A Model Ground State of Polyampholytes

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The ground state of randomly charged polyampholytes (polymers with positive and negatively charged groups along their backbone) is conjectured to have a structure similar to a *necklace*, made of weakly charged parts of the chain, compacting into globules, connected by highly charged stretched 'strings'[1,2]. Kantor and Ertaş [3] attempted to quantify the qualitative necklace model, by suggesting a zero approximation model, in which the longest neutral segment of the polyampholyte (PA) forms a globule, while the remaining part will form a tail. Expanding this approximation, we suggest [4] a specific necklace-type structure for the ground state of randomly charged PA's, where all the neutral parts of the chain compact into globules: The longest neutral segment compacts into a globule; in the remaining part of the chain, the longest neutral segment (the 2nd longest neutral segment) compacts into a globule, then the 3rd, and so on.
A random sequence of charges is equivalent to a random walk (RW), and a neutral segment is equivalent to a loop inside the RW. We use analytical and Monte Carlo methods to investigate the size distribution of loops in a one-dimensional RW. We show that the length of the nth longest neutral segment in a sequence of N monomers (or equivalently, the nth longest loop in a RW of N steps) is proportional to N/n^2, while the mean number of neutral segments increases as $\sqrt{N}$. The PA in the ground state within our model is found to have an average linear size proportional to $\sqrt{N}$, and an average surface area proportional to $N^{2/3}$.

[1] Y. Kantor and M. Kardar, Phys. Rev. E **51**, 1299 (1995).
[2] Y. Kantor and M. Kardar, Phys. Rev. E **52**, 835 (1995).
[3] D. Ertaş and Y. Kantor, Phys. Rev. E **53**, 846 (1996).
[4] S. Wolfling and Y. Kantor, Phys. Rev. E, in press (1998).