like structures, Janus tori, and uniform wrappings, arising from the long-range electrostatic interaction and the toroidal geometry. Their broken mirror symmetry is quantitatively characterized by introducing an order parameter, an integral of the torsion. The uniform packing, which breaks the mirror symmetry the least, has the lowest value of the order parameter. In addition, it is found that the electrostatic energy of confined chains on tori conforms to a power law regardless of the screening effect in some typical cases studied. Furthermore, we study random walks on tori that generate chain configurations in the large screening limit or at large thermal fluctuation; some features associated with the toroidal geometry are discussed.

12 10 (left) A double spiral structure is found under some initial 8 conditions. Ц 6 (right) The representation of 4 the left configuration in toroidal 2 coordinates. 0 2 3 5 6 4

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