

Electronic supporting information

Charge-controlled nano-structuring in partially collapsed star-shaped macromolecules

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K_A	$p = 2$	$p = 10$	$p = 20$
1×10^{-5}	0.196(1)	0.065(1)	0.043(1)
5×10^{-5}	0.396(1)	0.103(1)	0.059(1)
1×10^{-4}	0.478(1)	0.176(1)	0.090(1)
2×10^{-4}	0.566(1)	0.294(1)	0.144(1)
5×10^{-4}	0.685(1)	0.428(1)	0.291(1)
1×10^{-3}	0.770(1)	0.522(1)	0.415(1)

TABLE I. Values of the average degree of ionization, α , obtained from the simulations at different input values of K_A (with standard deviations on the last digit given in parentheses) for various numbers of arms, p . We systematically varied K_A of the weak PEs, and α was obtained from the simulation as a result of complex interplay between ionization and conformation of the macromolecules. In contrast, for the strong PEs we set the degree ionization to be $\alpha = 1/m$ using a repeating sequence of $m - 1$ uncharged monomers followed by one charged.

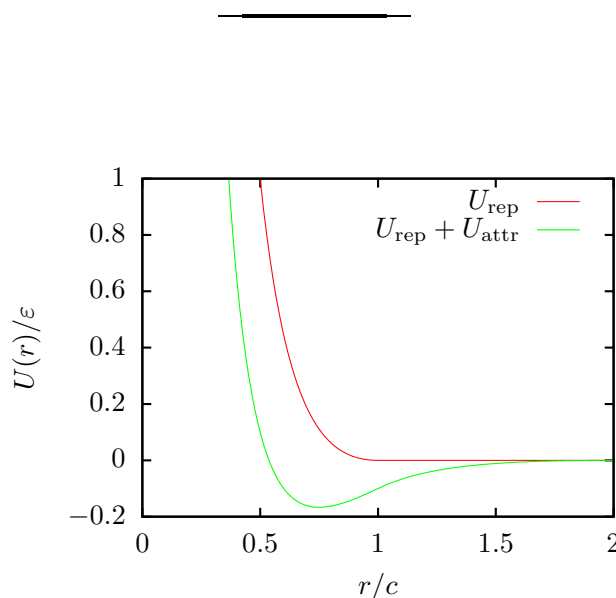


FIG. 1. The repulsive and attractive short-range interaction potentials.

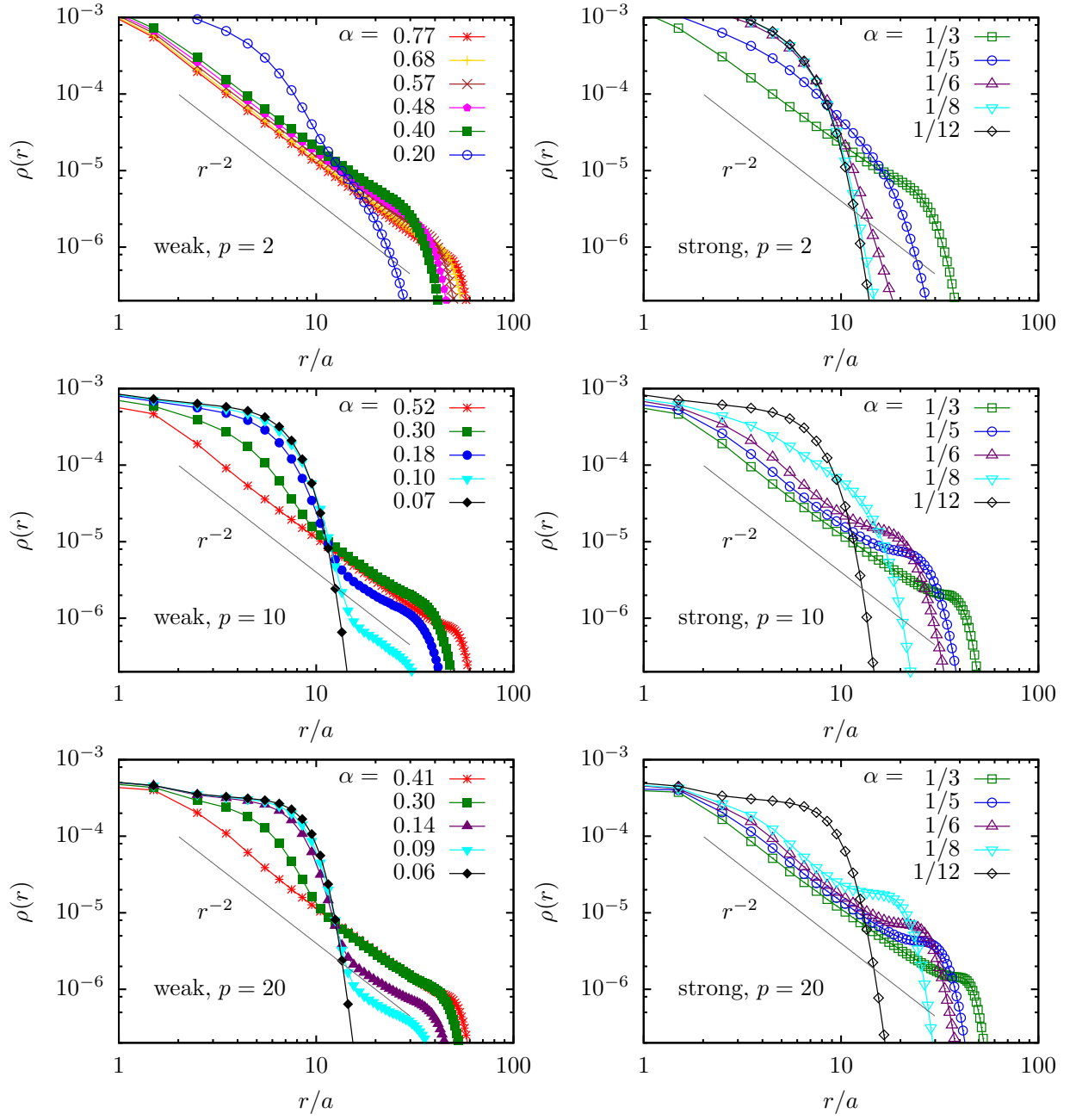


FIG. 2. Radial segment density profile for weak (left) and strong (right) PE stars with $p = 2$ (top), $p = 10$ (middle) and $p = 20$ (bottom).

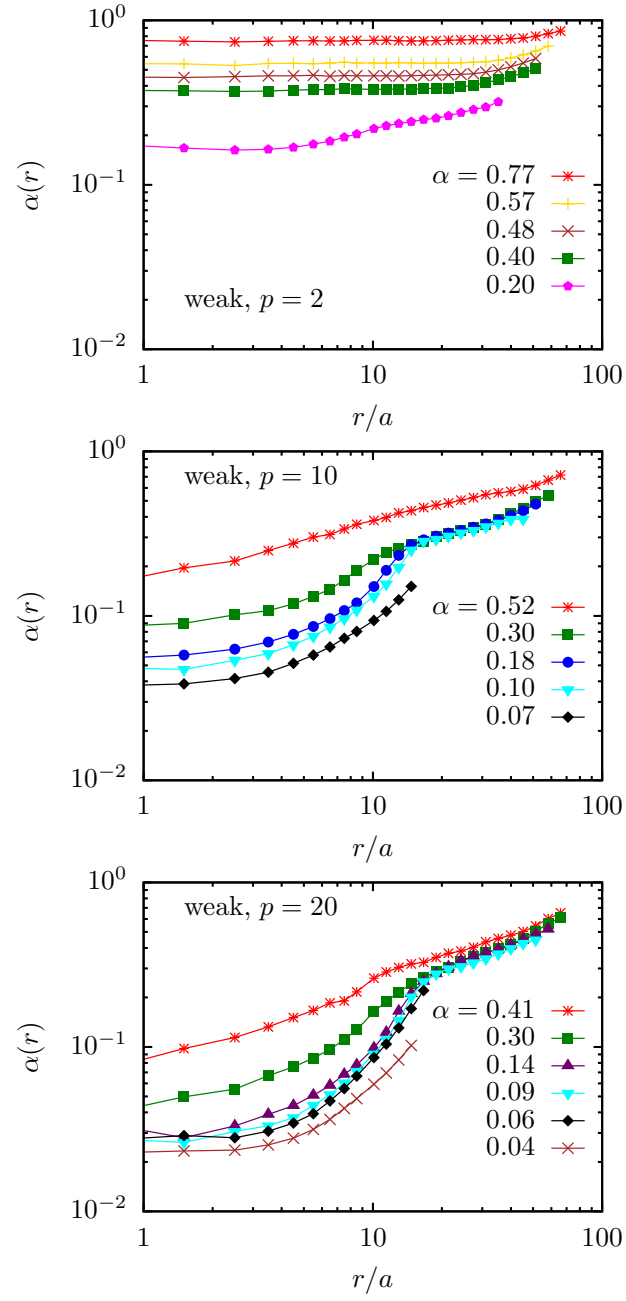


FIG. 3. Radial profile of degree of dissociation for weak PE stars with $p = 2$ (top), $p = 10$ (middle) and $p = 20$ (bottom).

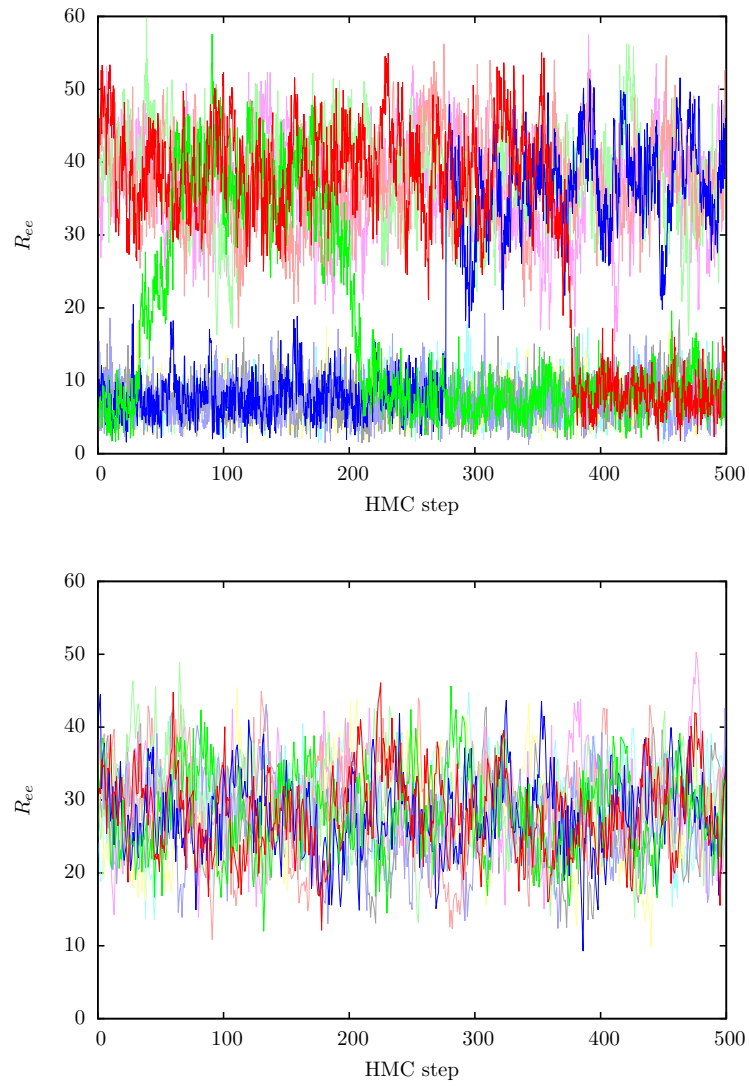


FIG. 4. Sample traces of the end-to-end distances of individual arms (in different colours) for the weak polyelectrolyte star (left) and the strong one (right) with $p = 10$ arms and $\alpha \approx 0.2$. In the weak case, clear bimodality is seen, which is absent in the strong case. Some arms repeatedly change their state between stretched and collapsed within the depicted frame, which confirms that the system is not frozen in the core-shell structure. The plots include about 1/20 of the whole simulation.